罗渝然 编著

化学键能数据手册

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作者简介

罗渝然博士，重庆人，曾任教于中国科学技术大学，现客居美国，是著名的大型工具书*Handbook of Chemistry and Physics*的执笔人之一。

- 第一本全面介绍化学键能测量数据的实用手册，是教学科研必备工具书
- 全书按照化学键的类型、功能团、键级、分子大小等安排数据，利于快速检索
- 每个化学键列出了5种不同来源，并用黑体字显示了推荐值，利于快速选用
- 提供了完整的原子和自由基的生成热（焓）的数据库，利于扩大使用范围
- 前三章介绍了化学键能的基本知识，为基础教学增添了最新的参考材料

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化学键能数据手册

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内 容 简 介

本书是化学键能的数据大全。前 3 章介绍了化学键能的基本知识，主要测量方法以及如何使用键能数据库等。第 4～11 章，介绍了 3700 个含碳、氢、氧、氮、硫、磷、硅、卤素元素等化合物中的 4300 个键能的测量数据。对每个化学键，列出了 5 种不同来源的数值，并用黑体字显示了推荐值。本书按照 C—H、C—C、C—X、O—X、N—X、S—X、Si—X、P—X 等化学键的次序排列。第 12 章列出了原子和大量自由基的生成热（焓）。

本书可供化学、化工、物理、材料、能源、生物、资源、环境等学科的大学生、研究生、教师、工程师、专业技术人员参考，是有关学科的必备工具书。

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前　言

2002年，美国CRC出版社出版了我的一本英文书："Handbook of Bond Dissociation Energies in Organic Compounds"。这本书收集、评选和推荐了2400个有机物中2700个化学键（离解）能的实验数据，是当时最完整的有机物键能参考手册。假如，仅仅是把那本英文书翻译成中文，虽然节省了时间，但实际效果肯定不好。因为它起点比较高，太简练，"阳春白雪"，不适合目前国内大学生与研究生的需要。所以，我进行了改写、加工，增加了新内容，提供了许多细节和解释，介绍了十余种测量键能的方法及其优缺点，补充了上千个最新的有机和无机分子的实验数据，扩大了键能和自由基生成热的数据库，包揽了3700种化合物中4300个化学键。我认为，这样处理后，可能比较适合更多的读者，能与更多的朋友们共同讨论、分享现代科技成果，或作为有关选修课或专业课的参考资料，或成为有关科研的必备工具书，或进一步开展实验测量和理论计算、开发物理模型、建立数据库和数据库联网等多方面研究工作。

通过CA（Chemical Abstracts）和ISI（Institute for Scientific Information）等网站检索，我了解到，近几年国内许多科学家，既用现代方法测量了许多分子的键能，又用高级理论方法预测了许多分子的键能，讨论了化学反应活性及其实际应用。但非常遗憾的是，我在海外读不到国内科技刊物，没有办法收集到国内所有科学家的成果并选编到本书内，再集中介绍给世界各国成千上万的读者。我诚恳地希望，国内的专家、学者能帮助我，邮寄或电邮你们已发表的论文抽印本。本书再版时，我一定将这些成果编写进去，以弥补本书的这一缺憾。

"理想的"化学数据库应当有化合物的结构式、英文名称、中文标准译名，也应当标明化合物的 CAS（Chemical Abstracts Service）登记号。在本数据库里，我们提供了全部分子的结构式，也介绍了大部分化合物的英文名称，但是没有列出中译名和 CAS 登记号。主要原因有二：①今天，被确认的化合物数目已经高达2400万，虽然它们的结构式已知，但国际纯粹和应用化学协会（IUPAC）还没有推荐这些新化合物的标准英文名称；②许多有标准英文名称的化合物，却无标准中文译名。此外，读者在访问数据库时遇到的符号、缩写、略语和常见术语，已在开卷前给出对应的中文译名。

中国科学技术大学是我的母校。我在那里求学、工作了多年，与许多老师、同窗好友、四川老乡和我的学生们有过深厚的友谊。我愿把十余年"磨一剑"才完成的书，奉献给中国科学家、工程师、教师、大学生和研究生们。

衷心感谢两位著名的科学家——南开大学程津培教授和中国科学技术大学郭庆祥教授。他们在百忙之中，为本书提供了极大的帮助，修正原稿里的错误，并写序言，直接和我交流讨论现代科学，拓展了我的视野，提高了本书质量。

非常感谢俞书勤、张允武、刘凡镇、刘铨良（中国科学技术大学），吕日昌、王秀岩（中国科学院大连化学物理研究所），孔繁敖、王殿勋（中国科学院化学研究所），赵新生、高盘良（北京大学），何学中、张志新（中国科学院力学研究所），秦启宗（复旦大学），赵学庄（南开大学），陈慧兰（南京大学）等教授，以及张先满博士（美国Yale大学）对本书出版的大力支持。诚恳欢迎读者对本书的任何批评、评论和

建议。电邮是我们联系的好途径。中国科学院科学出版基金委员会为本书提供了财务支持，科学出版社又很快地进行了认真细致的编辑加工，为我们提供了极好的服务，作者在此一并表示衷心感谢。

罗渝然

2004 年 3 月 7 日，于美国 Florida 州

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英文原版前言（中文译文）

有机化学有三大基本研究课题，这就是有机分子的结构、能量、反应活性，以及三者相互关系。化学家经常要查找化学键（离解）能的数据。有时候，查找可靠的数据，尤如大海捞针，徒劳无益。

1990 年，我开始收集化学键能的实验数据和理论计算预测值。4 年后，我的朋友，美国国家标准和技术研究院的 S.E. Stein 博士鼓励我继续做下去，因为它是化学反应动力学、自由基化学、有机热化学以及物理（或高等）有机化学最基本的工作。

现在有许多测量多原子分子中键能的方法，但是几乎没有实验精度进入 1 kcal/mol（化学精度：1 kcal = 4.184 kJ）的方法。很多重要有机分子中的键能，已经用现代技术多次测量。例如，甲烷中的 C—H 键能，从 20 世纪 30 年代以来，被测量过大约 50 次。所以，化学键能的可靠数据，今后将继续是科学家热烈争论的一个话题。

虽然我对理论计算有很大兴趣，但本书仅仅介绍键能的实验数值和各种测量方法。我觉得，收集化学键能的实验数据，就像是在进修一门化学历史课程，我们要认识在化学键能方面有过重大贡献的世界级科学家，例如 E.W.R. Steacie（加拿大），L. Pauling（美国），M. Szwarc（英国），N.N. Semonov（前苏联），以及我的恩师 S.W. Benson（美国）。

为了完成这本参考手册，“冷板凳”坐了十余年。作者衷心感谢许多科学家给予我的大量帮助和鼓励。他们是教授 S.W. Benson, F.W. Bordwell, 李远哲, R.H. Byrne, A.M. Dean, J.F. Liebman, V.D. Parker, I.R. Slagle（美国）；P.D. Pacey, J.L. Holmes, D.A. Armstrong, E. Tschuikow-Roux（加拿大）；J.A. Kerr, R. Walsh, M.J. Pilling（英国）；C. Rüchardt（德国）；K.D. King（澳大利亚）；赵学庄，程津培（南开大学）；A.J. Colussi（阿根廷）；J.A.M. Simões（葡萄牙）；J.A. Seetula（芬兰）。他们是博士 S.E. Stein, W. Tsang（美国国家标准和技术研究院）；T.J. Wallington（美国 Ford 汽车公司）；M. Tirtowidjojo（美国 Dow 化学公司）；K.U. Ingold, D.D.M. Wayner（加拿大科学院）以及 E.T. Denisov（俄国科学院）。

诚恳欢迎对本书的任何批评、意见和建议。电邮是我们联系的好途径。

罗渝然

2002 年 6 月

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序　一

化学是一门基础科学，它研究的对象是以分子为基础的物质的构建、变化及其性质。有关物质结构的知识告诉我们，分子由原子按一定的规则以化学键的形式构筑而成。化学键指的是分子内各原子之间的结合力，这种结合力的定量描述通常称为键能，即一个化学键发生断裂所需要的最低能量。由于化学反应作为化学科学的核心，研究的是物质分子化学键的变化过程，因此从一定意义上讲，化学在很大程度上是围绕着化学键的重组（即键的断裂与生成）而形成的一门学科。由此可见化学键研究在物质科学研究中的核心位置。化学键键能的知识对于理性判断化学反应能否发生和为何发生，判断或者预测反应进行的方向和速率，都具有十分重要的意义。

由于化学与物理、材料、能源、生物、资源、环境等许多学科的紧密相关性，键能数据一直是诸多领域的定量研究中非常需要的热力学参数。但以往受研究手段的限制，有较高可信度、可用作定量依据的键能数据并不很多，这不仅使得键能作为基本科学数据的巨大潜力难以得到充分展现和应用，也使物质科学定量研究的深入几十年来一直受到相当大的影响。所幸的是，最近十几年来键能的实验和理论研究方法得到了长足的发展，可靠的键能数据的产出大大加快，因此对繁杂的实验数据进行归纳整理出版，使大量重要键能数据发挥其应有效益的需求日益迫切。

在化学键键能研究方面，客居美国的罗渝然博士倾注了十余年的心血。不久前，他在工具书和数据库方面权威出版商美国CRC出版社的支持下，出版了该领域第一部，同时也是迄今为止涵盖面和摄纳量都最大的化学键键能数据库的专著——“Handbook of Bond Dissociation Energies in Organic Compounds”。现在他在该书的基础上，又增编了新的章节和数据，使内容更加丰富。罗博士怀着对祖国科学发展的深厚感情，以中文的版式，将他的新作献给国内的广大科技工作者，以报答祖国的养育之恩。我本人十分赞赏他这份浓厚的游子之情，故欣然同意为之作序。

此次在科学出版社付梓的这本著作，具有非常重要的科学参考价值。但一本这样的书工作量十分浩大，鲜有人愿意涉及，也是我从事键能研究二十余年来曾屡屡想做，但始终未能实现的工作。如今罗博士书的出版，了却了我的这项旧愿，所以我对罗博士对事业的执著十分钦佩，也对他对科学的奉献十分感谢。同时我还愿以一位长期从事有机物键能研究及应用的科学工作者的身份，向有兴趣利用键能这一有力工具，探索化学键重组内在规律的有机化学、物理化学、材料科学和生命科学的学生和学者推荐这本工具书。

程津培

2004年2月22日

序　二

化学的本质是变革分子。化学家通过各种各样的方法，根据人的意志实现分子间的相互转化。这种转化构成了合成化学的主体，转化过程几乎都涉及化学键的断裂和形成。合成化学家在确定目标分子的结构之后，就要制定合成策略，根据合成策略设计合成路线。在整个化学合成中，人们总是自觉不自觉地运用化学键能的知识，指导实现分子间的转化。反过来，化学键能的知识又可以解释许多化学现象，阐明反应机理。比如研究大气层中臭氧空洞的形成，就是一个应用化学键能的典型实例。氟里昂分子中的C—F键的键能超过110 kcal/mol，C—Cl键的键能低于84 kcal/mol。太阳光照在氟里昂分子上，使C—Cl键（而不是C—F键）断裂，形成氯原子。氯原子进攻臭氧（O_3），使O_3大量消耗，从而形成臭氧空洞。化学键能的知识还可以应用到材料科学、生命科学等领域，如研究材料的理化性质、强度、寿命，研究生命过程中的化学变化、疾病、衰老、生物抗氧化等。因此，化学键能的知识是化学的基础知识，是化学工作者应该“家喻户晓”的知识。然而，多年来缺乏这方面的专门著作，化学键能的数据散见于各种教科书和文献中，查阅极不方便。旅美化学家罗渝然博士出版了“Handbook of Bond Dissociation Energies in Organic Compounds”一书，受到学术界的极大欢迎和高度评价。为适应国内同行专家，尤其是广大研究生和大学生的需要，他又专门写了一本中文的《化学键能数据手册》。

这本书深入浅出，生动活泼，既有理论高度，又有可读性。该书收集了大量有机化合物和无机化合物的键能数据，集原理、方法、应用、数据库为一体，更具实用性。作者长期从事相关研究，功底深厚，成果丰硕。这本书是他多年辛勤劳动的结晶。该书的出版，相信一定深受国内同行和青年学生的欢迎。

我与罗渝然博士相识于20世纪70年代末、80年代初。那时，我在兰州大学读研究生，他在中国科学技术大学任教。我们在物理有机化学会议上经常见面，我常常向他讨教。严格地说，我们之间是师生关系。他思想活跃，学风严谨，知识面宽，性情直率，给我留下了深刻的印象。如今，他虽身在海外，但时时关心国内的大学教育和科学研究。他经常给国内同行打电话、写信、发电子邮件、邮寄图书资料，讨论学术问题。有时，他读到一篇好文章，怕我们没有看到，都要专门打个电话或发个电子邮件告知。他所做的这一切，用他的话说，都是“报答祖国的养育之恩”。从他朴实无华的语言中，我们可以领略到他的处世态度和治学精神，也可以感受到他这本书的分量和风格。愿广大读者从这本书中获得知识汲取营养。同时，感谢科学出版社为读者奉献了这样一本好书。

郭庆祥

2004年2月于中国科技大学

符号、缩写、略语和书中常见术语

AE	appearance energy, 呈现（出峰）能
AOP	acidity-oxidation potential，酸度-氧化势
AP	appearance potentials, 呈现（出峰）势
BDE	bond dissociation energy（or enthalpy）， 化学键离解能（或焓）
Bromination	溴化（法）
Chemiluminescene	化学发光（法）
Chlorination	氯化（法）
CID	collision-induced dissociation，碰撞诱导离解
Calorimetry	量热法
Correlation	相关法, 见第 2 章
DH°	i.c., BDE, where H emphasizes the BDE is an enthalpy change of thermochemistry, 即 BDE, 这里 **H** 强调 BDE 是热化学焓变
Derived	文献作者利用热化学循环导出的键离解能
Derived from $\Delta_f H^{\circ}$ in ref.	本书导出的值。根据第 1 章内公式（1.2），利用给定文献内的化合物生成热与本书 12 章内的自由基生成热，导出的键能
detect.	detection，检测
EA	electron affinity，电子亲和能
EI	electron impact method，电子冲击（法）
Electrochem.	electrochemical technique，电化学法
Electron capture	电子俘获（法）
Elimination	消去（法）
EPR	electron paramagnetic resonance spectrometry，电子顺磁共振谱
Equilibrium study	热平衡研究法，见第 2 章
ES MS	electrospray mass spectrometry, 电喷质谱
ESR	electron spin resonance spectrometry，电子自旋共振谱，即 EPR
Est. by exp.	按实验数据估计的
FA	flowing afterglow, 流动辉光（法）
FAB	fast atom bombardment，快速原子轰击质谱
Femtomole	毫微微（级）摩尔（10^{-15} mol）
Flash photolysis	闪光光解（法）
Fluorescence	荧光（法）
FT-ICR	Fourier transform ICR，Fourier 变换质子回旋共振谱
FT-MS	Fourier transform mass spectrometry, Fourier 变换质谱
FT-MW	Fourier transform microwave spectrometry, Fourier 变换微波谱

FT-IR	Fourier transform infrared spectrometry，Fourier 变换红外光谱
GIB MS	guided-ion beam，导向离子束质谱
GPA	gas-phase acidity，气相酸度
GC	gas chromatographic analysis，气相色谱分析
HPLC	high performance liquid chromatography，高压液相色谱
HPMS	high-pressure mass spectrometry，高压质谱
ICR	ion cyclotron resonance spectrometry，质子回旋共振谱
IE	ionization energy，电离能
Iodination	碘化（法）
Ion flow tube	离子流动管（质谱法）
IR	infrared spectrometry，红外光谱
IR MPD	infrared multiphoton dissociation，红外多光子离解
Isomerization	异构化（法）
KERD	kinetic energy release distribution，动能释放分布
Kinetics	动力学（法），见第 2 章
Laser photolysis	激光光解（法），见第 2 章
LIPAC	laser-induced photoacoustic calorimetry，激光诱导光声量热法
Microcalorimetry	微量热法
Mol. beam	分子束（法），见第 2 章
MS	mass spectrometry，质谱
NMR	nuclear magnetic resonance spectrometry，核磁共振谱
PA	proton affinity，质子亲和能
PAC	photoacoustic calorimetry，光声量热法
PD	photodissociation，光（致）离解
PES	photoelectron spectrometry，光电子谱
Photobromin.	photobromination，光溴化
Photochlorin.	photochlorination，光氯化
Photodetach.	photodetachment，光（致）分离
Photodissoc.	photodissociation，光（致）离解
Photoelectr.	photoelectron，光电子
Photoioniz.	photoionization，光（致）离解
Photolysis	光解（法），见第 2 章
Photosensitized	光敏（离解法）
PIMS	photoionization mass spectrometry，光离解质谱
Polanyi plot	Polanyi 相关图（法），见第 2 章
Proton affinity	质子亲势（法），见第 2 章
PTS	photofragment translational spectrometry，光碎片平动谱
Pulse radiolysis	脉冲射解（法）
Pulse shock tube	脉冲激波管（法）

Pulsed-laser	脉冲激光（光解法）
Pyrolysis	热解（法），见第 2 章
Radical buffer	自由基缓冲（法）
Re-anal.	re-analysis of experimental data, i.e., revised，重新分析计算
Re-cal.	re-calculated BDEs from experimental data, i.e., revised，重新计算
Recommend.	recommended，文献作者推荐
Re-evaluated	重新评议后的
Revised	修定了的
Review	文献作者评论
Shock tube	激波管法
Spectrometry	光谱测量法
Spectroscopy	光谱学法
SPST	single-pulse shock tube technique，单脉冲激波管技术
Thermolysis	热解（法），见第 2 章
Toluene carrier	甲苯载体（法）
TQ MS	triple-quadrupole mass spectrometry, 三元四极质谱
TR-PAC	time-resolved photoacoustic calorimetry，时间分辨光声量热法
VLPP	very low pressure pyrolysis technique，极低压热解技术
VLPR	very low pressure reactor method，极低压反应器法
UV/VIS	ultra-violet and visible spectrometry，紫外和可见光谱
UV absorption	紫外吸收
UV photoionizat.	紫外光（致）离解
UV photolysis	紫外光解（法）

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第一篇　化学键能

第1章　引　　言

1.1　什么是化学键能?

化学家研究化学反应是为了驾驭化学反应、造福人类。所以，化学家和化工工程师在动手之前，必须预先知道与该化学反应有关的许多物理量。例如，气体的压力，固体的溶解度，溶液的浓度，液体的沸点、蒸气压，有机溶剂闪点和可燃性，试剂的毒性，反应物对热、对光的稳定性，化学反应速度的快慢和产率等等。这类似于战争之前，军事家研究如何“知己知彼”、“心中有数”，从而妙计奇兵，旗开得胜。

所有化学和生物化学反应，都建立在化学键概念的基础上。大多数化学反应都包括旧化学键的断裂和新化学键的生成。因此，化学家、化工工程师、材料和安全工程师需要查阅、了解分子结构与化学键性质有关的物理量。其中，化学键（离解）能（bond dissociation energy 或 enthalpy, BDE）就是非常重要的数据之一。换句话说，键能数据应该是化学工作者“家喻户晓”的知识，“所有化学家都需要知道键能”（1994BER/ELL）。

大多数情况下，我们最关心的是化学键均相离解能。它被定义为如下离解反应的焓变：

$$R\text{—}X \longrightarrow R + X \qquad (1.1)$$

式中，R—X 是母体分子，R 和 X 是自由基或原子。R—X 键的键能可以由生成热（焓）推导出：

$$BDE(R\text{—}X) \equiv DH^\circ(R\text{—}X) = \Delta_f H^\circ(R) + \Delta_f H^\circ(X) - \Delta_f H^\circ(RX) \qquad (1.2)$$

式中，$\Delta_f H^\circ$（R）、$\Delta_f H^\circ$（X）和$\Delta_f H^\circ$（RX）分别是R 、X和RX为理想气体时，在热力学标准条件下（25℃, 101.325 kPa）的生成热（焓）。

在气相化学动力学的许多文献内，BDE（R—X）被记为DH°（R—X）。这符号来源于BDE的严格科学定义。其中，“D”表示化学键离解（dissociation），“H”强调BDE是属于热化学焓变（enthalpy），上标“°” 指出它们是在热力学标准条件下的数值。在物理学、化学、化工、生物化学、地学、材料、能源、环境和太空科学的绝大多数文献内，键离解能（焓）经常被简称为键能，更简单地记为D（R—X）。读者会发现，我们的这本有关化学键离解能（焓）的书名，也大众化了。

从式（1.2）知道，测量键能等价于测量自由基的生成热，反之亦然，因为许多有机物生成热的测量精度已经达到化学精度（±1 kcal/mol; 1 kcal = 4.184 kJ; 见3.2节）或更好。键能的实验值，既可以直接测量，又可以从式（1.2）推导出。例如，一旦$\Delta_f H^\circ$（CH_3）和 $\Delta_f H^\circ$（C_2H_5）被很好测量，我们能推导出许多CH_3—X和C_2H_5—X的键能值，这包括X = H, F, Cl, Br, I, OH, SH, NH_2, CN, NO, NO_2, CH_3 和 C_2H_5。

现在，大约 6000 多个有机物和 1000 多个无机物的生成热被测量过。它们的实验数

据人多数被收集在如下书籍中：1986PED/NAY，1988LIA/BAR，1989COX/WAG，1991GUR/VEY，1994PED 和 1996GUR/VEY，以及由美国国家标准和技术研究院（1998 NIST）和俄国莫斯科大学（2003YUN）支持的两个免费网站内。本书内，参考文献编码由两段构成，参考文献发表年代和作者姓氏的缩写。本书末的 1300 多条参考文献，按照其年代早晚和英文字母顺序先后排列。

今天，在美国《化学文摘》里，被确认了的化合物数目已超过 2400 万（2004CAS），而且每天都在快速增加。在 NIST 的数据库里（1998NIST），我们只能查到大约 7000 多个无机和有机化合物的生成热。因此，我们需要科学理论长期的、大力的帮助，利用各种理论方法估计化合物的生成热，包括利用从头计算分子轨道理论、密度泛函理论、半经验理论（如 PM3, AM1）、分子力学、原子团加和等等。这些理论方法是互相补充的，就像大米、玉米、小米和小麦等食品那样，有不同的基础和特点，适合不同的人群和用途。

1.2 为什么需要化学键能的数据？

我们生活在阳光，大气、土壤和水的环境里。许多化合物或材料对热对光是稳定的，但也有不少化合物或材料在加热或光照时，要发生明显的化学反应。许多化合物或材料对某些溶剂（例如，水）是惰性的，但对另外一些溶剂则要发生化学反应。许多化合物或材料在空气中能长期存储，但也有不少化合物或材料只能储存在氮气环境里，它们一接触空气，就发生化学转化。为什么人类的肉眼只对 380～760 nm 波长的光敏感？这些问题，都与分子内化学键能大小或强弱有关（1999LUO）。分子内化学键能的强弱,也是度量药物新陈代谢稳定性的尺度（2004LEW/CRA）。

常见化学反应总是先“破”后“立”。在加热、光照或催化剂等作用下，分子内许多化学键之中，那些弱键（或键能值低的键）最先断裂，并引发一系列后续过程，最后形成比较强的键，或键能值比较高、更稳定、性能不同的分子。所以，分子内的弱键是我们经常关心的课题。

表 1.1 给出了某些常见分子和材料内的最弱键的键能值范围。

表 1.1 常见分子和材料内最弱键的键能值范围

最弱键能的大小/（kcal/mol）	化学键强弱	例 子
<0, 或负值		现实中不能稳定存在
2～10	氢键	蛋白质分子内
10～30	极弱键	催化、生化（如血液循环和新陈代谢）过程
30～55	次弱键	碘酒，双氧水，聚合物的引发剂，催化过程
55～70	弱键	催化过程，不稳定的化合物（如炸药）
70～80	次强键	许多抗氧化剂（如维生素A、C、E）
80～95	中强键	燃料（如汽油、柴油），有机化工品
95～110	强键	燃料（如汽油、柴油），有机化工品
110～130	高强键	耐热材料，如不粘锅的涂料
>130	超强键	耐高温高热材料，如太空飞船表面材料

现实存在的分子内，化学键能的数值总是正值。它表示该化学键断裂时，需要外

界提供能量。键能值越高，表示它们需要吸收更多的能量才能断裂。反之，键能值越低，表示它们需要不多的能量就能断裂。所以，广泛流行一种近似的观点，即键能值越高的，表示化学稳定性越高；键能值越低的，表示化学稳定性越差。严格来讲，化学键能是负值的分子，它们只能瞬间存在，寿命极短（纳秒或更短），很快转变成另外的分子，不能稳定储存。

分子和材料的化学稳定性的高低，它们的化学活性或惰性，都是相对的。在阳光、大气、土壤和水的环境中，没有不发生化学反应的绝对惰性的原子和分子。任何金属、无机、有机材料和生物化学分子，都会氧化、老化、转化、衰变或腐蚀，任何食品都会腐败变质。当然，化学稳定性高的材料，其变化过程比较缓慢。许多极慢的化学变化过程，只有经过一段长时间后，才能观察到。

为什么需要化学键能的数据？让我们看一个重要例子。健康长寿，是人们最爱议论的话题。衰老和疾病的主要原因何在？在 20 世纪 50 年代，美国科学家提出一个假设，自由基是看不见的“隐形杀手”。这一观点已被动物试验证实，也被大多数人接收。人体新陈代谢需要氧气，体内有机物的氧化，变成二氧化碳和水等，提供我们生存需要的能量。自由基是氧化过程的副产品，这和煤、油、天然气、木材的燃烧过程非常相似。污染物、废气、毒物、吸烟、暴晒、偏食、受伤、感染、发烧、闹情绪、发脾气、剧烈运动都能使体内产生更多的自由基。在正常情况下，自由基是“功臣”，它将攻击外来微生物、细菌等有害物质，保护身体免受侵害。如果人体内自由基太多，不及时清除，自由基就会成为“杀手”，将攻击细胞膜、DNA、RNA，蹂躏人体器官，破坏免疫系统，伤害大脑和神经系统等等。随着年龄增加，人体自身的抵抗力逐渐降低，难以抵挡自由基的氧化破坏。自由基的氧化破坏，可以引发广泛分布的慢性病。这包括癌症、心脏病、心血管病、糖尿病、肾脏病、关节炎、白内障、未老先衰、老人痴呆症等等。这就是说，自由基氧化伤害导致我们衰老，大多数人都死于“自由基病”。我们通常的食物内，含有许多种抗氧化剂——自由基清除剂，如维生素 A、B_1、B_2、B_6、C、E、K、胡萝卜素、番茄素、儿茶素、类黄酮、前花色素和某些矿物质等等。它们犹如多兵种组合成的“武装力量”，在人体内的不同场合围剿体内的“隐形杀手”，清除不同类别的自由基。现在，科学家正在设计“超强功能”的抗氧化剂，为人类的健康与长寿造福。这类新分子（新保健品）内的最弱键能应当在一个适当的范围之内（即所谓的“键能 windows”），它低于 77 kcal/mol （维生素 E 内 O—H 键能），但又不能太低，70 kcal/mol （标准炸药 TNT 内的最弱 C—N 键能）也许是下限。若最弱键能太低了，化合物不稳定，容易被空气中的氧气氧化变质，反而伤害人体。所以，设计“超强功能”的抗氧化剂，要考虑所谓亲水性、亲油性、无抗原性、无毒、其最弱键能数值必须适当等这些关键的、重要的科学参数。

1.3 为什么需要可靠的键能数据？

利用分子和材料内最弱键的键能数据，我们可以定性地预测它们的化学稳定性的高低。为了定量预测，我们就需要可靠的键能数据。化学键能属于材料热化学量之一，本质上对应于键离解反应平衡常数或反应产率。化学键离解反应的平衡常数对键能值非

常敏感。在 25℃下，键能值误差 1 kcal/mol，平衡常数将变化 540%，即 5 倍多的误差。如键能值误差 2 kcal，平衡常数将变化 2920%，即 29 倍多的误差。如键能值误差 3 kcal，平衡常数将变化 15800%，即 158 倍多的误差。但是，在目前的实验水平下，测量得到的键能值误差大多在 1~3 kcal/mol，或更高。只有极少数分子的键能测量值的精度进入了 1 kcal/mol （化学精度）。因此，化学键能的测量，是化学科学中一个过去、现在和未来都很活跃、很吸引年轻科学家的领域。记得我在中国科技大学读书的时候，一位老师说过一则似乎是笑话、但又是事实的话：如果你们测量的反应速率常数与平衡常数的实验误差是 100%，那是好结果！顺便，希望青年读者回答两个问题：① 假如你们在室温时，测量的反应速率常数与平衡常数的实验误差是 100%，相应的活化能与键能实验值的不确定性是多少？② 假如你们在室温条件下，测量的反应活化能与键能的误差为 0.1 kcal/mol，它导致反应速率常数与平衡常数的不确定性是多少？

为了精确测量关键、重要分子内的化学键能，许多科学家（包括几位诺贝尔化学奖获得者）贡献了青春年华，长期不懈地努力工作。例如，我们可以检索到，从 20 世纪 30 年代以来，大约 50 篇原始文献报导了甲烷内 C—H 键能的测量值。经过近 60 年的不断工作，可以用多种方法测量甲烷内 C—H 的键能。其测量值精度现在进入了 0.1 kcal/mol （见 2.2 和 4.1 节）。科学家们的长期努力和百家争鸣，导致了化学键能测量值精度进一步提高，因此我们才能更好地定量预测分子和材料的化学反应能力。这里有一则好消息，利用高分辨激光光谱仪，氢分子和其同位素分子的键能的测量值已经精确到了小数点后第四位，或±0.0001 kcal/mol（2004ZHA/CHE）：

DH^{o}（H—H）= 104.1502±0.0001 kcal/mol 或 435.7644±0.0001 kJ/mol
DH^{o}（H—D）= 104.9729±0.0001 kcal/mol 或 439.2066±0.0002 kJ/mol
DH^{o}（D—D）= 105.9552±0.0001 kcal/mol 或 443.3038±0.0001 kJ/mol

目前，对人类很重要的化合物有一万多种，它们绝大多数的化学键能要么是不精确，要么是不知道。因此，我们“任重而道远”。

1.4 哪里能得到键能的数据？

通常，我们是通过查找有关书籍、综述评论文章以及原始文献获取键能的数据。但不幸的是，化学键能的原始测量数据中散布在化学、物理学、化工、生物化学、地学、材料、能源、环境和太空科学的许多文献中。有时候，查找可靠的数据，尤如大海捞针。有时候，会找到几个或更多互相冲突的数据。到底选用哪一个值，如果你不在行，会感到左右为难。在 20 世纪 70 年代，科学家开始建立化学键能的数据库。许多化学键能的实验数据，已经收集在“CRC Handbook of Chemistry and Physics （2002CRC）”中。这是一本物理和化学的大百科全书，从中我们可以查到 800 多个双原子分子的键能的实验数值，400 多个多原子分子内的键能实验数据。遗憾的是，这本信誉很好、每年都再版的手册，对键能实验数据的介绍，没有与时俱进，不断更新和补充。

1990 年，我开始收集化学键能的实验数据和理论计算预测值。在那些“坐冷板

凳”的漫长日子里，海内外的许多科学家帮助我、鼓励我坚持做下去，因为这项课题是化学反应动力学、自由基化学、有机热化学以及物理（或高等）有机化学最基本的工作。至 2002 年，我的编写工作终于定稿，由美国 CRC 出版社发行，它是头一本完整的化学键能参考书。

化学键能数据库是本书的主要内容。本书收集了大约 3700 余种多原子分子内的 4300 多个化学键的键能实验数据，比我于 2002 年出版的英文书更新和更丰富。什么是数据库？数据库就像百货商店和超级市场。在百货商店和超级市场里，我们能方便地采购到需要的东西和食品。在各种科学数据库里，我们能方便地查找到需要的各种科学数据。

第 2 章　得到键能数据的主要实验方法

如果你没有兴趣了解测量化学键能的方法，仅仅是希望访问键能数据库，那么可以跳开这一章，直接阅读下面的第3章，然后利用本书目录，检索数据库。

为了准确测量化学键能，科学家几乎使用了现代已有的、最好的实验手段。下面，我们将介绍最主要的实验方法。事实上，各种测量技术都在研究如下三种反应：

（1）化学键离解与重合反应

$$A—B \rightleftharpoons A^{\cdot} + B^{\cdot} \qquad (2.1)$$

（2）自由基夺取反应

$$A^{\cdot} + B—C \rightleftharpoons A—B + C^{\cdot} \qquad (2.2)$$

（3）自由基离解反应

$$A—B^{\cdot} \rightleftharpoons A + B^{\cdot} \qquad (2.3)$$

2.1　热解反应动力学法

这是提供键能数据最早期的方法。许多键能数据来源于在高压和高温下测量键离解反应（2.1）的活化能。这类方法存在四个问题。第一，它没有考虑化学反应机理的复杂性。自由基非常活泼，要引发许多后续反应。第二，化学键能DH°的数值并不等于键离解反应活化能的数值。第三，自由基重合反应的活化能比较小，但并不等于零，而且很难精确测定。第四，化学键能DH°的数值被定义在25℃，因此高温下活化能数值必须换算到25℃时的活化能数值。在几个近似假定的条件下，McMillen和Golden（1982MCM/GOL）提出了一个关联高温键离解反应活化能$E_{d,T}$与键能DH°的公式：

$$DH^{\circ} = \Delta H_{298} \approx E_{d,T} - <\Delta C_p^{\circ}> (T-298) + 0.5RT \qquad (2.4)$$

式中，T是热解温度（K），R是摩尔气体常量，$<\Delta C_p^{\circ}>$是离解反应前后反应物与产物（自由基）之间的平均比热容改变。从公式（2.4）得知，化学键能的数值通常低于键离解反应活化能的数值1～2 kcal/mol。一般地说，常见的热解方法不能提供精确的键能数据，实验偏差为1.5～3 kcal/mol。

早期最著名的热解方法是Szwarc等（1950SZW）发展的，叫做甲苯载体技术，它力图消除自由基的后续反应。Szwarc等提供了几百个键能数据。Benson等（1970ONE/BEN）很快发现，这些数据都偏低几到10 kcal/mol。现在，再也没有人接受Szwarc等提供的键能数据了。

单激波管热解。这是Tsang等（1981TSA，1999TSA）发展的一项非常简单和方便的测量分子热解的技术。在单激波管内，加热和冷却都很快（大约百万分之一秒），消除了许多后续反应，反应器表面的影响也很小。该技术的主要问题是不能提供明确的反应温度数值。为了克服这一缺点，做实验时，要引入参考分子，测量参考分子的相对反应速度。如果参考分子的反应速度与温度的关系是已知的，那么我们有

$$\lg A - E/RT = <\lg A' - E'/RT> + C \qquad (2.5)$$

式中，A（A'）与E（E'）分别是A因子与活化能；<lgA'–E'/RT>为Arrhenius图中的斜率；C为截距。这一方法能够提供比较可靠的键能数据，误差多在1～2 kcal/mol内。

流动管热解。热解反应器是一根柱状的石英管。反应分子在反应器内的平均停留时间，取决于反应器尺寸和流动速度。流出气体由色谱和质谱分析。通常，人们用自由基反应的稳态近似法计算反应速度。Pacey等（1984PAC/WIM）改进了这一技术，使得人们能够在反应还没有到达稳态的很短时间就可以测量。改进的方法提供了比较可靠的键能数据，误差进入了1 kcal/mol内。

极低压热解。这是Benson等（1979ROS/KIN, 1982MCM/GOL）开发的多用途的反应动力学研究技术。反应器内的压力为0.1～10 mtorr （1 torr = 1 mm Hg = 133.322 Pa），反应物连续通过反应区。如同激波管技术那样，极低压热解技术也能消除后续反应和反应器表面的影响。反应温度和停留时间是明确的，流出气体由质谱分析。因此，这一技术可以提供大量的、比较可靠的键能数据。

2.2 卤原子夺取反应动力学法

这是提供气相分子内键能数据的主要方法之一。热解反应动力学法主要是研究反应（1）和（3），这里我们主要研究反应（2）：

$$X + RH \rightleftharpoons HX + R \qquad (2.6)$$

式中，X代表卤原子，如Cl, Br和I原子，RH是有机分子。我们要分别测量正反应和逆反应的速度常数，以及它们与温度的关系、A因子与活化能。该反应焓变等于正反应和逆反应的活化能之差

$$\Delta H_T = E_f - E_b \qquad (2.7)$$

把反应温度T的ΔH_T换算到25℃下的ΔH_{298}：

$$\Delta H_{298} = \Delta H_T + <\Delta C_p>(298-T) \qquad (2.8)$$

式中，T是平均反应温度，$<\Delta C_p>$是反应前后平均比热容变化。我们有

$$\Delta H_{298} = DH^\circ(H—X) - DH^\circ(R—H) \qquad (2.9)$$

因为双原子分子卤化氢HX的键能DH°（H—X）已经高精度确定，所以我们能得到许多有机分子内的键能DH°（R—H）以及自由基R的生成热$\Delta_f H^\circ$（R），另外，还可以进一步推导出更多的有机分子内的键能DH°（R—X）。这一方法借助于van't Hoff 方程，故简称“第二定律”法。

如果正反应和逆反应速度常数仅在一个温度或一个很小的温度范围内（如50 K）测量，我们首先计算在该温度或平均反应温度下的平衡常数K_{eq}：

$$K_{eq} = k_f / k_b \qquad (2.10)$$

然后利用统计力学配分函数计算反应物与产物分子的生成熵，并计算该反应温度或平均反应温度下的熵变ΔS。因为该反应的Gibbs自由能变化为

$$\Delta G = -RT \ln K_{eq} = \Delta H - T\Delta S \qquad (2.11)$$

最后，我们计算出焓变ΔH，并换算到25℃下的ΔH_{298}，得到键能DH°（R—H）、自由基R的生成热$\Delta_f H^\circ$（R）以及更多的有机分子内的键能DH°（R—X）。这一方法借助于计算熵变，故简称“第二定律”法。通常，第二定律法比第二定律法能提供更可靠的数

据，原因是我们可以精确地计算许多分子和自由基的生成熵，大大减少了计算过程中的误差传递。

下面举一个例子。Benson等（1981HEN/KNO）在极低压反应器内，研究了反应

$$Cl + CH_4 \rightleftharpoons HCl + CH_3$$

利用第二定律法，他们得到

$$\Delta H_{298} = DH^\circ\ (H—Cl) - DH^\circ\ (CH_3—H) = 1.6\pm0.7\ kcal/mol$$

因为DH°（H—Cl）是已知的，为103.16 kcal/mol（2002CRC），最后我们有

$$DH^\circ\ (CH_3—H) = 104.8\pm0.7\ kcal/mol$$

$$\Delta_f H^\circ\ (CH_3) = 34.8\pm0.7\ kcal/mol$$

同样的反应，同样的实验数据，如果利用第三定律法，他们得到

$$DH^\circ\ (CH_3—H) = 105.0\pm0.1\ kcal/mol$$

$$\Delta_f H^\circ\ (CH_3) = 35.1\pm0.1\ kcal/mol$$

对于有机物键能和自由基生成热来说，这是目前最好的几个测量结果之一。

2.3 光解反应动力学法

光解动力学法包括紫外光解（1995BOY/NOZ）、射解（1990LIN/SHE）、激光光解（1997BEC/CAR）、光敏光解（1967LOU/LAI）等。光解反应动力学法和热解反应动力学法最根本的区别在于引发自由基的方式是光解还是热解。

光解技术可以很快引发自由基，这是一大优点。选择产物分析的方法比较多，例如，各种色谱、HPLC、各种质谱、FTIR、UV/VIS、EPR、NMR、共振荧光、化学发光等等。下面我们提供三个例子。

（1）乙基自由基热解平衡的细致研究。Pilling等（1986BRO/LIG, 1990DAV/LEE）研究了如下反应：

$$H + C_2H_4 \rightleftharpoons C_2H_5 \qquad (2.12)$$

他们利用一台ArF受激激光器，脉冲能量15～150 mJ，闪光光解乙烯，产生H原子，观察Lyman α共振荧光信号，分析产物，同时和直接地测量正、逆反应速度。因为H原子、乙烯和乙基自由基C_2H_5的生成熵是准确知道的，利用第三定律法，他们得到乙基自由基C_2H_5的生成热，$\Delta_f H^\circ\ (C_2H_5) = 28.36\pm0.40$ kcal/mol。我们导出，DH°（H—C_2H_5）= 100.5±0.5 kcal/mol。

（2）甲酰基的热化学。Walsh等（1997BEC/CAR）利用一台KX2激光器，用308 nm的光，闪光光解甲醛，产生甲酰基自由基CHO。研究在HI或HBr存在条件下的夺取反应

$$CHO + HI \longrightarrow CH_2O + I \qquad (2.13)$$

$$CHO + HBr \longrightarrow CH_2O + Br \qquad (2.14)$$

观察产物随时间的衰变信号，直接地测量夺取反应速度常数。他们利用第三定律法，得到甲酰基自由基的生成热$\Delta_f H^\circ\ (CHO) = 10.4\pm0.1$ kcal/mol，进一步导出DH°（H—CHO）= 88.6±0.1 kcal/mol。

（3）流动光解技术。Gutman等（1988RUS/SEE（b）,1990SEE/RUS）发展了这一新

技术。实验设备主要是一个流动反应器、一台受激激光器及光电离质谱仪。激光器提供未聚集的193或248 nm的激光，闪光光解卤素分子，引发卤原子夺取反应（2.6），产物由光电离质谱仪监测。通常，他们的DH°（R—H）既可用第二定律法推出，也可用第三定律法推出。

2.4 气相离子的热化学循环和质谱法

气相离子热化学循环和质谱法的研究，是提供键能数据的又一个主要来源。从热化学讲，我们至少有图 2.1 所示的三种热化学循环可以得到键能 BDE(R—H)：

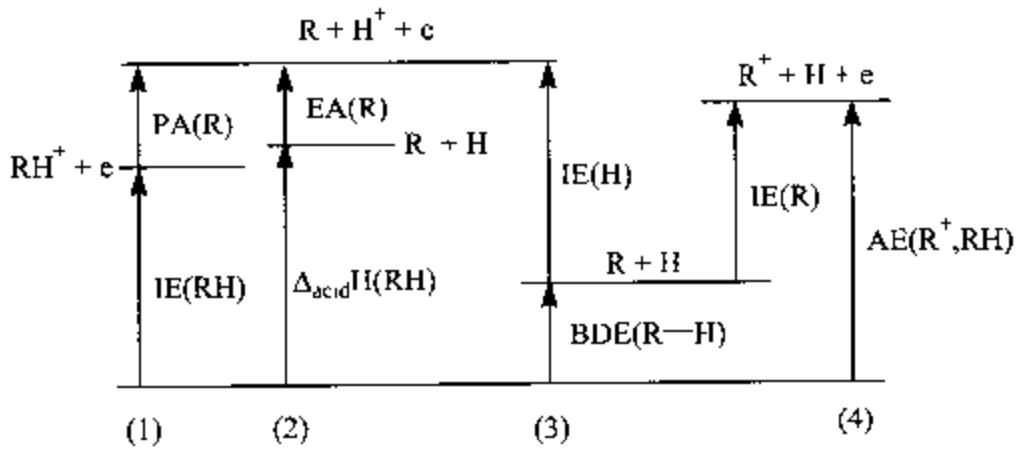


图 2.1 三种热化学循环

这里，IE, PA, EA, AE 和 $\Delta_{acid}H$ 分别代表电离能、质子亲和势、电子亲和势、呈现（出峰）能以及气相酸度。

利用质子亲和循环（1），我们有

$$BDE（R—H）= IE（RH）+ PA（R）- IE（H） \tag{2.15}$$

利用负离子或气相酸度循环（2），我们得

$$BDE（R—H）= \Delta_{acid}H（RH）+ EA（R）- IE（H） \tag{2.16}$$

利用呈现（出峰）能循环（4），我们有

$$BDE（R—H）= AE（R^{+},RH）- IE（R） \tag{2.17}$$

IE, PA, EA, AE 和 $\Delta_{acid}H$ 等都是 0K 时的焓变。从理论上讲，它们需要换算到 298 K 下的焓变，才能给出键能 BDE(R—H)。这种热效应修正非常之小，因为离子和中性物的结构与振动频率很相似。忽略这种修正后，带入的误差常低于 1 kcal/mol。另一方面，质子亲和势、气相酸度、电离能与呈现（出峰）能的数值都比键能大得多，根据方程（2.15）、（2.16）和（2.17），BDE 是这几个大数之间的差值。所以，这种代数差成为导出键能的主要误差来源。例如，气相酸度$\Delta_{acid}H$ 为 200±2 kcal/mol，误差 2 kcal，才 1% 的误差，是一个好结果！但它同时将导致键能误差高于 2 kcal/mol 以上，这就未必是好结果了。

观察正负离子，需要各种质谱仪。下面我们提供一张简表（表 2.1），列出了各种质谱方法、不同的观测量及有关参考文献。

表 2.1　各种质谱法简介

实验方法	观　测	参考文献
质谱法（MS）包括:	研究观测量与键能的关系	（1）2001ERV （2）2001GRO （3）2002SAB/FUJ
• electron impact （EI） 电子冲击质谱	ion intensities vs. electron energy	（1）1979BER （2）1984HOL/LOS （3）1992HOL
• guided ion beam （GIB） 导向离子束质谱	ion intensities vs. ion kinetic energy	（1）1995ARM （2）1998DET/ERV
• high pressure （HPMS）高压质谱	ion intensities vs. temperature	（1）1994BUS/KEM （2）1994BOW （3）1999MCM
• ion cyclotron resonance （ICR） 离子回旋共振质谱	ion intensities vs. time, electron, or photon energy	（1）1980DEF/MCI （2）2000BOR/ING （3）1999ABB/NOT
• time-of-flight （TOFMS） 时间飞行质谱	ion intensities vs. flight time	（1）1996ZHA/SHE
• high temperature 高温质谱	ion intensities vs. temperature	（1）1984MAR
• photoionization （PIMS） 光电离质谱	ion intensities vs. photon energy	（1）1994BER/ELL （2）1994BAR
• pulsed high pressure 脉冲高压质谱	ion intensities at one or several temperatures	（1）1989MEO （2）1993SHA/KEB
• kinetic method 动力质谱	ion intensities	（1）1994COO/PAT
• kinetic energy release distributions 动能质谱	ion intensities vs. product kinetic energy	（1）1992BEA/KOP

这里介绍一个例子。Holmes 等（1988HOL/LOS）利用电子冲击法测量自由基电离时的出峰电势（AP），得到了反应分子内的键能。它的基本原理是

$$\begin{array}{ll} e + AB \longrightarrow A^+ + B + 2e & AP\ (A^+) \\ 2e + A^+ \longrightarrow A + e & -IP\ (A) \\ \hline AB \longrightarrow A + B & BDE\ (A—B) = AP\ (A^+) - IP\ (A) \end{array} \tag{2.18}$$

或者，出峰电势是有关物种的生成热之和

$$AP(A^+) = \Delta_f H^\circ(A^+) + \Delta_f H^\circ(B) - \Delta_f H^\circ(AB) \qquad (2.19)$$

2.5 气相离子的热化学循环和光谱法

质谱法的特点是用高能电子撞击分子，然后分析其热化学循环，导出分子键能。我们也可以用光子撞击分子，使分子电离，通过热化学循环，最后利用方程（2.15），（2.16）或（2.17）导出分子键能。

下面，我们提供一张简表（表 2.2），列出这类方法的观察量以及参考文献。它们之中，碰撞诱导离解法（CID）和光电离质谱法（PIMS）比较常见。

表 2.2 光谱法简介

实验方法	观测	参考文献
光谱法 包括:	研究观测量与键能的关系	(1) 2001ERV
• photoelectron (PES) (光电子光谱)	electron count vs. electron kinetic energy	(1) 1984MEA (2) 1994BER/ELL
• electron photo-detachment (光电分离)	ion intensities vs. photon energy	(1) 1987WET/BRA (2) 1989CHE/ALB
• flowing afterglow (FA) (流动辉光)	ion intensities vs. time or ion kinetic energy	(1) 1992SQU (2) 1994BER/ELL
• collision-induced dissociation (CID) (碰撞诱导离解)	collision energy vs. cross section	(1) 1994WEN/SQU (2) 2001HAM/WEN
• photoionization MS (PIMS) (光电离质谱)	ions are detected by MS	(1) 1994BER/ELL (2) 1996ZHA/SHE

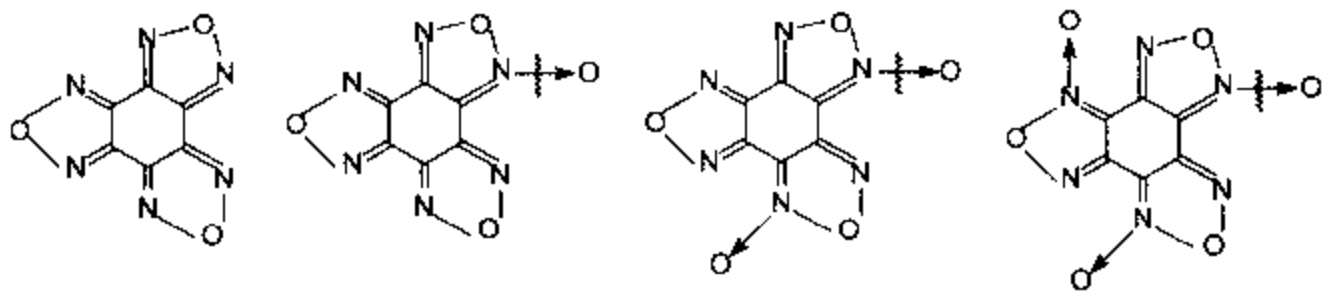
下面来看两例子。

李远哲等（1989NAT/MIN）测量 CF_2ICF_2—I 键能的实验。在交叉分子束装置内，用 308 nm 的紫外光光解 CH_2ICH_2I，产生自由基 CH_2ICH_2 和 I 原子，利用光碎片平动光谱监控它的离解。最初产生的 I 原子，有两个电子态，基态 I（$^2P_{3/2}$, 记为 I）和激发态 I（$^2P_{1/2}$, 记为 I*），后者的能量比前者高 21.7 kcal/mol。根据能量守恒定律，最初产生的自由基 CF_2ICF_2 的平动和内激发所用能量，应当等于光能减去 C—I 键能（0 K），再减去 I 激发的自旋能。利用光谱和质谱的组合技术测量有关各种能量，他们得到 BDE（CH_2ICH_2—I, 0 K）= 52±1.6 kcal/mol。

中国科技大学张允武、俞书勤等和他们的合作者们（1996ZHA/SHE, 1997QI/YAN, 2001LIU/LI），利用同步辐射加速器引出的单色紫外光，经过后置镜聚焦到光电离室。研究分子的光电离，利用质谱仪测量碎片离子的出现势。借助于理论计算，分析可能的离解通道，推导出离子、自由基、分子的热力学性质以及化学键能数据。他们的测量装置，提供了大量无机、有机、金属有机化合物和簇合物的键能数据。

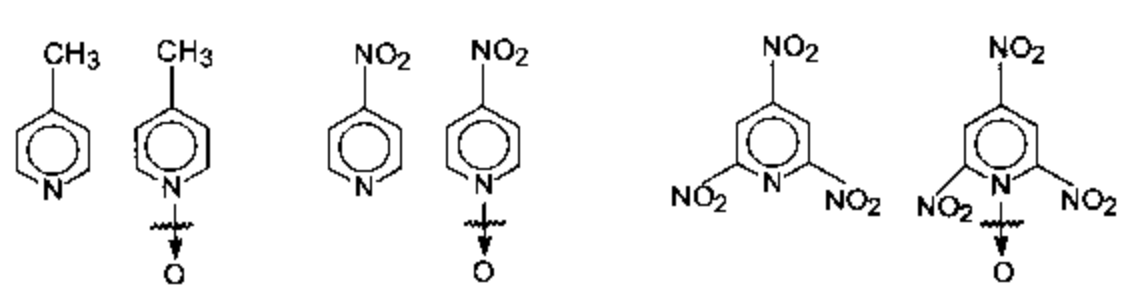
2.6 量 热 法

根据第1章的公式（1.2），只要我们知道了键离解反应中每个物种的生成热，即可导出键能。最近，Lebedev等（2002MAT/PEP）测量了如下每个物种（炸药）的燃烧热、气化热以及生成热$\Delta_f H^\circ$（RO）。从分子结构看，它们的差别在于氧原子。氧原子的生成热是59.555 kcal/mol。因此，我们可以计算出相应的N—O共价配键的键能。很有趣，三种N—O共价配键的键能基本相等，与分子结构几乎无关。



物种	1	2	3	4
$\Delta_f H^\circ$(RO)/kcal	174.5±1.1	175.9±1.5	177.7±1 0	179.9±1.1
BDE(N—O)/kcal		58.2±1 9	57 8±1.8	57.4±1.5

他们用同样的方法测量了如下固体炸药的N—O键能（1995LEB/CHI）：



$\Delta_f H^\circ$(RO)/kcal	23.9	17.8	30.2	24.1	32.5	49.8
BDE(N—O)/kcal		65.7		65.7		42.3

对比他们的测量结果，我们看到了邻位NO_2基的位阻排斥效应导致该N—O键能明显降低。

2.7 光声量热法

这是Griller和Wayner等（1989GRI/WAY，1999LAA/MUL）发展的新量热技术。上面介绍的各种动力学、质谱和光谱测量键能的技术，主要适合于气相或蒸气压比较高的液相分子。光声量热法（PAC）是专门为测量蒸气压比较低的液相分子键能设计的。

光声量热的实验设备是比较简单的。一个流动反应池，一台氮激光器，提供337 nm的激光，引发在四氯化碳中的如下反应

$$t\text{-BuO—Ot-Bu} \longrightarrow 2\ t\text{-BuO}$$

$$t\text{-BuO} + RH \longrightarrow t\text{-BuOH} + R$$

释放的热量进入溶剂，引起激波，以声速传递到反应器壁，引起器壁振动，用有微秒分

辨率的高灵敏的压电传感器检测信号。

因为该反应的热量是

$$\Delta H_{total} = 2\Delta_f H(\text{t-BuOH}) + 2\Delta_f H(\text{R}) - 2\Delta_f H(\text{RH}) - \Delta_f H(\text{t-BuOOt-Bu}) \quad (2.20)$$

利用已知的分子生成热数据，我们可以计算出自由基的生成热$\Delta_f H$（R）。许多液相有机、有机金属和生化分子内的键能，已经被光声量热技术测定，其精度可以达到1～2 kcal/mol。为了提高测量精度，现在正在开发时间分辨的光声量热技术（2002SAN/MUR）。南京大学陈慧兰、张淑仪等与他们的合作者们，利用激光诱导时间分辨光声量热法，测量了维生素B_{12}辅酶中的C—Co键能（2003CHE/LI）。

2.8 液相自由基缓冲法

为了研究液相自由基动力学和测量键能，Griller和Wayner（1990WAY/GRI）发展了这一方法。碘原子交换反应

$$CH_3 + RI \longrightarrow CH_3I + R$$

是一快过程。如果碘代物RI的浓度是1 mol，这一反应将更快，自由基的其他竞争反应可以忽略不计。这好像是建立了一个自由基的“缓冲”体系。

用热或光引发自由基，用ESR监测自由基浓度及CH_3/R 比例，根据已知的RI分子生成热，估计反应焓变，最后可以导出反应分子的键能。他们发现，溶剂效应比较小，得到的键能数值可以与气相技术得到的相比较。

2.9 电化学法

在各种各样测量键能的方法之中，电化学方法出现的时间比较短，但它提供的数据远比其他方法多得多，极大地丰富了键能数据库。电化学法有两大优点：（1）能够测量许多蒸气压非常低的液相有机、有机金属和生化分子内的键能。这一优点非常重要，可用于研究生化反应、催化反应、开发新药物。（2）实验设备惊人地简单只需要一台循环伏安（CV）计。

程津培、张先满和Bordwell（1988BOR/CHE,1993BOR/ZHA）等发展了化学键能的电化学测量技术。它的基本原理是测量酸性离解常数（pK_{HA}）和氧化还原电位[E_{OX}（A^-）]，利用如下热化学循环，导出键能：

$$\begin{array}{ll} R{-}H \rightleftharpoons R^- + H^+ & pK_{RH} \\ R^- \rightleftharpoons e + R & E_{ox}(R^-) \\ H^+ \rightleftharpoons H & E_{red}(H^+) \\ \hline R{-}H \longrightarrow R + H & DH^\circ(R{-}H) \end{array}$$

$$\begin{aligned} BDE(R{-}H) &= 2.303\,RT\,pK_{RH} + 23.06\,E_{ox}(R^-) + C \\ &= 1.37\,pK_{RH} + 23.06\,E_{ox}(R^-) + C \end{aligned} \quad (2.21)$$

式中，E_{ox}（R^-）的单位用eV（1 eV = 23.06 kcal/mol），BDE（R—H）的单位用kcal/mol；对于同类反应，C是一个常数，包含反应熵变、溶剂化效应等。这一方法又简称AOP （acidity-oxidation potentials）法。程津培等发现（1989BOR/CHE），RH在Me_2SO中的酸性离解常数和在气相中的酸度（或酸性离解常数）有近似的线性关系。所以，从减少误差的观点看，利用同类反应的相对测量值更好：

$$\Delta BDE（R—H）= 1.37\,\Delta(pK_{RH}) + 23.06\,\Delta E_{ox}（R^-）\qquad（2.22）$$

Parker等（1991PAR/HAN）分析了方程（2.21）的可能误差，如果考虑到溶剂化、不可逆电位等修正，导出的键能值很可能往上调高1或3 kcal/mol，与从气相反应动力学技术测量的键能数值相当接近。

2.10 相关估计法

2.10.1 活化能、速率常数、生成热与键能的相关

夺取反应（2.2）的活化能与该反应生成热或键能BDE（B—C）之间的线性关系（或图），叫Evans-Polanyi关系（图）。如果BC分子是同系列化合物，它们的实验活化能已经知道，它们的键能也已经知道，我们就可以利用这一线性关系，内插或外推某些未知的同类BC分子内的键能。

这一经验关系，简单、方便，但使用时必须小心。我们要注意两点：①是否为同系列化合物；②Evans-Polany图中各点的实验误差到底有多大。

因为反应活化能E与lg$k$（速率常数）之间是线性的，所以我们也可以利用lg$k$ - BDE（B—C）作图，内插或外推某些未知的同类BC分子内的键能。相对而言，速率常数与活化能比较容易测量，所以Evans-Polany图较受欢迎。

2.10.2 利用速率常数与活化能数据估算键能的抛物线相交模型

在化学数据库里，自由基夺取反应的速率常数与活化能的实验数据非常之丰富。相比之下，化学键能的数据库却太小，原因是测量键能的工作更困难。如果我们能从自由基夺取反应的速率常数或活化能数据出发，通过一个物理模型，估计一系列反应分子的键能，这样的研究工作很有价值。10年前，Denisov等（1995DEN, 2000DEN/DEN）假定，自由基夺取反应

$$A + HB \rightleftharpoons AH + B$$

的过渡态势能曲线可以用两个相交的抛物线近似描述，如图2.2所示。

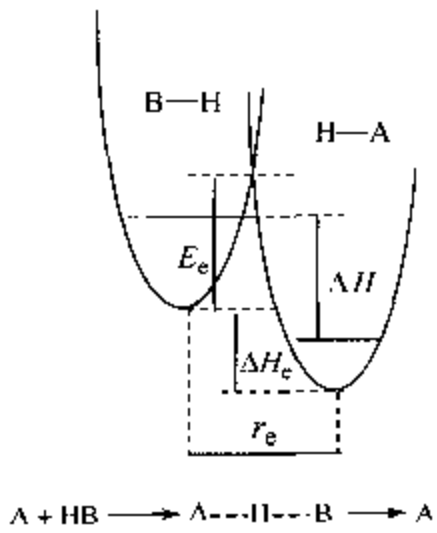


图2.2 自由基夺取反应的过渡态势能曲线

他们利用几个近似假设，计算同类反应的模型参数，最后估算了好几百个分子的键能，特别是酚类化合物的O—H键能、芳烃化合物的C—H键能以及卤素化合物的C—X键能，误差多在1～3 kcal/mol。

在利用这类物理模型时，我们要注意如下三个物理量的区别：D_e，D°和本书的键能

DH°。D_e是势能曲线（面）上的势阱深度，D°是0 K时的键能，而DH°是热力学标准条件下的键能。对双原子分子，DH°的数值比D°要高$3RT/2$（即0.89 kcal/mol）。对碳氢化合物，DH°的数值比D_e大约低6.2 kcal/mol（1965BEN）。在我们知道了D_e和D°之后，还需要考虑各种自由度从0～298K的温度效应，才能得到DH°。如果读者希望知道其详细解释，可以阅读赵学庄主笔的教材《化学反应动力学原理》（1990ZHA/LUO）。

2.10.3 氟代烃的^{19}NMR化学位移与C—F键能

Mercader和Castro（2001MER/CAS）发现，氟代烃的^{19}NMR化学位移Φ与C—F键能有线性关系：

$$\mathrm{BDE}\ (\mathrm{C}\quad \mathrm{F}) \propto \Phi^{0.5} \tag{2.23}$$

氟代烃是大气环境污染物，能破坏大气臭氧保护层，引发皮肤癌。目前，氟代烃^{19}NMR化学位移Φ的数据非常多，而C—F键能数据相对来说很少，所以简单的经验（2.23）关系式是有价值的。但使用这类关系式，必须小心，可能包括了原因不明的误差，约2~4 kcal/mol。

2.10.4 自由基的ESR光谱与键能

Ruchardt等（1997WEL/BEC，1998BRO/BEC）发现，自由基R的α-质子ESR超精细分裂常数（proto hyperfine splitting constants）a（H_α）、β-质子ESR超精细分裂常数a（$H_\beta Me$）都和键能BDE（R—H）有线性关系：

$$\mathrm{BDE}(\mathrm{R—H}) = A\,a\ (\mathrm{H}_\alpha) + B \tag{2.24}$$

$$\mathrm{BDE}(\mathrm{R—H}) = A'\,a\ (\mathrm{H}_\beta\mathrm{Me}) + B' \tag{2.25}$$

式中，A（A'）是斜率，B（B'）是截距。相对于键能来说，自由基的ESR超精细分裂常数还比较容易测量。因为键能值很重要，但数据少，直接测量困难，所以这类经验关系是有用的。

2.10.5 C—C键长与C—C键能

乙烷、乙烯和乙炔内的C,C键，分别是单键、双键和三键。从乙烷到乙烯到乙炔，C,C键长愈来愈短，但C,C键能愈来愈强。这三点有一个很好的线性关系。最近，Zavitsas（2003ZAV）发现，这一线性关系可以推广到许多其他C,C键：

$$r(\mathrm{C,C}) = 1.748 - 0.002371[\mathrm{BDE}(\mathrm{C,C})] \tag{2.26}$$

式中，r（C,C）是C,C键长，单位用Å（1 Å = 10 nm）。

2.10.6 键伸缩频率、自旋耦合常数、力常数和C—X键能

Batt等（1973MCK/DUN）发现，许多有机分子内的C—H键长r（C—H）、C—H键的伸缩振动频率$\nu_{C\ H}$（cm^{-1}）、C—H键自旋耦合常数J_{C-H}（Hz）与C—H键能有近似的线性关系。

Zavitsas（1987ZAV）也发现，C—X键的未耦合的红外（uncoupled infrared）伸缩振动频率ν（cm^{-1}）与C—X键能（kcal/mol）有如下关系：

$$\nu = 143.3\ (\mathrm{BDE} - c_1)^{0.5} \tag{2.27}$$

式中，c_1 是成键原子C和X的特征常数：c_1 = 39.7（C—C 键），26.7（C—N 键），33.8（醇和羰基化合物内的C—O键），24.2（醚和酯内的C—O键），51.4（C—F键），42.5（C—Cl键）和40.6（C—Br 键）。

Zavitsas（1987ZAV）发现，C—X键的力常数（mdyn[1]/Å）和C—X键能（kcal/mol）有关：

$$k/\mu = 0.0121\ (\mathrm{BDE} - c_1) \tag{2.28}$$

式中，k是力常数，μ是折合质量（amu）。

使用这些粗糙的经验关系，必须十分小心，估算误差可能有2～4 kcal/mol。其实，数据库内，C—C, C—N, C—O, C—Cl 和C—Br键能的数据比较多，经验关系（2.27）和（2.28）的实际价值比较小。

2.10.7 自由基的内转动能垒与键能

ESR技术可以测量自由基的内转动能垒。Nonhebel和Walton（1984NON/WAL）发现，某些RCH_2—H键能DH°（C—H）和自由基内围绕化学键R—CH_2·的内转动能垒V_o有线性关系：

$$\mathrm{BDE\ (C—H)} \propto V_o \tag{2.29}$$

他们试图利用这近似关系估计某些分子内的键能。事实上，这一关系很不精确。

2.10.8 二元参数法

Errede（1960ERR）认为，键能BDE（X—Y）可以表示为

$$\mathrm{BDE\ (X—Y)} = \lambda \varepsilon_X \varepsilon_Y \tag{2.30}$$

式中，λ是物种X—Y的特征参数，ε_X和ε_Y分别是X和Y的结构参数。Neale（1964NEA）发现，结构参数ε和自由基的电离能和电子亲和势有关。这些经验关系不够精确，引用极少。

2.11 其他测量方法

化学键能还可以用另外一些方法进行测量，如化学活化法（1973ONE/BEN），产物能量分配法（1980KIA/ZAR, 1981SLO/WAT）等。这些方法提供的键能数据比较少，我们不详细介绍了。

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1) dyn 为非法定单位。1dyn=10^{-5}N，1mdyn=10^{-8} N。

第 3 章　如何在键能数据库中查找需要的数据

3.1　键能数据库的范围

一个理想的化学键能数据库,应当包括如下几个部分:

（1）气相原子的生成热;

（2）双原子分子的生成热;

（3）多原子分子（无机、有机、元素有机和簇合物）的生成热;

（4）自由基的生成热;

（5）双原子分子内的键能;

（6）多原子分子内的键能。

“CRC Handbook of Chemistry and Physics”（2002CRC）提供了800多个双原子分子的键能的实验数值。这是关于该课题目前最完整的数据库。美国国家标准和技术研究院的免费网站（1998NIST）http://webbook.nist.gov，介绍了大约7 000多个双原子和多原子分子的生成热的实验数据。这是当前最完整的无机和有机分子的热化学数据库。

这两个高质量的数据库，为我们提供了很好的基础。对于上面六部分工作，第（4）部分,自由基的生成热，以及第（6）部分,多原子分子内的键能,是空白领域，也是化学数据库研究工作的前沿。为了建立完整的化学键能数据库，我们必须完整地检索和收集从20世纪30年代开始的实验文献。我们应当收集所有实验数据，而不应当把所有实验数据不经过评选就奉献给读者。举一个典型例子，甲烷内的C—H键能，被报道50多次，从最早的98 kcal/mol到今天接受的（105.0±0.1）kcal/mol。饭店的大师傅，把生冷的原料，通过烹调手艺，变成了色鲜味美的食品，才奉献给顾客。我们应当向他们学习，把最好的、比较可靠的数据奉献给读者。什么数据比较可靠？这是一个很难准确回答的问题，通常最近的实验数据或许比较可靠。如果读者愿意知道更多、更早期的实验结果，可以利用本书的参考文献进一步检索。

本书内，全部多原子分子内的键能数据，是按照自由基中心原子种类组织排列的。它们被区分为C—X, O—X, N—X, S—X, Si—X, Ge—X, Sn—X, Pb—X, P—X和Se—X键能。

无机物、元素有机化合物、无机生物化合物、簇合物、氢键合物、van der Waals键合物以及金属表面键合物的键能数据，内容丰富多彩。对于这些化合物，我们已搜集到了101种元素、1万多个键、2万多个测量数据。我们计划在另外一本书内，按照元素周期表，系统、全面、分门别类地介绍它们，为将来的电子网络检索，走出第一步。

3.2　能 量 单 位

在国际单位制（SI）内，能量单位是焦耳（J），不是卡（cal）。原则上，我们有三种能量表示的方法：① 仅用 J；② 仅用 cal；③ 二元单位，既用 J，又用 cal。我们认

为，对于键能（或分子能量）的数据库来说，二元单位表示比较好。为什么呢？

我们至少有三个非常现实的理由。首先，过去和现在，报道实验键能的大部分文献都使用 kcal/mol。国际科学组织提倡使用国际单位制，宣传使用国际单位制的好处。但是，各国科学家仍然使用非国际单位发表他们的实验结果。其次，常见化学键能的范围，从 40（如 RO—OR）到 110（如 H—C_6H_5, H—C_2H_3）kcal/mol。大家知道，在日常生活里，我们比较容易记住小一点的数字。在科学技术领域，也是这样。例如，我们比较容易记住甲烷 C—H 键能是 105.0 kcal/mol，但很难记住对等的 439.3 kJ/mol。第三，二元单位最容易被绝大多数人接受。

直到今天，海内外不少科学家仍然在使用 eV （电子伏特）、cm^{-1}（波数）或 nm（波长）等能量单位发表他们的文章。这时，我们需要对它们进行转换：

1 eV = 23.060 kcal/mol = 96.483 kJ/mol

1 cm^{-1} = 2.85914×10^{-3} kcal/mol = 1.196264×10^{-2} kJ/mol

在物理学上，波长（λ）=1/波数（ω）因此，可见光的红区端 760 nm 对应于 37.62 kcal/mol （157.4 kJ/mol），它的紫区端 380 nm 对应于 75.24 kcal/mol（314.81 kJ/mol）。这就是为什么不少化合物能被可见光分解，许多化学试剂应当储藏在暗处。

书末，附有 SI 能量单位 kJ 和常见能量单位 kcal，K（Kelvin 温度），cm^{-1}，eV，au（哈特里）之间的转换表。

3.3 建立化学键能数据库的基本方法

在百货商店和超级市场里，为什么我们能采购到满意的东西？一是因为货物与食品相当丰富多样，二是货物与食品都被放置在合理的货架或位置上。同样的道理，我们收集、评价和选择了几万个数据，它们还应当根据某些原则，被组织和归类，被“安放”在不同的“货架”上，方便读者快速“采购”。

在本书内，化学键能数据是根据不同类别管理的。有相似结构环境的化学键，被“安放”到同一个“货架”——表格内。本书有 63 个表格。所有被表列的键能数据，按照下面七条规则系统地排列和“安放”：

（1）化学键类别，如像 C—H, C—C, C—O, C—N, C—S, C—F, C—Cl, C—Br, C—I 键等等。

（2）该化学键的α位置有没有杂原子和功能团，如像 O，CO，C（O）O，N，CN，NO，NO_2，NN，S，SS，SO，SO_2 等等。杂原子和功能团强烈地影响α位置该化学键能的大小。众所周知，许多有机化学书籍，就是按照杂原子和功能团来组织内容的。因此，我们查阅键能数据之前，必须事先知道该化学键的α位置有没有杂原子和功能团，如果有，是什么杂原子和功能团。例如：

- $C_6H_5CH_2$—**H** 内的 C—H 键能，被安放在本书的表 4.4，因为这是一个芳烃分子内的一级 C—H 键能。这里的黑体字，强调了该离解的原子或原子团，一个 H 原子从 CH_3 原子团上离解。
- $PhCH_2COCH_3$ 内的 C—H 键能，被安放在本书的表 4.6.1。注意，在该 C—H 键的α位置，有一个 CO 原子团。

- $PhCOCH_2NMe_2$ 内的 C—H 键能，被安放在本书的表 4.6.3。注意，在该 C—H 键的α位置，既有一个 CO 原子团，又有一个 N 原子。
- $PhCOCH_2SO_2Ph$ 内的 C—H 键能，被安放在本书的表 4.6.4。注意，在该 C—H 键的α位置，既有一个 CO 原子团，又有一个 SO_2 原子团。

（3）键级（bond order；triple, double or single）以及键度（bond degree; primary, secondary or tertiary）。含三键的化合物的键能、一级键能，首先安排。

（4）饱和化合物与不饱和化合物。饱和化合物内的键能，首先安排。

（5）分子大小。小分子内的键能，首先安排。

（6）分子形状（链状或环状）。链状分子内的键能，首先安排。

（7）是否含有取代基。没有取代基的母体分子内的键能，首先安排。例如，取代甲苯内的 C—**H** 键能，安排在母体分子 $C_6H_5CH_2$—**H** 键能的后面。

3.4 如何在本书的键能数据库中查找数据？

本书内，4300 多个化学键的数据都被安排进入 63 个不同的表格。要交待的是：①数据库里的名词、术语和化合物名称，没有对译成中文。我们认为，这并不妨碍读者访问查询。②数据库里的符号、缩写和略语，已经在本书开卷时，提供了说明。我们怎样才能检索出需要的键能数据？这里举一个例子，检索甲烷内的 C—H 键能（表 3.1）。

表 3.1 甲烷的 C—H 键能

断裂键 (**黑体** = 离解原子) Δ_fH°(R)，kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methane CH_3—**H** Δ_fH°(R) – 35 06±0.1 (146 69±0.4)	(1) **105.0±0.1** (2) 105.3±0.7 (3) 104.8±0.2 (4) 105.3±0.6 (5) 104.99±0.03	**439.3 ±0.4** 440.6±2.9 438.5±0.8 440.6±2.5 439.28±0.13	(1) VLPP (2) PIMS detect. (3) Spectrometric detection (4) Resonance fluorescence detection (5) AE, revised	(1) 1987DOB/BEN (2) 1988RUS/SEE(b) (3) 1990SEE/RUS (4) 1991NIC/DLJ (5) 1999RUS/LIT

这个表格的第一列指出了被断裂的化学键。表中的黑体字，强调了该离解的原子或原子团，一个 **H** 原子从甲烷分子内离解。化学键离解后，形成的自由基 R 的生成热，也被显示在小框里面。本书的第三篇，收集了许多多原子自由基的生成热数据。它是目前最完整的自由基的生成热数据库。

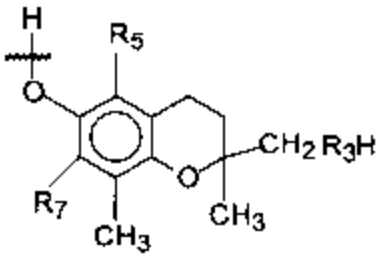
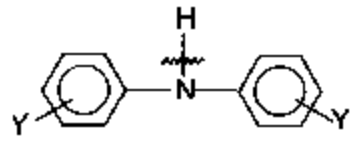
这个表格的第二列指出了该化学键能的实验值。编号（1），（2），（3），（4）和（5）代表 5 个不同的数据来源或参考文献。我们使用了二元单位（kcal 和 kJ）。为了方便大部分读者，我们提供了一个推荐值，它用黑体字加以强调。我们最多介绍 5 个该键能的实验值。这样考虑可以满足大多数用户。如果希望知道更多实验值，你可以借助于本书提供的参考文献，进一步检索。

表格的第三列指出了为了得到这些键能数据，采用了什么方法。

表格的第四列列出了相应的参考文献。

让我们再看以下三个例子（表 3.2）。

表 3.2　键能数据库示例

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methoxybenzene or anisole	(1) 64.8	271.1	(1) VLPP	(1) 1989SUR/KAF
	(2) 65.2	272.8	(2) Tubular flow reactor	(2) 1993ARE/LOU
CH_3—OC_6H_5	(3) 65.3	273.2	(3) VLPP	(3) 2001PRA/HEE
	(4) **64.2±1.7**	**268.6±7.1**	(4) Derived from $\Delta_f H^\circ$ in ref	(4) 1986PED/NAY
α-tocopherol				
				
	(1) 78.9	330.1	(1) EPR	(1) 1992JAC/HOS
	(2) 78.9	330.1	(2) EPR	(2) 1994LUC/PED
	(3) 80.9±1, in sol.	338.5±4.2	(3) AOP	(3) 1996BOR/LIU
	(4) **79.3**, in sol.	**331.8**	(4) PAC	(4) 1996WAY/LUS
R = $CH_2CH_2CH(CH_3)$ CH_2	(4) **77.3**, in gas	**323.4**		
$R_5 = R_7 = CH_3$	(5) 78.23±0.25	327.31±1.05	(5) EPR	(5) 2003VAL/BRI
(vitamin E)				
δ-tocopherol	(4) 82.2, in sol.	343.9		
$R_5 = R_7 = H$	(4) 80.2, in gas	335.6		
	(6) 81.9	342.8	(6) Correlation	(6) 2000DEN/DEN
β-tocopherol $R_5 = CH_3$, $R_7 = H$	(6) 80.2	335.6		
γ-tocopherol $R_5 = H$, $R_7 = CH_3$	(6) 80.1	335.1		
diphenylamine, substituted				
				
Y = p-Br	(1) 88.1	368.6	(1) AOP	(1) 1993BOR/ZHA
	(2) 87.0	364.2	(2) Correlation	(2) 2000DEN/DEN
p-MeO	(1) 84.2	352.3		
	(2) 83.3	348.6		
	(4) 81.8	342.2		
p-Me	(2) 85.4	357.5		
	(3) 86.3, in sol.	361.1	(3) PAC	(3) 1997MAC/WAY
	(3) **86.2**, in gas	**360.7**		
	(4) 83.3	348.5	(4) EPR	(4) 2002PRA/DIL
p-tBu	(2) 85.8	358.8		
p-$N(CH_3)_2$	(4) 79.5	332.6		

（1）它介绍了 methoxybenzene （anisole）内 C—O 键能的实验值。我们给出了相互独立的 4 个不同结果。推荐值用黑体字强调。这里导出值（derived）是根据方程（1.2）推导出来的。自由基的生成热数据取自本书的第三篇——自由基的生成热数据库，分子生成热数据取自所列出的参考文献。如果巧妙地利用这一自由基的生成热数据库，你可以导出极其大量的化学键能的数据。

（2）它介绍了 4 种不同构形的 tocopherols （vitamin E）内最弱的 H—O 键能的实验值。这里也强调了气相和液相实验条件下得到的不同结果，溶剂效应是存在的。

（3）它介绍了取代 diphenylamine 内 H—N 键能的实验值。这些结果表明了远程取代基 Y 对键能的影响。

作为一个优秀的化学数据库，既应当有化合物的英文名称，又应当有化合物的中文译名，还应当有化合物的 CAS 登记编号。在本书的数据库里，我们只有化合物的英文名称。主要原因之一是，不少化合物的英文名称还没有标准的中文译名。为此，我们征求了许多专家学者的意见，大家普遍认为暂不译成中文名，利多于弊，并不妨碍当前科研、教学与学术交流。由此带来的不理想或弊处，待日后逐步解决。

现在，你可以利用本书目录，检索化学键能数据库了。

第二篇　多原子分子中化学键能的数据库

第 4 章　C—H 键能

4.1　链状饱和碳氢化合物

表 4.1　链状饱和碳氢化合物内的 C—H BDEs

断裂键 （黑体 – 离解原子） $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs （黑体　推荐值； 括号内数字 = 文献编号）		方法	文献
	kcal/mol	kJ/mol		
methane	(1) **105.0±0.1**	**439.3 ±0.4**	(1) VLPP	(1) 1987DOB/BEN
CH_3 **H**	(2) 105.3±0.7	440.6±2.9	(2) PIMS detect.	(2) 1988RUS/SEE(b)
$\Delta_f H^\circ$（R）= 35.06±0.1	(3) 104.8±0.2	438.5±0.8	(3) Spectrometric detection	(3) 1990SEE/RUS
（146.69±0.4）	(4) 105.3±0.6	440.6±2.5	(4) Resonance fluorescence detect.	(4) 1991NIC/DIJ
	(5) 104.99±0.03	439.28±0.13	(5) AE, revised	(5) 1999RUS/LIT
ethane	(1) 100.5±0.5	420.5±2.1	(1) Kinetics	(1) 1984PAC/WIN
CH_3CH_2–**H**	(2) 100.5±0.5	420.5±2.1	(2) Resonance fluorescence detect.	(2) 1986BRO/LIG
$\Delta_f H^\circ$(R) = 28.4±0 3				
(118.8±1.3)	(3) 100.8±0.7	421.7±2.9	(3) PIMS detect	(3) 1988RUS/SEE(b)
	(4) 101.0±0.4	422.6±1.7	(4) PIMS detect.	(4) 1992SEA/PIL
	(5) **100.5±0.3**	**420.5±1.3**	(5) VLPP	(5) 1997DOB/BEN
propane	(1) 99.9±1.0	418 0±4 2	(1) Radical buffer	(1) 1982CAS/GRI
$CH_3CH_2CH_2$–**H**	(2) 99.8±2	417.6±8.4	(2) AE	(2) 1992HOL
$\Delta_f H^\circ$(R) = 23.8±0.5	(3) **100.9±0.5**	**422.2±2.1**	(3) SPST	(3) 1996TSA
(100±2)	(4) 101.2±0.5	423.4±2.1	(4) PIMS detect.	(4) 1997SEE/SLA
propane	(1) **98.1±0.7**	**410.5±2.9**	(1) PIMS detect.	(1) 1988RUS/SEE(b)
$CH_3CH_2CH_3$	(2) 98.9±0.6	413.8±2 5	(2) PIMS detect.	(2) 1990SEE/RUS
$\Delta_f H^\circ$(R) = 21.0±0 7	(3) 98.6±0.4	412.5±1 7	(3) PIMS detect.	(3) 1992SEA/PIL
(88±3)	(4) 97.8±0.5	409.2±2.1	(4) PIMS detect.	(4) 1997SEE/SLA
	(5) 97.4±1.0	407.5±4.2	(5) SPST	(5) 1999TSA
butane	(1) 101±2	422.6±8.4	(1) Electron impact	(1) 1958COT
$CH_3CH_2CH_2CH_2$–**H**	(2) 100.2	419.2	(2) AE	(2) 1988HOL/LOS
$\Delta_f H^\circ$(R) = 18.6±0.5	(3) **100.7**	**421.3**	(3) SPST	(3) 1990WAL/TSA
(77.8±2.1)	(4) 101.7±0.5	425.5±2.1	(4) PIMS detect.	(4) 1997SEE/SLA
butane	(1) 99.1±0.4	414.6±1.7	(1) PIMS detect.	(1) 1990SEE/RUS
$CH_3CH_2CH_2CH_3$	(2) **98.3±0.5**	**411.1±2.2**	(2) Resonance fluorescence detect.	(2) 1992SEA/PIL
$\Delta_f H^\circ$(R) = 16.2±0.5				
(67.8±2.1)	(3) 98.6±0.5	412.5±2.1	(3) Review	(3) 1996TSA
	(4) 98.3±0.5	411.3±2.1	(4) PIMS	(4) 1997SEE/SLA
	(5) 97.4±1.0	407.5±4.2	(5) SPST	(5) 1999TSA

续表

断裂键 (黑体　离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值， 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
isobutane $(CH_3)_2CHCH_2$-**H** $\Delta_f H^\circ$(R) = 16.7±1.0 (70±4)	(1) **100.2±1** (2) 99.3±2 (3) 101.6±0.5 (4) 100.9±1	**419.2±4.2** 415.5±8.4 425.1±2.1 422.0±4.2	(1) Exp analysis (2) AE (3) PIMS detect. (4) SPST	(1) 1976BEN (2) 1992HOL (3) 1997SEE/SLA (4) 1999TSA
isobutane $(CH_3)_3C$-**H** $\Delta_f H^\circ$(R) = 11.5±0.7 (48±3)	(1) 95.6±0.7 (2) 95.0 (3) 95.5±0.7 (4) 95.5±0.3 (5) **95.7±0.7**	400.0±2.9 397.5 399.6±2.9 399.6±1.3 **400.4±2.9**	(1) SPST (2) VLPP (3) Resonance fluorescence detect. (4) Resonance fluorescence detect. (5) Recommend.	(1) 1985TSA (2) 1987BEN/KON (3) 1991SEA/PIL (4) 1992SEA/PIL (5) 1996TSA
neopentane $(CH_3)_3CCH_2$-**H** $\Delta_f H^\circ$(R) = 8.7±2 (36.4±8.2)	(1) 99.4±1 (2) **100.3±1** (3) 99.4±1 (4) 101±2 (5) 101.1	415.9±4.2 **419.7±4.2** 415.9±4.2 422.6±8.4 423	(1) Polanyi plot (2) Kinetics (3) SPST (4) Review (5) Laser photolysis	(1) 1966KER (2) 1969LAR/HAR (3) 1969TSA (4) 1982MCM/GOL (5) 2001IMR/DOB
2-methylbutane (CH_3CH_2) C**H**$(CH_3)_2$ $\Delta_f H^\circ$(R) = 7 (29)	(1) 91.6±2 (2) 96.5±1 (3) 92.6 (4) **95.8**	383.3±8.4 403.8±4.2 387.4 **400.8**	(1) SPST (2) SPST (3) PES (4) SPST	(1) 1969TSA (2) 1981TSA (3) 1986KRU/BEA (4) 1999TSA
pentane nC_5H_{11}–**H** $\Delta_f H^\circ$(R) = 13 (54.4)	100.2	419.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pentane $CH_3CH_2(CH_2)_2CH_3$ $\Delta_f H^\circ$(R) = 12 (50.2)	99.2	415.1	Derived from $\Delta_f H^\circ$ in ref	1986PED/NAY
2-methylpentane (C_3H_7) C**H**$(CH_3)_2$ $\Delta_f H^\circ$(R) = 0.8±2 (3.3±8.2)	94.7±2	396.2±8.4	Pyrolysis	1983SER/GOR
2,3-dimethylbutane $CH_3CH(CH_3)$ C**H**$(CH_3)_2$ $\Delta_f H^\circ$(R) = 0.7±2.4 (3.1±10)	95.4±3.1	399.2±13.0	Equilibrium study	2000KIR/KOR
hexane nC_6H_{13}-**H** $\Delta_f H^\circ$(R) – 8 (33.5)	99.0	414.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
hexane $CH_3CH_2(CH_2)_3CH_3$ $\Delta_f H^\circ$(R) = 7 (29.3)	98.0	410.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
heptane $CH_3CH_2(CH_2)_4CH_3$ $\Delta_f H^\circ$(R) = 2 (8.2)	98.0	410.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

4.2 链状非饱和碳氢化合物

表 4.2 链状非饱和碳氢化合物内的 C—H BDEs

断裂键 (黑体 = 离解原 *f*) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Acetylene HC≡C–**H** $\Delta_f H^\circ$(R) = 135.6±0.2 (567.4±0.8)	(1) 134.9±1.2 (2) 132.9±0.7 (3) 133.1±0.7 (3) 132.8±0.7 (4) **133.32±0.07** (5) 131.3±0.7	564.4±5.0 556.1±2.9 556.9±2.9 556.6±2.9 **557.81±0.30** 549.4±2.9	(1) AE (2) Photoelectron detachment (3) GPA (3) Recommended (4) Photolysis (5) Electr. affinity	(1) 1979BER (2) 1990ERV/GRO (3) 1994BER/ELL (4) 1994MOR/ASH (5) 2002KIR/TSC
acetylene, substituted X–C≡C–**H** X = CH_3 $\Delta_f H^\circ$(R) = 121±3.0 (506.3±12.6)	(1) 130.2±3, at 0 K	544.8±12.6	(1) PES	(1) 1995ROB/POL
BF_3	(2) 130.8	547.3	(2) MS	(2) 1999HIL/POU
Ph	(3) 133±5	556.5±21	(3) GPA	(3) 2003REE/HAR
C(O) OCH_3	(3) 132±5	552.2±21		
CC(O) $N(CH_3)_2$	(3) 132±5	552.3±21		
diacetylene HC≡C–C≡C–**H**	128.8±2.9, at 0 K	539±12	CID	2000SHI/ERV
Propyne CH≡C–CH_2–**H** $\Delta_f H^\circ$(R) = 81.0±1.0 (339±4)	(1) 89.2±2.4 (2) 87.2±2 (3) 90.3±3 (4) **88.9±1.0** (5) 91.8±1.0	373.2±10.0 364.8±8.4 377.8±12.6 **372.0±4.2** 384.1±4.2	(1) VLPP (2) AE (3) GPA (4) Recommended (5) SPST	(1) 1979KIN/NGU (2) 1988HOL/LOS (3) 1995ROB/POL (4) 1996TSA (5) 1999TSA
2-butyne CH_3C≡C–CH_2–**H** $\Delta_f H^\circ$(R) = 70.2±2 (293.7±8.4)	(1) 90.7 (2) **87.4±2** (3) 84.8	379.5 **365.7±8.4** 354.8	(1) SPST (2) VLPP (3) Correlation	(1) 1978TSA (2) 1982NGU/KIN (3) 2000DEN/DEN
1-butyne HC≡C–CH_2–CH_3 $\Delta_f H^\circ$(R) = 70.5±2.2 (295.0±9.2)	(1) **85.0** (2) 87.3 (3) 83.1±2.2 (4) 82.9	**355.6** 365.3 347.7±9.2 346.8	(1) VLPP (2) SPST (3) Review (4) Correlation	(1) 1981NGU/KIN (2) 1981TSA (3) 1982MCM/GOL (4) 2000DEN/DEN
1-penten-3-yne CH_2=CH–C≡C–CH_2–**H** $\Delta_f H^\circ$(R) = 84.0 (351.5)	86.8	363.3	VLPP	1992STA/KIN

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
2-pentyne $CH_3C{=}C{-}C\mathbf{H}_2{-}CH_3$ $\Delta_f H^\circ$(R) = 65.2±2.2 (272.8±9.2)	87.3±2.3	365.3±9.6	VLPP	1981KIN/NGU
1-pentyne $HC{\equiv}C{-}C\mathbf{H}_2CH_2CH_3$ $\Delta_f H^\circ$(R) = 66.2±2.0 (277.0±8.4)	83.6±2	349.8±8.4	AE	1976LOS/TRA
3-methyl-1-butyne $HC{\equiv}C{-}C\mathbf{H}(CH_3)_2$ $\Delta_f H^\circ$(R) = 61.5±2.2 (257.3±9.2)	(1) **82.5±2** (2) 81.0±2.3	**345.2±8.4** 338.9±9.6	(1) AE (2) VLPP	(1) 1976LOS/TRA (2) 1977KIN
4-methyl-2-pentyne $CH_3C{=}C{-}C\mathbf{H}(CH_3)_2$ $\Delta_f H^\circ$(R) = 53.0±2.2 (221.8±9.2)	82.3±2 7	344.3+11.3	VLPP	1981KIN/NGU
5-decyne $CH_3(CH_2)_3C{\equiv}CC\mathbf{H}_2(CH_2)_2CH_3$	83.2	348.0	Correlation	2001TUM/DEN
triacetylene $HCCCCCC{-}\mathbf{H}$	(1) 126.8±1.6 (2) **~129.8±3**	530.5±6.7 **~543±13**	(1) GPA (2) Re-evaluated	(1) 1994NAT/KOC (2) 2001ERV
ethylene $H_2C{=}CH{-}\mathbf{H}$ $\Delta_f H^\circ$(R) = 71.6±0.8 (299.6±3.3)	(1) 110.1±2 (2) 110.2±2 (3) **111.2±0.8** (4) 110.2±0.4 (5) 110.7±0.6	460.7±8.4 461.1±8.4 **465.3±3.3** 461.1±1.3 463.0±2.7	(1) Kinetics (2) Review (3) Recommended (4) FT-IR-GC detection (5) GPA, revised	(1) 1981STE/ROW (2) 1982MCM/GOL (3) 1994BER/ELL (4) 1996KAI/WAL (5) 2002ERV/DET
allene $CH_2{=}C{=}CH{-}\mathbf{H}$ $\Delta_f H^\circ$(R) = 81.0±1 (338.9±4)	(1) 92.4±1.2 (2) **88.7±3**	386.6±5.0 **371.1±12.6**	(1) Kinetics (2) GPA	(1) 1971WAL (2) 1995ROB/POL
propene $CH_3CH{=}CH{-}\mathbf{H}$ $\Delta_f H^\circ$(R) = 63.8±1.5 (266.9±6)	(1) 109±2.4 (2) **111.1**	456.1±10.0 **464.8**	SPST	(1) 1988CUI/HE (2) 1999TSA
propene $CH_2{=}CH{-}CH_2{-}\mathbf{H}$ $\Delta_f H^\circ$(R) = 40.8±0.7 (171±3)	(1) 87.2±0.5 (2) 88.8±0.4 (3) **88.2±0.7** (4) 88.8±0.4 (5) 87 0±1.1	364.8±2.1 371.5±1.7 **369±3** 371.5±1.7 364.0±4.6	(1) Pulse shock tube (2) GPA (3) Recommended (4) PES (5) PIMS detect.	(1) 1991ROT/BAU (2) 1996ELL/DAV (3) 1996TSA (4) 1996WEN/POL (5) 1997SEE/SLA
(Z) -2-butene (Z) $-CH_3CH{=}CH{-}CH_2{-}\mathbf{H}$ $\Delta_f H^\circ$(R) = 34.9±2 (146±8)	(1) 89.7 (2) 85.0	375.3 355.8	(1) SPST (2) Correlation	(1) 1999TSA (2) 2000DEN/DEN

续表

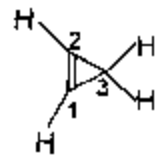
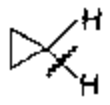
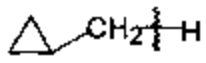
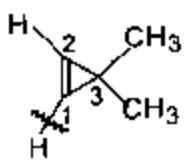
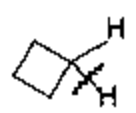
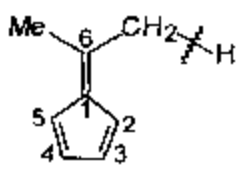
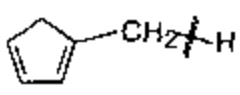
断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
(E) -2-butene (E) -CH_3CH=CH–CH_2–**H**	85.3	356.8	Correlation	2000DEN/DEN
1-butene CH_2=CH–CH_2–CH_2 **H** $\Delta_f H^\circ$(R) = 46.0 (192.5)	98.1	410.5	PES	1984SCH/HOU
1-butene CH_2–CH–CH_2 CH_3 $\Delta_f H^\circ$(R) = 31.8±1.5 (133.1±6.3)	(1) 82.3 (2) 81.5±1.5 (3) 82.6±1.3 (4) **83.8** (5) 83.5	344.3 341.0±6.3 345.6±5.4 **350.6** 349.2	(1) SPST (2) Pyrolysis (3) Review (4) Proton affinity (5) Correlation	(1) 1969TSA (2) 1970TRE (3) 1982MCM/GOL (4) 1987LIA/AUS (5) 2001TUM/DEN
isobutene CH_2=C(CH_3)–CH_2–**H** $\Delta_f H^\circ$(R) = 30.6±0.6 (128.0 ±2.5)	(1) 86 2±1 (2) 85±2 (3) **86.7±0.6** (4) 88.3±2.3 (5) 89.1	360.7±4.2 355.6±8.4 **362.8±2.5** 369.4±9.6 372.8	(1) Pyrolysis (2) MS (3) Shock tube (4) PES (5) SPST	(1) 1977TRE/WRI (2) 1977LIA/AUS (3) 1991ROT/BAU (4) 1996WEN/POL (5) 1999TSA
1,3-pentadiene CH_2=CHCH=$CHCH_2$–**H** $\Delta_f H^\circ$(R) = 49±3 (205±12 6)	(1) 79.8±1.0 (2) 79.7±1.0 (3) **83±3**	333.9±4.2 333.5±4.2 **347.3±12.6**	(1) Iodination (2) Pyrolysis (3) Review	(1) 1973ONE/BEN (2) 1980TRE (3) 1982MCM/GOL
2,3-pentadiene CH_3CH=C=$CHCH_2$ -**H**	87.2	365.0	Correlation	2000DEN/DEN
1,4-pentadiene (CH_2=CH) $_2$CH–**H** $\Delta_f H^\circ$(R) = 49.7±1.0 (207.9±4.2)	(1) 79.5±1.7 (2) 76.4 (3) **76.6±1.0** (3) 76.6±1.0	332.6±7.1 319.7 **320.5±4.2** 320.5±4.2	(1) Isomerization (2) Pyrolysis (3) PAC (3) AE	(1) 1970EGG/JOL (2) 1982TRE (3) 1991CLA/CUL
1-pentene CH_2=CH–CH_2- CH_2CH_3 $\Delta_f H^\circ$(R) = 26.2±2 (109 6±8.4)	(1) 82.5±2 (2) 83.4	345.2±8.4 348.8	(1) AE (2) Correlation	(1) 1976LOS/TRA (2) 2000DEN/DEN
2-methyl-1-butene CH_2=C(CH_3) –CH_2CH_3	83 0	347.3	Correlation	2000DEN/DEN
3-methyl-1-butene CH_2- CH–CH(CH_3) $_2$ $\Delta_f H^\circ$(R) = 20.8±2 (87 0±8.4)	(1) **79.5±1.7** (2) 76.4 (3) 83.1 (4) 81.2	**332.6±7.1** 319 7 347.7 339.6	(1) Isomerization (2) Pyrolysis (3) Re-anal. of pyrolysis data (4) Correlation	(1) 1970EGG/JOL (2) 1982TRE (3) 1998BRO/BEC (4) 2000DEN/DEN
3-methyl-2-butene CH_3CH=C(CH_3) CH_2–**H**	84.2	352.4	Correlation	2000DEN/DEN
2-ethyl-1-propene CH_2=C(CH_3CH_2) –CH_2 **H** $\Delta_f H^\circ$(R) = 26.2±2.0 (109.6±8.4)	85.1±2	356.1±8.4	AE	1976LOS/TRA
(E) -2-pentene (E) -CH_3CH–CHC**H**$_2CH_3$	(1) 81.7±1.5 (2) 82.6	341.8±6.3 345.4	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2000DEN/DEN

续表

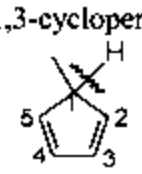
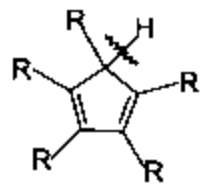
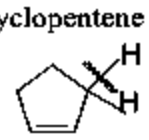
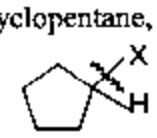
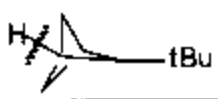
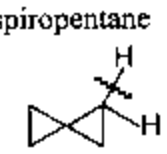
断裂键 (黑体　离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字　文献编号) kcal/mol	kJ/mol	方法	文献
(Z) -2-pentene (Z) -CH_3CH=$CHCH_2CH_3$	(1) 80.6±1.5 (2) 82.5	337.2 345.2	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2000DEN/DEN
1-hexene CH_2=$CHCH(CH_2)_2CH_3$	83.4	348.8	Correlation	2001TUM/DEN
3-methyl-1,4-pentadiene $(CH_2$=$CH)_2C(CH_3)$–**H** $\Delta_f H^\circ$(R) = 46.3 (202.0)	77	322.2	PAC	1999LAA/MUL
(Z) -4-methyl-2-pentene (Z) -$(CH_3)_2CHCH$=$CHCH_3$	79.8	333.9	Correlation	2001TUM/DEN
4-methyl-3-pentene $(CH_3)_2C$=$CHCH_2CH_3$	79.3	331.9	Correlation	2001TUM/DEN
2,3-dimethyl-2-butene $(CH_3)_2C$=$C(CH_3)$–CH_2–**H** $\Delta_f H^\circ$(R) = 9.5±1.5 (39.7±6.3)	(1) 78.0±1.0 (2) 84.7	326.4±4.2 354.3	(1) Iodination (2) Correlation	(1) 1973ROD/WU (2) 2001TUM/DEN
2,3-dimethy-1-butene CH_2=$C(CH_3)$–$CH(CH_3)_2$ $\Delta_f H^\circ$(R) = 9±1.5 (37.7±6.3)	(1) 76.3±1.0 (2) 84.3	319.2 352.8	(1) Iodination (2) Correlation	(1) 1973ROD/WU (2) 2001TUM/DEN
(Z) -2,5-dimethyl-3-hexene (Z) -$(CH_3)_2CHCH$=$CHCH(CH_3)_2$	80.3	336.1	Correlation	2001TUM/DEN
1,3-octediene CH_2=$CHCH$=$CHCH_2(CH_2)_2CH_3$	79.3	332.0	Correlation	2001TUM/DEN
1-octene CH_2=$CHCH_2(CH_2)_4CH_3$	83.4	348.9	Correlation	2000DEN/DEN
(E) -2-octene (E) -CH_3CH=$CHCH_2(CH_2)_3CH_3$	81.9	342.7	Correlation	2000DEN/DEN
1,8-nonediene CH_2=$CHCH_2(CH_2)_4CH$=CH_2	83.6	349.8	Correlation	2001TUM/DEN
Z,Z-2,8-decediene CH_3CH=$CH(CH_2)_4CH$=$CHCH_3$	81.6	341.6	Correlation	2001TUM/DEN
1-hexadecene CH_2=$CHCH_2(CH_2)_{13}CH_3$	83.4	348.8	Correlation	2001TUM/DEN
allyl triphenyl phosphonium bromide $Ph_3P^+CH_2CH$=CH_2 Br^-	85.9	359.4	AOP	1996ZHA/FRY
3-phenyl-allyl triphenyl phosphonium bromide $Ph_3P^+CH_2CH$=$CHPh$ Br^-	81.0	338.9	AOP	1996ZHA/FRY

4.3 环状碳氢化合物

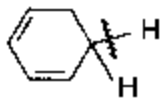
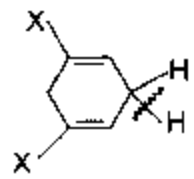
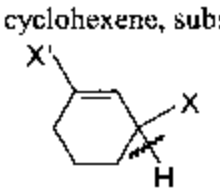
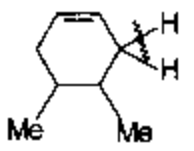
表 4.3 环状碳氢化合物内的 C—H BDEs

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
cyclopropene  C–H at *1 site* $\Delta_f H^\circ$(R) = 105.1±4.1 (439.7±17.2)	103±3	431.0±12.6	GPA	2002KAS/BRO
C–H at 3	90.4±4	378.3±12.6	ICR	1980DEF/MCI
cyclopropane  $\Delta_f H^\circ$(R) = 66 9±0 3 (279.9±1.3)	(1) 101±3 (2) 100.2±0.4 (3) **106.3±0.25** (4) 105.9±2.7 (5) 102.5	422 6±12.6 419.3±1.7 **444.8±1.0** 443.1±11.3 429.0	(1) Polanyi plot (2) Kinetics (3) VLPP (4) ICR (5) Correlation	(1) 1966KER (2) 1978APP/KLU (3) 1979BAG/BEN (4) 1980DEF/MCI (5) 2001TUM/DEN
methylcyclopropane  $\Delta_f H^\circ$(R) = 51.1±1.6 (213.8±6.7)	97.4±1.6	407.5±6.7	Iodination	1971MCM/GOL
3,3-dimethylcyclopropene 	106.7±3.7	446.4±15.5	GPA	2003FAT/MCC
cyclobutane  $\Delta_f H^\circ$(R) = 51.4±1.0 (215.1±4.2)	(1) 95±3 (2) 96.5 (3) **96.8±1.0** (4) 97.8±0.3 (5) 100.0	397.5±12.6 403.8 **405.0±4.2** 409.2±1.3 418.5	(1) Polanyi plot (2) Polanyi plot (3) Iodination (4) Kinetics (5) Correlation	(1) 1966KER (2) 1971FER/WHI (3) 1972MCM/GOL (4) 1978APP/KLU (5) 2001TUM/DEN
6,6-dimethylfulvene 	84.5	353.5	AOP	1989BOR/HAR
1,3-cyclopentadienes, substituted 	86.5±2	361.9±8.4	VLPP	1981STE

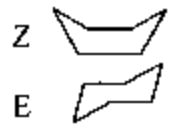
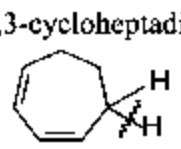
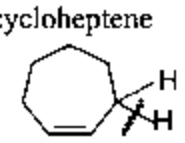
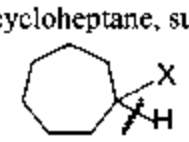
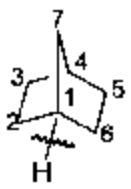
续表

断裂键 (**黑体** 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1,3-cyclopentadiene, substituted  at 1 site H $\Delta_f H^\circ$(R) = 63.9±2 (267.4±8.4)	(1) 82.9±2.2 (2) 81.2 (3) **83.9±0.5** (4) 81.5±2.7 (5) 82.5±1	346.9±9.2 339.7 **351.0±2.1** 341.0±11.3 345.2±4.2	(1) ICR (2) AOP (3) Electrochem. (4) ICR (5) Reflected shock tube	(1) 1980DEF/MCI (2) 1988BOR/CHE (3) 1991PAR/HAN (4) 1997ROM/JAN (5) 2001ROY/BRA
at 1,4 site Ph	(6) 75	313.8	(6) AOP	(6) 1991BOR/CHE
1,3-cyclopentadienes, substituted  R = Me $\Delta_f H^\circ$(pentamethyl-cyclo-pentadienyl) = 16.1±1.0 (67.4±4.2)	(1) 77	322.2	(1) AOP	(1) 1989BOR/HAR
Ph	(1) **78** (2) 74.1	**326.4** 310.0	(2) Pyrolysis	(2) 1995ROT/HUN
cyclopentene  $\Delta_f H^\circ$(R) = 38.4±1.0 (160.7±4.2)	(1) 82.3±1 (2) 82±2 (3) 81.9	344.3±4.2 343.1±8.4 342.5	(1) Iodination (2) AE (3) Correlation	(1) 1970FUR/GOL(b) (2) 1976LOS/TRA (3) 2000DEN/DEN
cyclopentane, substituted  X = H $\Delta_f H^\circ$(R) = 25.3±1.0 (105.9±4.2)	(1) 94.9±1 (2) 95.0±2 (3) 96.0±0.2 (4) **95.6±1** (5) 97.6	397.1±4.2 397.5±8.4 401.7±0.8 **400.0±4.2** 408.5	(1) Iodination (2) AE (3) Kinetics (4) Radical buffer (5) Correlation	(1) 1970FUR/GOL (2) 1976LOS/TRA (3) 1978APP/KLU (4) 1982CAS/GRI (5) 2001TUM/DEN
Me	(5) 93.7	392.2		
Et	(5) 93.7	392.3		
Ph	(6) 81.9	342.7	(6) Correlation	(6) 1995TUM/DEN
3-tert-butylbicyclo(1.1.1) - pentane 	109.7±3.3	459.0±13.8	GPA	2002REE/KAS
spiropentane  $\Delta_f H^\circ$(R) = 91.0±1.0 (380.7±4.2)	98.8±1	413.4±4.2	Polanyi correlation	1971FER/WHI

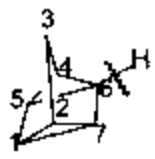
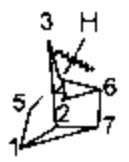
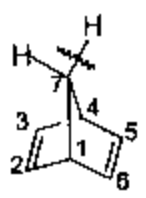
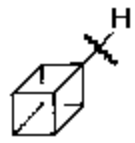
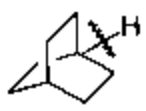
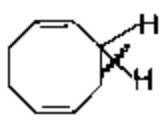
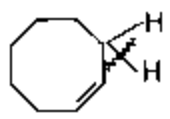
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1,3-cyclohexadiene  $\Delta_f H^\circ$(R) = 47.6 (199.2)	(1) 73±5 (2) 73.2 (3) **74.3** (4) 74.3 (5) 79.1	305.4 306.3 **310.9** 310.9 331.1	(1) Review (2) Kinetics (3) VLPP (4) PAC (5) Correlation	(1) 1982MCM/GOL (2) 1985DEA (3) 1991STE/BRO (4) 1997LAA/MUL (5) 2001TUM/DEN
1,4-cyclohexadiene, substituted  X = H $\Delta_f H^\circ$(R) = 48.2±1.2 (201.7±5.0)	(1) 70 (2) **76.0±1.2** (3) 73±2 (4) 77 (5) 75.0	292.9 **318.0±5.0** 305.4±8.4 322.2 313.7	(1) Pyrolysis (2) SPST (3) PAC (4) PAC (5) Correlation	(1) 1968JAM/SUA (2) 1986TSA (3) 1989GRI/WAY (4) 1999CIR/KOR (5) 2001TUM/DEN
Me	(5) 80.4	336.4		
cyclohexene, substituted  X = H, X′ = H $\Delta_f H^\circ$(R) = 28.6 (119.7)	(1) 81.9 (2) 87±3 (3) 81.6	342.7 364±13 341.4	(1) AOP (2) Mol. beam (3) Correlation	(1) 1988BOR/CHE (2) 1989ZHA/CON (3) 2000DEN/DEN
H Me	(4) 81.0	338.9	(4) Correlation	(4) 2001TUM/DEN
Me H	(4) 79.5	332.7		
cyclohexene, substituted 	78.0	326.2	Correlation	2001TUM/DEN
cyclohexane, substituted  X = H $\Delta_f H^\circ$(R) = 18±1.5 (75.3±6.3)	(1) 96.2 (2) **99.5** (3) 96.4±0.6 (4) 98 (5) 97.6	402.5 **416.3** 403.3±2.5 410.0 408.4	(1) Kinetics (2) SPST (3) EPR (4) PAC (5) Correlation	(1) 1978APP/KLU (2) 1981TSA (3) 1982CAS/GRI (4) 1999CIR/KOR (5) 2001TUM/DEN
Me	(5) 94.3	394.6		
Et	(5) 94.5	395.4		
$CH{=}CH_2$	(5) 81.7	341.8		
Ph	(6) 85.2	356.4	(6) Correlation	(6) 2000DEN/DEN

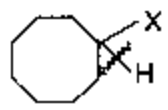
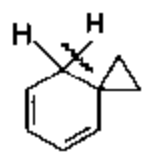
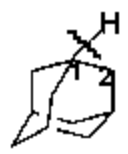
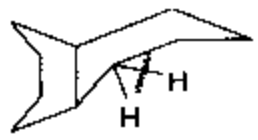
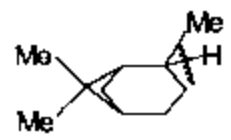
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
cyclohexane, substituted  				
(Z) -1,2-Me_2	93.9	392.9	Correlation	2001TUM/DEN
(E) -1,2-Me_2	97.4	407.5		
(Z) -1,3-Me_2	93.9	392.9		
(E) -1,3-Me_2	93.2	389.9		
(Z) -1,4-Me_2	93.7	392.0		
(E) -1,4-Me_2	94.8	396.6		
1,3,5-cycloheptatriene  $\Delta_f H^\circ$(R) – 68.2±3 (285.3±12.6)	(1) 82.9±7 (2) 73±1 (3) 73±2 (4) **76.6±3** (5) 73.2±2	346.9±29.3 305 4±4 2 305.4±8.4 **320.5±12.6** 306.3±8.4	(1) Electron impact (2) Pyrolysis (3) ICR (4) ICR (5) Review	(1) 1960HAR/HON (2) 1969VIN/DAU (3) 1979BAR/SCO (4) 1980DEF/MCI (5) 1982MCM/GOL
1,3-cycloheptadiene 	83.0	347.3	Correlation	2001TUM/DEN
cycloheptene 	82.9	346.9	Correlation	2001TUM/DEN
cycloheptane, substituted  X = H $\Delta_f H^\circ$(R) = 12.1±1 (50.6±4.2)	(1) 93±3 (2) **94.0** (3) 92.5±1 (4) 92.5±1 (5) 96.5	389.1±12.6 **393.3** 387.0±4.2 387.0±4.2 403.8	(1) Polanyi plot (2) Kinetics (3) Photobromin. (4) Review (5) Correlation	(1) 1966KER (2) 1970JON/WHI (3) 1971FER/WHI (4) 1982MCM/GOL (5) 2001TUM/DEN
Me	(5) 93.0	389.0		
Et	(5) 93.8	392.4		
norbornane  $\Delta_f H^\circ$(R) = 32.6±2.5 (136 4±10.5)	(1) **96.7±2.5** (2) 99.4	**404.6±10.5** 415.9	Iodination	(1) 1970ONE/BAG (2) 1971DAN/TIP

续表

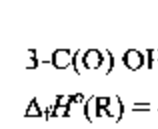
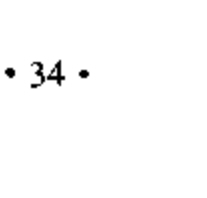
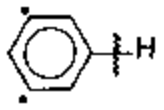
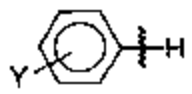
断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
quadricyclane  $\Delta_f H^\circ$(R) = 138.3±1.3 (578.6±5.4)	109.4±1.3	457.7±5.4	Ion flow tube	1996LEE/DEP
quadricyclane  $\Delta_f H^\circ$(R) = 140.4±1.3 (587.4±5.4)	111.5±1.3	466.5±5.4	Ion flow tube	1996LEE/DEP
norboradine  $\Delta_f H^\circ$(R) = 122.3±1.9 (511.7±7.9)	115.6±1.9	483.7±7.9	Ion flow tube	1996LEE/DEP
cubane  $\Delta_f H^\circ$(R) = 198.6±4 (830.9±16.7)	102±4	426.8±16.7	GPA	1997HAR/EMR
bicyclooctane  $\Delta_f H^\circ$(R) = 22.0 (92.0)	97.7	408.8	Kinetics	1971DAN/TIP
cyclooctadiene 	79.3	331.8	Correlation	2001TUM/DEN
cyclooctene 	85.4	357.2	Correlation	2001TUM/DEN

续表

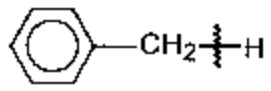
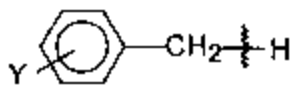
断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
cyclooctane, substituted  				
X = H	95.7	400.2	Correlation	2001TUM/DEN
Me	94.4	395.0		
Et	93.7	392.2		
spiro(2.5) -octa-4,6-diene  	70.7	295.6	Correlation	2001TUM/DEN
cyclononane cyclo-C_9H_{17}–**H**	96.3	402.9	Correlation	2001TUM/DEN
adamantane  				
$\Delta_f H^\circ$(R, at 1 site) = 12.3 (51.5)	(1) 97.0 (2) **96.2** (3) 98.5 (4) 93.0	405.8 **402.5** 412.0 389.0	(1) Kinetics (2) AP (3) Correlation (4) Derived	(1) 1971DAN/TIP (2) 1998AUB/HOL (3) 2001TUM/DEN (4) 2002MIR/LEB
$\Delta_f H^\circ$(R, at 2 site) = 14.8 (61.9)	(2) 100.2 (3) 98.5 (5) **98.4**	419.2 412.0 **411.7**	(5) PES	(5) 1986KRU/BEA
cyclodecane cyclo-$C_{10}H_{19}$–**H**	96.7	404.5	Correlation	2001TUM/DEN
cycloundecane cyclo-$C_{11}H_{21}$–**H**	96.7	404.7	Correlation	2001TUM/DEN
cyclododecane cyclo-$C_{12}H_{23}$–**H**	98 0	410.0	Correlation	2001TUM/DEN
(Z) decalin  	93.5	391.1	Correlation	2001TUM/DEN
(E) -decalin  	95.6	400.0	Correlation	2001TUM/DEN
(Z) -pinane  	90.2	377.4	Correlation	2001TUM/DEN

4.4 芳香碳氢化合物

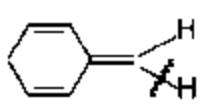
表 4.4 芳香碳氢化合物内的 C—H BDEs

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
benzene  $\Delta_f H°$(R) = 78.9±0.8 (330.1±3.3)	(1) 112.3±1 (2) 111.2±0.8 (3) 113.5±0.5 (4) 113.3±2 (5) **112.9±0.5**	469.9±4.2 465.3±3.3 474.9±2.1 474±8 **472.2±2.2**	(1) Iodination (2) GPA, Recommended (3) Ion flow tube (4) Recommend. (5) GPA, revised	(1) 1967ROD/GOL (2) 1994BER/ELL (3) 1995DAV/BIE (4) 1996TSA (5) 2002ERV/DET
C_6D_5–**D**	(6) 113.5±0.5	478.9±2.1	(6) GPA	(6) 2003REE/HAR
phenyl  C–H at site 2	79.9±3.1	334.3±13.0	CID	1994WEN/SQU
3	95.3±3.2	398.7±13.4		
4	110.6±3.4	462.8±14.2		
3,5-didehydrophenyl 	109.2±5.6	456.9±23.4	CID	2002LAR/NAS
benzene, substituted 				
Y = 2-C(O) O	113.9	476.6	Correlation	1998WEN/SQU
3-C(O) O^-	110.4	461.9		
4-C(O) O	112.3	469.9		
2-C(O) OH $\Delta_f H°$(R) = –7.9 (–33.1)	114.5	479.1		
3-C(O) OH $\Delta_f H°$(R) = –8.4 (–35.1)	114.0	477.0		
4-C(O) OH $\Delta_f H°$(R) = –8.6 (–36.0)	113.8	476.1		

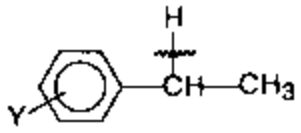
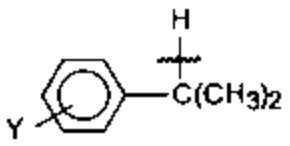
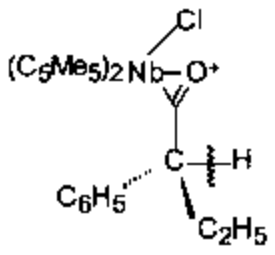
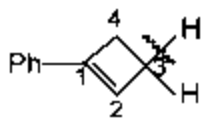
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^o$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
toluene  $\Delta_f H^o$(R) = 48.4±1.5 (202.5±6.3)	(1) 88.1±2.2 (2) 88.6 (3) **88.5±1.5** (4) 89.6±1.0 (5) 90.9±1.2, in sol (5) 89.7±1.2, in gas	368.6±9.2 370.7 **370.3±6.3** 375±4 380.5±5.1 375.5±5.0	(1) ICR (2) SPST (3) Recommend. (4) Recommend. (5) TR- PAC	(1) 1980DEF/MCI (2) 1990WAI/TSA (3) 1994BER/ELL (4) 1996TSA (5) 2004MUR/SAN
toluene, substituted 				
Y = 3-F	(1) 88.8±2.1 (3) 89.3	371.5±8.8 373.6	(1) PES (2) PES	(1) 1999KIM/WEN (2) 1986HAY/KRU
4-F	(1) 87.6±2.1 (3) 89.7	366.5±8.8 375.1	(3) Correlation	(3) 2000DEN/DEN
2-Cl	(1) 89.0±3.1	372.4±13.0	(4) Correlation	(4) 2002KRO/TUM
3-Cl	(1) 89.8±2.1 (3) 89.1	375.7±8.8 373.0	(5) AOP (6) AOP	(5) 1995BOR/ZHA(c) (6) 1993ZHA/BOR
4-Cl	(1) 87.5±2.1 (3) 88.7	366.1±8.8 371.3	(7) CID	(7) 2000HAM/WEN
2-Br	(1) 90.2±3.1	377.4±13.0	(8) CID	(8) 2001HAM/WEN
3-Br	(1) 90.1±3.1 (3) 89.7	377.0±13.0 375.4		
4-Br	(1) 88.5±3.1 (4) 90.8	370.3±13.0 380.1		
2-CH_3	(2) 87.3 (3) 89.6	365.3 375.0		
3-CH_3	(2) 87.8 (3) 88.8	367.4 371.4		
4-CH_3	(2) 87.7 (3) 88.4	366.9 369.7		
4-Et	(4) 87.0	363.9		
2-Pr	(4) 87.6	366.6		
3-Pr	(4) 86.8	363.2		

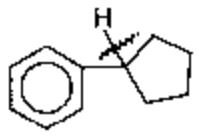
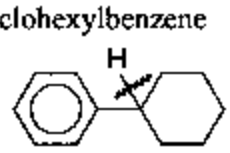
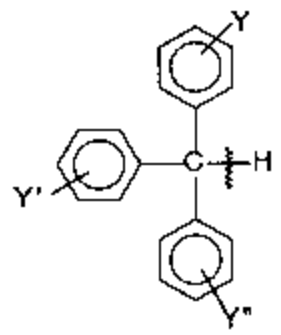
续表

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 文献编号)		方法	文献
	kcal/mol	kJ/mol		
4-Pr	(4) 87.0	363.9		
4-tBu	(3) 89.4	374.1		
3-CN	(4) 88.7	371.0		
4-CN	(4) 88.0	368.0		
3-NO_2	(4) 89.6	375.0		
4-NO_2	(3) 89.2 (5) 86.5	373.4 361.9		
4-PhO	(3) 89.7	375.4		
4-$PhSO_2$	(6) 88	368.2		
4-CH_2OCH_3	(4) 85.4	357.5		
3-MeO	(4) 90.5	378.8		
4-MeO	(4) 86.6	362.5		
3-EtOC(O)	(4) 89.1	372.7		
4-EtOC(O)	(4) 89 4	374.1		
2,4-Cl_2	(4) 88.6	370.9		
3,4-Cl_2	(4) 88.3	369.6		
2,3-Me_2	(4) 89.5	374.3		
2,4-Me_2	(3) 89.1	373.0		
3,5-Me_2	(3) 89.5	374.3		
2,3,4,5,6-Me_5	(3) 88.6	370.9		
3-CH_2·	(7) 90.7±2.9	379.5±12.1		
3,5-(CH_2·)	(8) 88.2±5.0	369.0±20.9		
p-isotoluene 	64±3	267.8±12.6	Derived	1990BAR/GRI
toluene bromide $C_6H_5CH_2H^+Br^-$	87.7	367	AOP	1997CHE/LIU

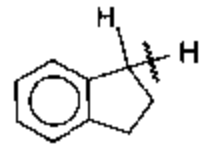
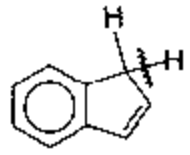
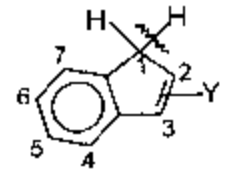
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ethylbenzene, substituted  Y = H $\Delta_f H^\circ$(R) = 40.4 (169 0)	(1) 84.6 (2) 86.2 (3) **85.4±1.5** (4) 90.3 (5) 87.0	354.0 360.7 **357.3±6.3** 377.8 364.1	(1) VLPP (2) Proton affinity (3) Review (4) Re-anal. of pyrolysis data (5) Correlation	(1) 1981ROB/STE (2) 1982MEO (3) 1982MCM/DOL (4) 1998BRO/BEC (5) 2000DEN/DEN
p-C_2H_5	(6) 86.3	361.1	(6) Correlation	(6) 2002KRO/TUM
p-Br	(6) 87.1	364.4		
p-tBu	(6) 86.5	361.9		
p-MeOC(O)	(6) 87.0	364.1		
prop-2-enylbenzene $PhCH_2CH{=}CH_2$	84.4	353.1	Correlation	1995TUM/DEN
n-propylbenzene $PhCH_2C_2H_5$	(1) 86.1 (2) 87.5	360.2 366.2	(1) Proton affinity (2) Correlation	(1) 1982MEO (2) 2000DEN/DEN
i-propylbenzene, substituted  Y = 2,5-Me_2	86.7	362.8	Correlation	2002KRO/TUM
4-t-Bu	83.5	349.3		
t-butylbenzene $C_6H_5C(CH_3)_2CH_2$–**H**	98.7	413.0	Correlation	2002KRO/TUM
(E) -1-phenylpropene (E) -Ph CH=CH-CH_2–**H**	78.9±2.6	330.1±10.9	FT-MS	2002GLA/MAK
phenylacetonitrile $PhCH_2CN$	81.5	341.0	AOP	1991BAU/FAS(b)
1-methoxyphenylacetonitrile PhC**H**(CN) MeO	76.2	318.8	AOP	1991BAU/FAS(b)
cationic niobium η^2-acyl 	82±3	343.1±12.6	Electrochemical	1997KER/ZHA
1-phenylcyclobutene 	85.6±2.6	358.2±10.9	FT-MS	2002GLA/MAK

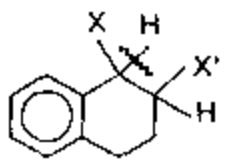
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值, 括号内数字 文献编号) kcal/mol	kJ/mol	方法	文献
cyclopentylbenzene 	88.0	268.2	Correlation	2002KRO/TUM
cyclohexylbenzene 	85.2	356.4	Correlation	2002KRO/TUM
diphenylmethane Ph_2CH_2 $\Delta_f H^\circ$(R) = 72.2±1.0 (302.1±4.2)	(1) 84±2 (2) **84.5±0.5** (3) 85.8 (4) 85.3 (5) 81.8	351.5±8.4 **353.5±2.1** 359.0 356.9 342.3	(1) VLPP (2) Electrochem. (3) Re-anal. of pyrolysis data (4) Correlation (5) AOP	(1) 1991STE/BRO (2) 1991PAR/HAN (3) 1998BRO/BEC (4) 2000DEN/DEN (5) 2002ALN/ZHA
diphenylmethane, substituted (p-$PhC_6H_4)_2CH_2$	80	334.7	AOP	1989BOR/HAR
1,2-diphenylethane $PhCH_2CH_2Ph$	87.0	364.1	Correlation	2000DEN/DEN
2-phenylpropane $PhCH(CH_3)_2$ $\Delta_f H^\circ$(R) = 32.0±1.0 (133.9±4.2)	(1) 83.6 (2) 84.4±1.5 (3) **83.2±1** (4) 87.3 (5) 84.8	349.8 353.1±6 3 **348.1±4.2** 365.3 354.7	(1) VLPP (2) Review (3) PAC (4) Re-anal. of pyrolysis data (5) Correlation	(1) 1981ROB/STE (2) 1982MCM/GOL (3) 1997LAA/BOR (4) 1998BRO/BEC (5) 2000DEN/DEN
1,1-diphenylethane $Ph_2C(CH_3)$ C-**H**	(1) 81±2 (2) **82.8** (3) 83.9	338.9±8.4 **346.4** 351.0	(1) VLPP (2) Re-anal. of pyrolysis data (3) Correlation	(1) 1981STE (2) 1998BRO/BEC (3) 2000DEN/DEN
thiphenylmethane, substituted  Y = p-H, Y′ = p-H, Y″ = p-H $\Delta_f H^\circ(Ph_3C)$ = 93.7±2 (392.0±8.4)	(1) **81±2** (2) 80.8±3 (3) 79.0 (4) 82.7 (5) 85.4	**338.9±8.4** 338.1±12.6 330.5 346.0 357.3	(1) AOP (2) AOP (3) AOP (4) Correlation (5) Correlation	(1) 1991PAR/HAN (2) 1993BOR/ZHA(b (3) 1997ARN/FLO (4) 2000DEN/DEN (5) 2002KRO/TUM
p-MeO, p-MeO, p-MeO	(3) 78.1	326.8		
p-MeO, p-MeO, p-H	(3) 79.3	331.8		
p-Me, p-Me, p-Me	(3) 79.0	330.5		
p-MeO, p-H, p-*H*	(3) 80 7	337.6		

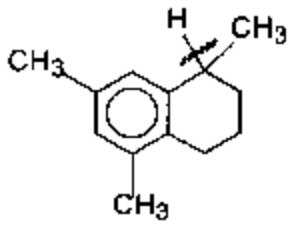
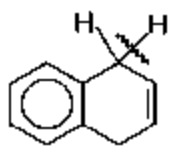
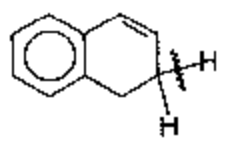
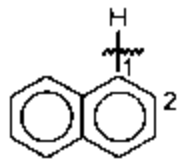
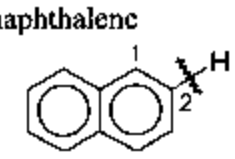
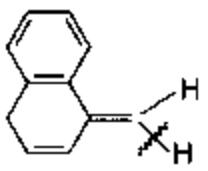
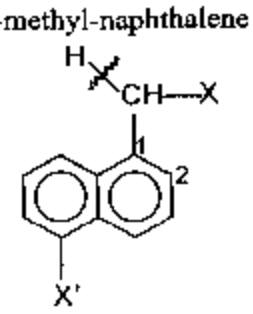
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
p-Me, p-Me, p-H	(3) 80.3	336.0		
p-Me, p-H, p-H	(3) 79.1	331.0		
p-tBu, p-tBu, p-tBu	(3) 74.4	311.3		
thiphenylmethane, substituted $(p\text{-}HC_6F_4)_3C\text{-}\mathbf{H}$	82.3	344 3	AOP	1993BOR/ZHA(b)
1,1,3,3-tetraphenylpropene $Ph_2C{=}CHC(Ph)_2\text{–}\mathbf{H}$	77	322.2	AOP	1989BOR/HAR
1,1,3,5,5-pentaphenyl-1,4-pentadiene $Ph_2C{=}CH\mathbf{C}H(Ph)\,CH{=}CPh_2$	75.1	314.2	AOP	1991BOR/CHE
benzocyclobutene 	92±4	384.9±16.7	GPA	2000GLA/MAK
benzocyclobutadiene 	114±4	477.0±16.7	GPA	2000BRO/KAS(b)
indane  $\Delta_f H^\circ$(indanyl) = 48.8±2 (204.2±8.4)	85.9	359.4	Correlation	2000DEN/DEN
indene  $\Delta_f H^\circ$(indenyl) = 71 (297.1)	(1) 84±3 (2) 81.5±0.5 (3) 81.1±2.4 (4) **83.0** (5) 81.2	351.5±12.6 341.0±2.1 339.3±10.0 **347.3** 339.7	(1) Review (2) Electrochem. (3) ICR (4) Re-anal. of pyrolysis data (5) Correlation	(1) 1982MCM/GOL (2) 1991PAR/HAN (3) 1997ROM/JAN (4) 1998BRO/BEC (5) 2001TUM/DEN
indene, substituted 				
Y = 2-Br	(1) 80.9	338.5	(1) AOP	(1) 1992BOR/SAT
3-Me	(1) 77 6	324.7		
3-t-Bu	(1) 78.5	328.4		
2-Ph	(1) 79.3 (2) 84±3	331.8 351.5±12.6	(2) VLPP	(2) 1981STE

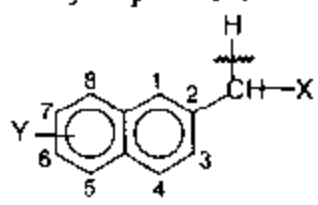
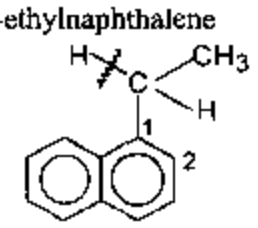
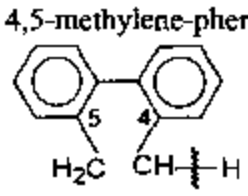
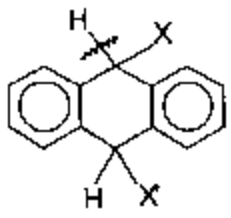
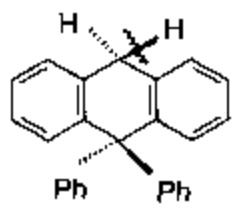
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
3-Ph	(1) 75.3	315.1		
3-MeO	(1) 76.4	319.7		
3-MeS	(1) 74.1	310.0		
2-PhS	(1) 80.2	335.6		
3-CN	(1) 77.9	325.9		
3-c-C_4H_8N	(1) 70.3	294.1		
2-c-C_4H_8N	(1) 83.5	349.4		
3-c-$C_5H_{10}N$	(1) 72.3	302.5		
2-c-$C_5H_{10}N$	(1) 82.5	345.2		
3-c-OC_4H_8N	(1) 73.4	307.1		
2-c-OC_4H_8N	(1) 82.8	346.4		
2-(4-$MeOC_6H_4$)	(1) 79.3	331.8		
2-(4-MeC_6H_4)	(1) 79.1	331.0		
3-C(O) NH_2	(1) 77.7	325.1		
2-C(O) OMe	(1) 79.2	331.4		
3-C(O) OMe	(1) 77.6	324.7		
6-NO_2-3-Me	(1) 78.4	328.0		
1,2,3-Ph_3	(1) 75.8	317.1		
tetralin  X = H X' = H $\Delta_f H^\circ$(R) = 37±1.2 (54.8±5.0)	(1) 82.9±1.2 (2) 83.6 (3) 82.6	346.9±5.0 349.6 345.6	(1) PAC (2) Correlation (3) Correlation	(1) 1997LAA/MUL (2) 2000DEN/DEN (3) 2002KRO/TUM
Me *H*	(3) 80.4 (4) 79.3	336.4 331.8	(4) Correlation	(4) 1995TUM/DEN
Me *Me*	(4) 80.5	336.8		

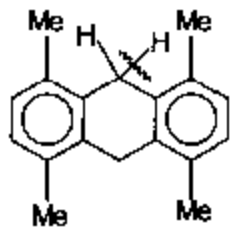
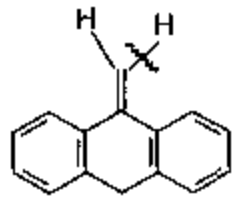
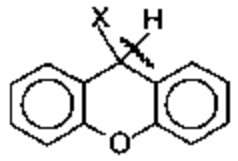
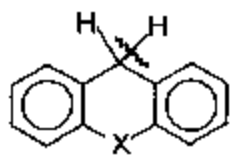
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1,5,7-trimethyltetralin 	80.9	338.4	Correlation	2002KRO/TUM
1,4-dihydronaphthalene 	83.0	347.3	Re-anal. of pyrolysis data	1997RUC/GER
1,2-dihydronaphthalene 	(1) 86.0 (2) 80.4	359.8 336.4	(1) Re-anal. of pyrolysis data (2) Correlation	(1) 1997RUC/GER (2) 2002KRO/TUM
naphthalene  $\Delta_f H^\circ$(R) = 96.0±1.3 (401.7±5.4)	(1) **112.2±1.3** (2) 113.4±5.2 (3) 112.8±3.3	**469.4±5.4** 474.5±21.8 472±14	(1) FT MS (2) Negative ion cycle (3) Negative ion spectroscopy	(1) 2000REE/KAS (2) 2001LAR/SQU (3) 2001ERV/RAM
naphthalene  $\Delta_f H^\circ$(R) = 95.7±1.4 (400.4±5.9)	(1) **111.9±1.4** (2) 115.4±4.9 (3) 113.8±4.8	**468.2±5.9** 482.8±20.5 476±20	(1) FT MS (2) Negative ion cycle (3) Negative ion spectroscopy	(1) 2000REE/KAS (2) 2001LAR/SQU (3) 2001ERV/RAM
1-methylene-1,4-dihydronaphthalene 	69±3	288.7±12.6	Derived	1990BAR/GRI
1-methyl-naphthalene  X = H X′ = H $\Delta_f H^\circ$(1-naphthylmethyl) = 60.4 (252.7)	(1) 84.3±1.5 (2) **85.1±1.5** (3) 87.3	352.7±6.3 **356.1±6.3** 365.1	(1) VLPP (2) Review (3) Correlation	(1) 1980MCM/TRE (2) 1982MCM/GOL (3) 2000DEN/DEN
CN X′ = H	(4) 81.3	340.2	(4) AOP	(4) 1988BOR/CHE(b)
H X′ = Me	(5) 86.8	363.3	(5) Correlation	(5) 2002KRO/TUM

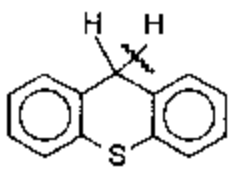
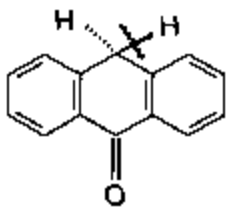
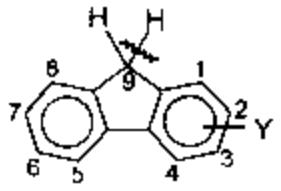
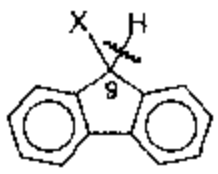
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断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
2-methyl-naphthalene 				
X = H Y = H	(1) 85.6	358.3	(1) Correlation	(1) 2002KRO/TUM
Me H	(1) 87.1	364.6		
SO_2Ph H	(2) 89	372.4	(2) AOP	(2) 1988BOR/BAU
CN H	(3) 81.4	340.6	(3) AOP	(3) 1988BOR/CHE(b)
H 3-Me	(1) 86.8	363.1		
H 6-Me	(1) 87.3	365.2		
1-ethylnaphthalene 	87.1	364.4	Correlation	2000DEN/DEN
4,5-methylene-phenathrene 	81	338.9	AOP	1989BOR/HAR
9,10-dihydroanthracene, substituted 				
X = H, X' = H	(1) 78	326.4	(1) AOP	(1) 1988BOR/CHE
	(2) 78	326.4	(2) PAC	(2) 1989GRI/SIM
	(3) 77	322.2	(3) Kinetics	(3) 1990MAL/MCM
	(4) **76.3**	**319.2**	(4) VLPP	(4) 1991STE/BRO
	(5) 83.0	347.3	(5) Re-anal. of pyrolysis data	(5) 1997RUC/GER
$\Delta_f H^\circ$(9,10-dihydroanthracen-9-yl) = 62.4 (261.1)				
H Ph	(5) 84.5	353.5		
	(6) 79	330.5	(6) AOP	(6) 1991BOR/CHE
Me Me	(5) 81.5	341.0		
	(7) 77	322.2	(7) PAC	(7) 1989GRI/SIM
9,10-dihydroanthracene, substituted 	84.9	355.2	Re-anal. of pyrolysis data	1997RUC/GER

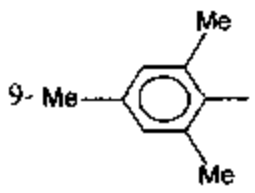
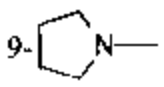
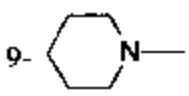
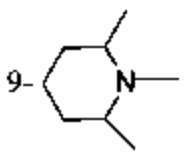
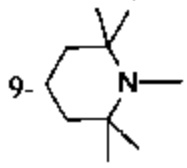
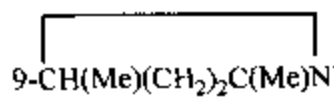
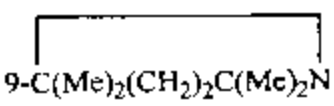
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值, 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
9,10-dihydroanthracene, substituted 	83.3	348.5	Re-anal. of pyrolysis data	1997RUC/GER
9-methylene-6,10,-dihydroanthracene 	77±3	322.2±12.6	Derived	1990BAR/GRI
xanthene, substituted 				
X = H	(1) 74 (2) 75.5 (3) 75.2 (4) 80.7	309.6 315.9 314.6 337.6	(1) VLPP (2) AOP (3) AOP (4) Re-anal. of pyrolysis data	(1) 1991STE/BRO (2) 1991BOR/CHE (3) 1997ARN/FLO (4) 1997RUC/GER
Me	(4) 77.6	324.7		
CN	(5) 69	288.7	(5) AOP	(5) 1992ZHA/BOR
SO_2Ph	(6) 82	343.1	(6) AOP	(6) 1988BOR/CHE
Ph	(5) 76 (3) 74.6 (7) 76.7	318.0 312.1 320.9	(7) AOP	(7) 1993ARN/FLO
p-MeC_6H_4	(5) 75.6	316.3		
p-$MeOC_6H_4$	(5) 74.3 (7) 76.2	310.9 318.8		
p-FC_6H_4	(5) 76.8 (7) 76.4	321.3 319.7		
p-ClC_6H_4	(5) 73.9 (7) 78.1	309.2 326.8		
p-$CF_3C_6H_4$	(5) 78.3 (7) 78.1	327.6 326.8		
9,10-dihydroacridine, substituted 				

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
X = NH	80.0	334.7	Re-anal. of pyrolysis data	1997RUC/GER
NCH_3	80 0	334.7		
thioxanthece 	74.6	312.1	AOP	1997ARN/FLO
10-hydroanthracen-9-one 	80.2	335.6	Re-anal. of pyrolysis data	1997RUC/GER
fluorene, substituted 	(1) 80.1	335.1	(1) VLPP	(1) 1991STE/BRO
	(2) 82.2	343.9	(2) Electrochem.	(2) 1992PAR
	(3) 81.2±2.4	339.7±10.0	(3) ICR	(3) 1997ROM/JAN
	(4) 82.0±2	**343.1±8.4**	(4) Re-anal. of pyrolysis data	(4) 1994RAK/VER
Y = H $\Delta_f H^\circ$(9-fluorenyl) = 71.7±2 (300.0±8.4)	(5) 82.6	345.6	(5) Re-anal. of pyrolysis data	(5) 1997RUC/GER
Y = 2-$PhSO_2$	(6) 80	334.7	(6) AOP	(6) 1992ZHA/BOR
2-CN	(6) 80	334.7		
2-NO_2	(6) 81	338.9		
2-MeO	(7) 80	334.7	(7) AOP	(7) 1994ZHA/BOR(b)
2-Me_2N	(6) 80	334.7		
2-$PhSO_2$	(8) 79.7	333.5	(8) AOP	(8) 1993ZHA/BOR
2,7-Br_2-9-CO_2Me	(6) 76.5	320.1		
fluorene, substituted 				
X = 9-CN	(1) 74.8	313.0	AOP	(1) 1991BOR/ZHA
9-SO_2Ph	(1) 81.9	342.7		
9-PhS	(1) 74.6	312.1		

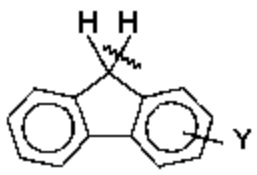
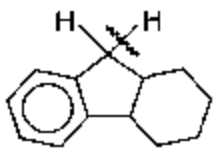
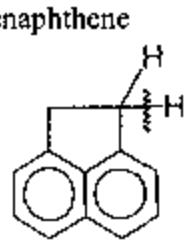
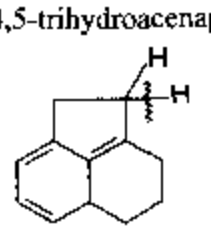
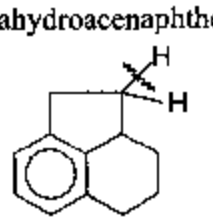
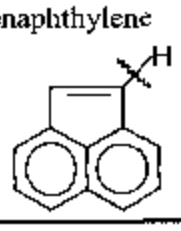
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
9-Me_2N	(1) 71.5	299.2		
9-(2,4,6-$Me_3C_6H_2$)	(2) 74.5	311.7		(2) 1991BOR/ZHA
9-$PhCH_2$(Me) N	(3) 72.5	303.3		(3) 1992ZHA/BOR
9-(iPr) $_2$N	(3) 73	305.4		
	(3) 76	318.0		
	(3) 68	284.5		
	(3) 72	301.2		
	(3) 72	301.2		
	(3) 71	297.1		
9-Ph	(6) 74	309.6		
9-C_6F_5	(4) 78.2	327.2		(4) 1993ZHA/BOR
9-mesityl	(6) 74.5	311.7		(5) 1994ZHA/BOR(b)
9-MeOCO	(6) 76	318.0		(6) 1994ZHA/BOR(c)
9-c-C_4H_8N	(6) 68	284.5		
9-c-$C_5H_{10}N$	(6) 72	301.2		
9-PhCH(Me) N	(6) 72.5	303.3		
	(6) 72	301.2		
	(6) 71	297.1		
9-Me $\Delta_f H^\circ$(R) = 64.1±2 (268.2±8.4)	(7) 75.4 (8) 79.7±2 (9) 78.5	315.5 333.5 328.4		(7) 1994BOR/ZHA (8) 1998BRO/BEC (9) 2002KRO/TUM

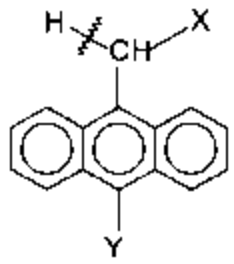
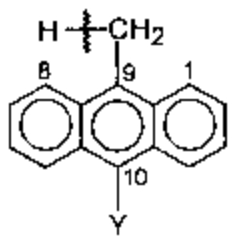
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
9-Et	(7) 76.2	318.8		
9-n-Pr	(7) 76.1	318.4		
9-iPr	(7) 77.3	323.4		
9-sBu	(7) 75.1	314.2		
9-tBu	(7) 79.9	334.3		
9-neoC_5H_{11}	(7) 73.6	307.9		
9-PhC(Me)$_2$$CH_2$	(7) 73.8	308.8		
9-$PhCH_2$	(7) 75.9	317.6		
9-MeS	(7) 74.6	312.1		
9-EtS	(7) 74.3	310.9		
9-iPrS	(7) 74.3	310.9		
9-tBuS	(7) 74.8	313.0		
9-PhS	(7) 74.8	313.0		
9-$MeSO_2$	(7) 82.1	343.5		
9-$EtSO_2$	(7) 81.4	340.6		
9-i$PrSO_2$	(7) 81.1	339.3		
9-$PhSO_2$	(7) 79.7	333.5		
9-(p-BrPh) SO_2	(7) 82.0	343.1		
9-MeO	(7) 73.0	305.4		
9-EtO	(7) 72.9	305.0		
9-iPrO	(7) 72.7	304.2		
9-tBuO	(7) 74.0	309.6		
9-PhO	(7) 74.3	310.9		
9-Me_3SiCH_2	(9) 76.3	319.2		(9) 1996ZHA/BOR
9-$Me_3N^+Cl^-$	(5) 84.6	354.0		
9-PyN^+Br	(4) 80.9	338.5		

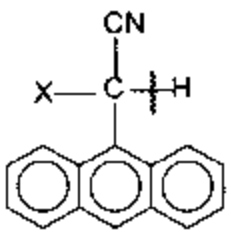
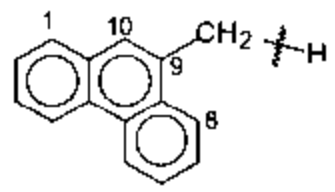
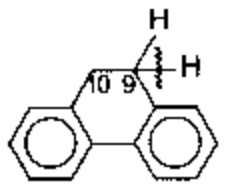
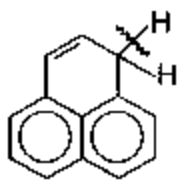
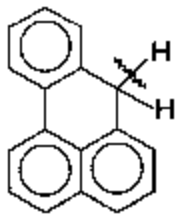
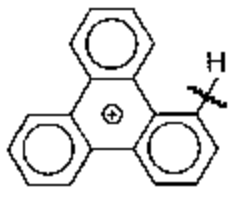
续表

断裂键 （**黑体**　离解原子） $\Delta_f H^0$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
9-nBu_3P^+, Br^-	(10) 83.0	347.3		(10) 2000CHE/LIU
9-Ph_3P^+, Br^-	(5) 81.6	341.4		
9-Ph_3As^+, Br^-	(10) 82.6	345.6		
9-Me_2S^+, Br	(10) 77.6	324.7		
9-Me_2Se^+, Br^-	(10) 78.7	329.3		
9-tBu_2Te^+, Br^-	(10) 77.3	323.4		
9-$Me_3N^+(2\text{-}PhSO_2)$, Br^-	(4) 85.7	358.6		
fluorene, substituted 				
Y = π-$Cr(CO)_3$	80	334.7	AOP	1994ZHA/BOR(b)
π- $Mn(CO)_3$	81	338.9		
π-$^+Fe(C_5H_5)$	80	334.7		
1,2,3,4,4a,9a-hexahydrofluorene 	79.3	332.0	Correlation	2002KRO/TUM
acenaphthene 	83.7	350.0	Correlation	2000DEN/DEN
3,4,5-trihydroacenaphthene 	78.8	329.7	Correlation	1995STUM/DEN
tetrahydroacenaphthene 	75.8	317.0	Correlation	2002KRO/TUM
acenaphthylene 	117±4	489.5±16.7	GPA	2002KAS/BRO

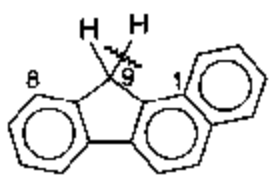
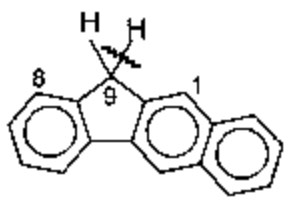
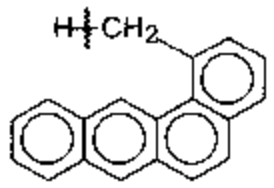
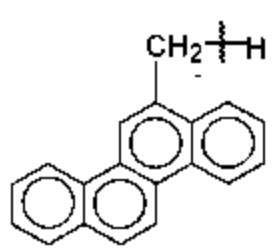
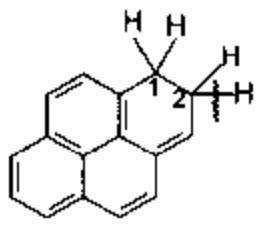
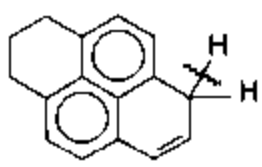
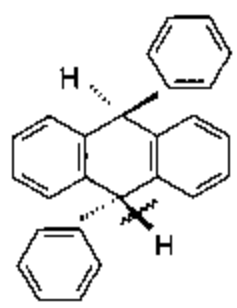
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
9-anthracenylmethane, substituted  				
	(1) 81.0	338.9	(1) Analysis of exp.	(1) 1980MCM/TRE
			(2) Review	(2) 1982MCM/GOL
	(2) 81.8	342.3	(3) AOP	(3) 1991BOR/CHE
Y = H, X = H	(3) 81.5	341.0	(4) Electrochem.	(4) 1991PAR/HAN
$\Delta_f H^\circ$(9-anthracenylmethyl) = 80.7 (337.6)	(4) **84.1±0.5**	**351.9±2.1**	(5) AOP	(5) 2002ALN/ZHA
	(5) 81.5	341.0		
CN	(6) 78.7	329.3	(6) AOP	(6) 1991BAU/FAS(b)
	(7) 78.9	330.1	(7) AOP	(7) 1993ZHA/BOR(b)
MeO	(6) 77.4	323.8		
	(7) 77.5	324.3		
PhO	(6) 78.6	328.9		
	(7) 79.9	334.3		
PhCO	(7) 84.2	352.3		
NO_2	(7) 86.1	360.2		
PhS	(7) 81.0	338.9		
$PhSO_2$	(7) 84 7	354.4		
Y = CN, X = MeO	(6) 73.7	308.4		
PhO	(6) 72.9	305.0		
anthracene, substituted  				
Y = Cl	(1) 80.8	338.1	(1) AOP	(1) 1993ZHA/BOR(b)
Me	(1) 81.8	342.3		
	(2) 78.1	326.7	(2) Correlation	(2) 2002KRO/TUM
MeO	(1) 81.4	340.6		
Ph	(1) 81.8	342.3		
CHO	(1) 80.4	336.4		
PhCO	(1) 82.3	344.3		

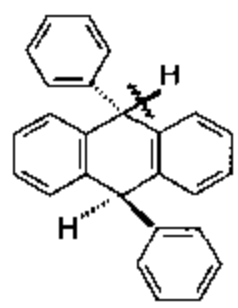
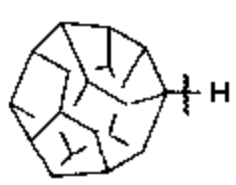
续表

断裂键 (黑体　离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值， 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
CN	(1) 80	334.7		
NO_2	(1) 82.6	345.6		
PhS	(1) 80.8	338.1		
anthracene, substituted 				
X = H	78.7	329.3	AOP	1991BAU/FAS(b)
MeO	78.0	326.4		
9-phenanthrenylmethane  $\Delta_f H^\circ$(9-phenanthrenylmethyl) = 74.4 (311.3)	85.1±1.5	356.1±6.5	VLPP	1982MCM/GOL
9,10-dihydrophenanthrene 	(1) 89.6 (2) 82.1 (3) 81.6	374 9 343.7 341.6	(1) Re-anal. of pyrolysis data (2) Correlation (3) Correlation	(1) 1997RUC/GER (2) 2000DEN/DEN (3) 2002KRO/TUM
phenalene 	(1) 64±3 (2) 74.0	267.8±12.6 309.6	(1) AOP (2) Re-anal. of pyrolysis data	(1) 1990BAU/GOS (2) 1997RUC/GER
benzanthrene 	(1) 66±3 (2) 76.0	276.1±12.6 318.0	(1) AOP (2) Re-anal. of pyrolysis data	(1) 1990BAU/GOS (2) 1997RUC/GER
triphenylene radical cation 	86.0±4.8	359.9±20	PIMS	1997LIN/LIF

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** 推荐值: 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1,2-benzofluorence 	78.7	329.3	AOP	1991BOR/CHE
2,3-benzofluorence 	(1) 78.8 (2) 78.4 (3) 78	329.7 328.0 326.3	(1) VLPP (2) AOP (3) AOP	(1) 1991STE/BRO (2) 1991BOR/CHE (3) 2002ALN/ZHA
methylbenzo(b) phenanthrene 	88.6	370.8	Correlation	2002KRO/TUM
6-methylchrysene 	85.7	358.7	Correlation	2002KRO/TUM
1,2-dihydropyrene 	81.6	341.4	Correlation	2000DEN/DEN
1,2,3,6-tetrahydropyrene 	81.6	341.4	Correlation	2002KRO/TUM
(E) -9,10-diphenyl-9,10-dihydroanthracene 	81.5	341.0	Re-anal. of pyrolysis data	1997RUC/GER

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
(*Z*) -9,10-diphenyl-9,10-dihydroanthracene 	79.4	332.2	Re-anal. of pyrolysis data	1997RUC/GER
dodecahedrane 	92±3	384.9±12.6	FT-MS	2000BRO/KAS(a)

4.5 卤代碳氢化合物

表 4.5 卤代碳氢化合物内的 C—H BDEs

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 文献编号)		方法	文献
	kcal/mol	kJ/mol		
trifluoromethane **H**–CF_3 $\Delta_f H^\circ$(R) = –111.2±0.4 (–465.3±1.7)	(1) 106.7±1 (2) 107 (3) 107.4 (4) **106.4±0.7** (5) 108.9	446.4±4.2 447.7 449.4 **445.2±2.9** 455.6	(1) Photolysis (2) Review (3) Derived (4) Derived (5) SPST	(1) 1972BAS/WHI (2) 1982MCM/GOL (3) 1997ASH/RUS , (4) 1998RUS/MIC (5) 1999TSA
difluoromethane **H**–CHF_2 $\Delta_f H^\circ$(R) = - 57.1±1 (–238.9±4.2)	(1) 97.4±1.3 (2) 101±2 (3) **103.2±1** (4) 101±2 (5) 101.8±1.1	407.5±5.4 422.6±8.4 **431.8±4.2** 422.6±8.4 425.8±4.6	(1) Kinetics (2) Elimination (3) Iodination (4) Kinetics (5) Review	(1) 1969PRI/PER (2) 1971KER/TIM (3) 1983PIC/ROD (4) 1983MAR/PAR (5) 2001LAZ/PRO
fluoromethane **H**–CH_2F $\Delta_f H^\circ$(R) = –7.6±1 (–31.8±4.2)	(1) **101.3±1** (2) 100±2	**423.8±4.2** 418.4±8.4	(1) Iodination (2) Kinetics	(1) 1983PIC/ROD (2) 1983MAR/PAR

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
chlorodifluoromethane **H**–$CClF_2$ $\Delta_f H^\circ$(R) = –66.7±2 (–279.1±8.4)	(1) 101.6±1 (2) **100.7±2**	425.1±4.2 **421.3±8.4**	(1) Review (2) Photobromin.	(1) 1982MCM/GOL (2) 1992MIY/TSC
dichlorofluoromethane **H**–CCl_2F $\Delta_f H^\circ$(R) = -21.3±2 (–89.0±8.4)	(1) 98.9±1.2 (2) **98.2±2** (3) 97.7	413.8±5.0 **410.9±8.4** 408.8	(1) Bromination (2) Photobromin. (3) Review	(1) 1987TSC/PAD (2) 1992MIY/TSC (3) 1997POU/PAU
difluorobromomethane **H**–$CBrF_2$	99.3±3	415.5±12.6	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
chlorofluoromethane **H**–CHClF $\Delta_f H^\circ$(R) = –14.5±2.4 (–60.7±10.0)	(1) **100.8±2.4** (2) 99.4	**421.7±10.0** 415.9	(1) Bromination (2) Review	(1) 1987TSC/PAD (2) 1997POU/PAU
trichloromethane **H**–CCl_3 $\Delta_f H^\circ$(R) = 17.0±0.6 (71.1±2.5)	(1) 95.8±1 (2) 95.2 (3) 94.9±2 (4) **93.8±0.6**	400.8±4.2 398.3 397.1±8.4 **392.5±2.5**	(1) Bromination (2) Review (3) Electron impact (4) PIMS detect.	(1) 1973MEN/GOL (2) 1983WEI/BEN (3) 1988HOL/LOS (4) 1991HUD/JON
dichloromethane **H**–$CHCl_2$ $\Delta_f H^\circ$(R) = 22.3±1.0 (93.3±4.2)	(1) 99.0±2 (2) 98.4±1.2 (3) 97.2±2 (4) 96 2±0.6 (5) **97.3±1.0**	414.2±8.4 411.7±5.0 406.7±8.4 402.5±2.7 **407.1±4.2**	(1) Toluene carrier tech. (2) Bromination (3) Electron impact (4) PIMS detect. (5) Review	(1) 1958PRI/TRO (2) 1987TSC/PAD (3) 1988HOL/LOS (4) 1996SEE (5) 1997POU/PAU
chloromethane **H**–CH_2Cl $\Delta_f H^\circ$(R) = 28.0±0.7 (117.2±2.9)	(1) 100.8±1 (2) 99.4±2 (3) **100.1±0.6** (4) 100±2 (5) 99.9	421.7±4.2 415.9±8.4 **419.0±2.3** 418.4±8.4 418	(1) Bromination (2) Electron impact (3) PIMS detect. (4) Review (5) FT-ICR	(1) 1987TSC/PAD (2) 1988HOL/LOS (3) 1996SEE (4) 1997POU/PAU (5) 2000BOR/ING
bromochlorofluoromethane **H**–CFClBr	98.6±5	413±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
bromochloromethane **H**–CHClBr $\Delta_f H^\circ$(R) = 34.2±1.4 (143±6)	(1) 93.9 (2) **97.0±0.6**	393 **406.0±2.4**	(1) FT-ICR (2) PIMS detect.	(1) 2000BOR/ING (2) 2003SEE
bromodichloromethane **H**–CCl_2Br	92.5±5	387±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
dibromochloromethane **H**–$CClBr_2$	88.7±5	371±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
tribromomethane **H**–CBr_3 $\Delta_f H^\circ$(R) = 49.0±2 (205.0±8.4)	(1) 96.0±1.6 (2) 95.4±2	401.7±6.7 399.2±8.4	(1) Bromination (2) Electron impact	(1) 1971KIN/GOL (2) 1988HOL/LOS

续表

断裂键 (黑体　离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
dibromomethane **H**–$CHBr_2$ $\Delta_f H^\circ$(R) = 45.0±2.2 (188.3±9.2)	(1) 103.7±2 (2) **99.7±1.8** (3) 97.9±2 (4) 98.2	433.9±8.4 **417.1±7.5** 409.6±8.4 411	(1) Toluene carrier tech (2) Bromination (3) Electron impact (4) Review	(1) 1958PRI/TRO (2) 1987TSC/PAD (3) 1988HOL/LOS (4) 2000BOR/ING
bromomethane **H**–CH_2Br $\Delta_f H^\circ$(R) = 40.9±0.6 (171.1±2.7)	(1) 102.0±2 (2) 101.6±1 (3) 100.8±2 (4) **102.1±0.6**	426.8±8.4 425.1±4.2 421.7±8.4 **427.2±2.4**	(1) Toluene carrier tech. (2) Bromination (3) Electron impact (4) PIMS detect.	(1) 1958PRI/TRO (2) 1987TSC/PAD (3) 1988HOL/LOS (4) 2003SEE
tetraiodomethane **H**–CI_3	101.1±7	423±29	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
diiodomethane **H**–CHI_2 $\Delta_f H^\circ$(R) = 79.8±2.2 (333.9±9.2)	103±2	431.0±8.4	Review	1970ONE/BEN
iodomethane **H**–CH_2I $\Delta_f H^\circ$(R) = 54.9±2 (229.7±8.4)	(1) 103±2 (2) 103.5±2 (3) 103.2±0.7	431.0±8.4 433.0±8.4 431.6±2.8	(1) Review (2) Electron impact (3) Kinetics	(1) 1970ONE/BEN (2) 1988HOL/LOS (3) 2002SEE
pentafluoroethane CF_3CF_2–**H** $\Delta_f H^\circ$(R) = –213.4±1 (–892.9±4.2)	(1) 103.1±1.5 (2) **102.7±0.5**	431.4±6.3 **429.7±2.1**	(1) Kinetics (2) Photolysis	(1) 1972BAS/WHI (2) 1981EVA/WHI
1,1,2,2-tetrafluoroethane CHF_2CF_2–**H** $\Delta_f H^\circ$(R) = –158.9±4.5 (–664.8±18.8)	103.0±4.5	431.0±18.8	Review	1996ZAR/WES
1,2,2-trifluoroethane CH_2FCF_2–**H** $\Delta_f H^\circ$(R) = –107.5±3.5 (–449.8±14.6)	103.5±3.5	433.0±14.6	Review	1996ZAR/WES
1,2,2-trifluoroethane CHF_2CFH–H $\Delta_f H^\circ$(R) = –109±3.5 (–456.1±14.6)	102.0±3.5	426.8±14.6	Review	1996ZAR/WES
1,1,1-trifluoroethane CF_3CH_2–**H** $\Delta_f H^\circ$(R) = –123.6±2 (–517.1±8.4)	106.7±1.1	446.4±4.5	Kinetics	1974WU/ROD
1,1-difluoroethane CH_3CF_2–**H** $\Delta_f H^\circ$(R) = –72.3±2 (–302.5±8.4)	99.5±1	416.3±4.2	Iodination	1977PIC/ROD

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** 推荐值; 括号内数字 · 文献编号) kcal/mol	kJ/mol	方法	文献
1,2-difluoroethane CH_2FCHF–**H** $\Delta_f H^\circ$(R) = –57.0±3 (–238.5±12.6)	98.8±3	413.4±12.6	UV-flash photolysis	1983MAR/PAR
1,1-difluoroethane CHF_2CH_2–**H** $\Delta_f H^\circ$(R) = –68.3±3.5 (–285.8±14.6)	103.5±3.5	433.0±14.6	Review	1996ZAR/WES
fluoroethane CH_2FCH_2–**H** $\Delta_f H^\circ$(R) = –14.2±2 (–59.4±8.4)	(1) **103.6±2** (2) 100.8±2	**433.5±8.4** 421.7±8.4	(1) Review (2) Photobromin.	(1) 1996ZAR/WES (2) 1996MIY/OZA
fluoroethane CH_3CHF–**H** $\Delta_f H^\circ$(R) = –16.8±2 (–70.3±8.4)	(1) 97.3±2 (2) **98.2±2**	407.1±8.4 **410.9±8.4**	(1) Bromination (2) Photobromin.	(1) 1987TSC/SAL(b) (2) 1996MIY/OZA
1-chloro-2,2,2-trifluoro-ethane CF_3CHCl–**H**	101.8±1.5	425.9±6.3	Review	1982MCM/GOL
1-bromo-1-chloro-2,2,2-trifluoroethane CF_3CClBr–**H** $\Delta_f H^\circ$(R) = –120.5±2 (-504.2±8.4)	96.6±1.5	404.2±6.3	Review	1982MCM/GOL
2-chloro-1,2,2-trifluoro-ethane $CClF_2CHF$–**H** $\Delta_f H^\circ$(R) = –107.7±3 (-450.6±12.6)	98.5±0.5	412.1±2.1	Pyrolysis	1998SKO/DYM
pentachloroethane CCl_3CCl_2–**H** $\Delta_f H^\circ$(R) = 8.4±1.3 (35.1±5.4)	(1) 95.8 (2) 95±2	400.8 397.5±8.4	(1) Photochlorin. (2) Shock tube	(1) 1969FRA/HUY (2) 1976LEW
1,1,2,2-tetrachloroethane $CHCl_2CCl_2$–**H** $\Delta_f H^\circ$(R) = 5.6±2 (23.4±8.4)	94±2	393.3±8.4	Shock tube	1976LEW
1,1-dichloroethane CH_3CCl_2–**H** $\Delta_f H^\circ$(R) = 10.2±0.4 (42.7±1.7)	(1) 93.4±0.4 (2) 95.1±1.2	390.6±1.5 397.9±5.0	(1) PIMS detect. (2) Kinetics	(1) 1996SEE (2) 1999MIY/TSC
chloroethane CH_3CHCl–**H** $\Delta_f H^\circ$(R) = 18.3±0.4 (76.6±1.5)	(1) 95.7 (2) 98.2±2 (3) 96.5±1 (4) **97.2±0.4**	400.4 410.9±8.4 403.8±4.2 **406.6±1.5**	(1) Bromination (2) Electron impact (3) Photobromin. (4) PIMS detect.	(1) 1987TSC/SAL(b) (2) 1988HOL/LOS (3) 1990MIY/TSC (4) 1996SEE

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
chloroethane CH_2ClCH_2–**H** $\Delta_f H^\circ$(R) = 22.2±0.6 (93.0±2.4)	(1) 101.7±2 (2) 100.7±1 (3) **101.1±0.6**	425.5±8.4 421.3±4.2 **423.1±2.4**	(1) Electron impact (2) Photobromin. (3) PIMS detect.	(1) 1988HOL/LOS (2) 1990MIY/TSC (3) 1998SEE
1,1-dibromoethane CH_3CBr_2 **H** $\Delta_f H^\circ$(R) = 33.5±1.3 (140.2+5.4)	94.9±1.2	397.1±5.0	Kinetics	1999MIY/TSC
bromoethane CH_2BrCH_2–**H** $\Delta_f H^\circ$(R) = 32.3 (135.1)	99.2±2	415.1±8.4	Electron impact	1988HOL/LOS
bromoethane CH_3CHBr **H** $\Delta_f H^\circ$(R) = 30.3 (126.8)	(1) 96.4 (2) 94.2±2 (3) **97.2±1**	403.3 394.1±8.6 **406.7±4.2**	(1) Bromination (2) Electron impact (3) Photobromin.	(1) 1987TSC/SAL(b) (2) 1988HOL/LOS (3) 1990MIY/TSC
trifluoroethylene CF_2=CF–**H**	111±2	464.4±8.4	Correlation	1981STE/ROW
1,1-difluoroethylene CF_2=CH –**H** $\Delta_f H^\circ$(R) = –22.2±2 (92.9±8.4)	110±2	460.2±8.4	Correlation	1981STE/ROW
(E) -1,2-difluoroethylene CHF=CF–**H** $\Delta_f H^\circ$(R) = –12.1±2 (–50.6±8.4)	110±2	460.2±8.4	Correlation	1981STE/ROW
1,1-difluoro-2-chloroethylene CF_2=CCl–**H**	109±2	456.1±8.4	Correlation	1981STE/ROW
(Z) -1,2-chloro-2-fluoro-ethylene CFCl=CCl–**H**	108±2	451.9±8.4	Correlation	1981STE/ROW
(E) -1,2-dichloroethylene CHCl=CCl **H** $\Delta_f H^\circ$(R) = 56.1±2 (234.7±8.4)	107±2	447.7±8.4	Correlation	1981STE/ROW
chloroethylene CH_2=CCl–**H**	(1) >103.6 (2) 116.0±1.2	>433.5 485.3±2.8	PIMS	(1) 1989RUS/SEN (2) 1995SHE/QI
1,1,1,2,2,3,3-heptafluoro-propane $CF_3CF_2CF_2$–**H**	(1) 104±2 (2) 103.3	435.1±8.4 432.2	(1) Review (2) Bromination	(1) 1982MCM/GOL (2) 1983EVA/WEE
1,1,1,2,3,3,3-hepta-fluoropropane CF_3CFHCF_3	103.5±0.6	433.0±2.5	Kinetics	1983EVA/WEE
1-chloropropane CH_3CH_2CHCl-**H** $\Delta_f H^\circ$(R) = 13.5±0.8 (56.6±3.3)	97.3±0.8	407.0±3.5	Derived	1998SEE

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1-chloropropane $CH_2ClCH_2CH_3$	97.8±0.9	409.3±3.9	Derived	1998SEE
1-fluoropropene CH_2=CH-CHF-**H**	88.6±1.1	370.7±4.6	VLPP	1973ALF/GOL
1-chloropropene CH_2=CH-CHCl-**H**	88.6±1.1	370.7±4.6	VLPP	1973ALF/GOL
1-bromopropene CH_2=CH-CHBr-**H** $\Delta_f H^\circ$(R) − 48.1±1.1 (201.3±4.6)	89.4±1.1	374.0±4.6	VLPP	1973ALF/GOL
pentafluorobenzene **H**-C_6F_5 $\Delta_f H^\circ$(R) = −130.9±2 (−547.7±8.4)	116.5	487.4	Toluene carrier tech.	1974KRE/PRI
9-pentafluorophenyl fluorene 9-C_6F_5Fl**H**	78.2	327.2	AOP	1993BOR/ZHA(b)
tri(2,3,5,6-tetrafluoro-phenyl) phenyl methane (p-HC_6F_4)$_3$C**H**	82.3	344.3	AOP	1993BOR/ZHA(b)

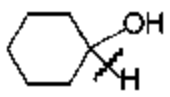
4.6 含杂原子的碳氢化合物

4.6.1 α位是—O、—OR、—CO、—C(O) O的C—H键

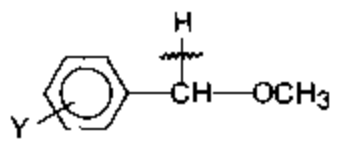
表 4.6.1 α位是—O、—OR、—CO、—C(O) O 的碳氢化合物内的 C—H BDEs

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
methanol **H**-CH_2OH $\Delta_f H^\circ$(R) = −4.08±0.8 (−17.07±3.35)	(1) 95.9±1.5 (2) 96.0 (3) 96.2±0.2 (4) **96.06±0.15** (5) 96.2±0.3	401.2±6.3 401.7 402.5±0.8 **401.92±0.63** 402.5±1.3	(1) Iodination (2) SPST (3) PIMS detect. (4) Recommend. (5) Resonance fluorescence	(1) 1973ONE/BEN (2) 1981TSA (3) 1993RUS/BER (4) 1994BER/ELL (5) 1996DOB/BER
ethenol CH_2CHO**H** $\Delta_f H^\circ$(R) −28.9±2.6 (121±11)	111.6±2.6	467±11	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
ethanol CH_3CH_2O**H** $\Delta_f H^\circ$(R) = −13.3±0.8 (−55.6±3.5)	(1) 93±1.0 (2) 94.6 (3) **94.8** (4) 95 9±1	389.1±4.2 395.8 **396.6** 401.2±4.2	(1) Iodination (2) SPST (3) Electron impact (4) Review	(1) 1973ALF/GOL (2) 1981TSA (3) 1991HOL/LOS (4) 1999ATK/BAU

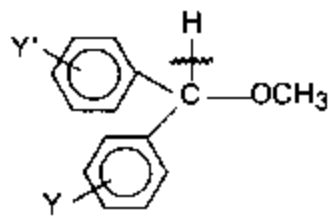
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 - 推荐值: 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
ethanol CH_3CH_2OH $\Delta_f H^\circ$(R) = –7.5±1.7 (-31±7)	(1) 101.3 (2) 98±2 (3) 100.8±2	423.8 410.0±8.4 421.7±8	(1) MS (2) PIMS detect. (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1990TAK (2) 1994RUS/BER (3) 1998NIST
propanol $CH_3CH_2CH_2OH$ $\Delta_f H^\circ$(R) = -19.4±1 (–81±8)	(1) 93.7 (2) 93.2	392.0 389.9	(1) SPST (2) Correlation	(1) 1999TSA (2) 2000DEN/DEN
propanol $CH_3CH_2CH_2OH$ $\Delta_f H^\circ$(R) = –18.8±2 (- 78.7±8.4)	94.3±2	394.6±8.4	AE	1992HOL
propanol $CH_3CH_2CH_2OH$ $\Delta_f H^\circ$(R) = –16.0±2 (–66.9±8.4)	97.1±2	406.3±8.4	AE	1992HOL
propan-2-ol $(CH_3)_2CHOH$ $\Delta_f H^\circ$(R) = –26.3±1 (–110.0±4.2)	(1) **91±1** (2) 89.3±1.7 (3) 91.7±2 (4) 93.0	**380.7±4.2** 373.6±7.1 383.7±8.4 389.1	(1) Review (2) PAC (3) AE (4) Correlation	(1) 1982MCM/GOL (2) 1989KAM/GRI (3) 1992HOL (4) 2000DEN/DEN
propan-2-ol $(CH_3)_2CHOH$ $\Delta_f H^\circ$(R) = -23.0±1 (–96.2±4.2)	94.3±2	394.6±8.4	AE	1992HOL
allyl alcohol CH_2=$CHCH_2OH$ $\Delta_f H^\circ$(R) = 0±2 (0±8.4)	(1) **81.6±1.8** (2) 80.1 (3) 85.2	**341.4±7.5** 355.1 356.5	(1) Iodination (2) PAC (3) Correlation	(1) 1973ALF/GOL (2) 1992ARN/CAL (3) 2000DEN/DEN
2-methylpropan-2-ol $(CH_3)_3COH$ $\Delta_f H^\circ$(R) = –26.8±2 (–112.1±8.4)	(1) **100±2** (2) 99.1 (3) 100.0	**418.4±8.4** 414.6 418.6	(1) Review (2) PAC (3) Correlation	(1) 1982MCM/GOL (2) 1989KAM/GRI (3) 2000DEN/DEN
penta-1,4-dien-3-ol $(CH_2$=$CH)_2CHOH$ $\Delta_f H^\circ$(R) = 22.1±2 (92.5±8.4)	89	372.4	PAC	1991CLA/CUL
cyclohexanol 	92.4	386.7	Correlation	2000DEN/DEN
benzyl alcohol $C_6H_5CH_2OH$	87.5	366.3	Correlation	2000DEN/DEN
1-phenylethanol PhMeC(OH) –**H**	88.3	369.4	Correlation	2000DEN/DEN

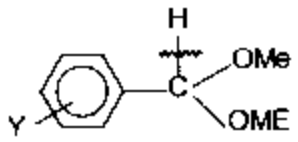
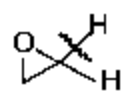
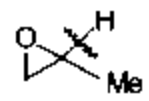
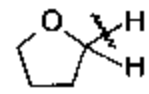
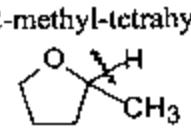
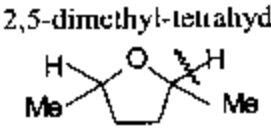
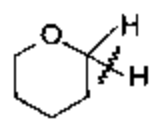
续表

断裂键 (**黑体** = 离解原子) Δ_fH°(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
diphenylmethn-1-ol Ph_2CHOH Δ_fH°(R) = 36.4±1.5 (152.3±6.3)	(1) 78 (2) **75.4±1.5**	326 **315.5±6.3**	PAC	(1) 1983ROT/SIM (2) 1992ARN/CAL
ethane-1,1-diol $CH_3CH(OH)_2$	~ 92	~ 385	Electrochemical	1991MER/LIN
ethane-1,2-diol $(CH_2OH)_2$ Δ_fH°(R) = - 52.6±2 (–220.1±8.4)	(1) 89.6±2.2 (2) **92.1** (3) 95.6	374.9±9.2 **385.3** 400.0	(1) PAC (2) AE (3) Correlation	(1) 1989KAM/GRI (2) 1992HOL (3) 2000DEN/DEN
1,4-butanediol $HOCH_2(CH_2)_2(OH)$ CH–H	95.4	399.2	Correlation	2000DEN/DEN
dimethyl ether CH_3OCH_3 Δ_fH°(R) = 0±1 (0±4.2)	(1) 95.5 (2) 93±1 (3) **96.1** (4) 95.3	399.6 389.1 **402.1** 398.7	(1) Photosensitized dissociation (2) Review (3) Review (4) Correlation	(1) 1967LOU/LAI (2) 1969GOL/BEN (3) 1999ATK/BAU (4) 2000DEN/DEN
difluoromethyl trifluoromethyl ether CHF_2OCF_3	106±1	443.5±4.2	Kinetics	1995HSU/DEM
bis(difluoromethyl) ether CHF_2OCHF_2	104±1	435.1±4.2	Kinetics	1995HSU/DEM
methyl trifluoromethyl ether CH_3OCF_3	102±1	426.8±4.2	Kinetics	1995HSU/DEM
ethyl methyl ether $CH_3OCH_2CH_3$ Δ_fH°(R) = –10.8±2 (–45.2±8 4)	93 0	389.1	AE	1991HOL/LOS
ditertbutyl ether $(CH_3)_3COC(CH_3)_3$	96.1	402.1	Correlation	2002TUM/KRO
diethyl ether $CH_3CH_2OCH_2CH_3$ Δ_fH°(R) = –19.4±1 (-81.2±4.2)	(1) 91.7±0.4 (2) **93** (3) 95.5±0.6	383.7±1.7 **389.1** 399.5±2.4	(1) VLPP (2) PAC (3) Correlation	(1) 1984KON/BEN (2) 1986BUR/MAJ (3) 2000DEN/DEN
ethyl tert-butyl ether $CH_3CH_2Ot\text{-}C(CH_3)_3$	96.9	405.4	Re-anal. of pyrolysis data	1998BRO/BEC
methyl phenyl ether CH_3OPh	92.0	385.0	Correlation	2002TUM/KRO
benzyl methyl ether, substituted 				

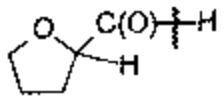
续表

断裂键 (黑体：离解原子) $\Delta_f H°$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
Y = H	85.8	359.0	Correlation	2002TUM/KRO
3-Cl	86.3	360.9		
4-Cl	85.9	359.5		
4-Me	85.4	353.2		
4-Pr	84.4	353.2		
4-MeO	84.7	354.5		
dibenzyl ether, substituted				
Y = H	85.8	359.0	Correlation	2002TUM/KRO
4- MeO	83.7	350.0		
cyclohexyl methyl ether cyclo-C_6H_{11}–OMe	89.9	376.3	Correlation	2000DEN/DEN
dimethoxymethane $(MeO)_2CH_2$	92.9	388.7	Correlation	2000DEN/DEN
diethoxymethane $(EtO)_2CH_2$	93.2	390.1	Correlation	2002TUM/KRO
diprooxymethane $(PrO)_2CH_2$	93.6	391.8	Correlation	2002TUM/KRO
dibutoxymethane $(BuO)_2CH_2$	93.3	390.2	Correlation	2002TUM/KRO
1,1-dimethoxyethane $(MeO)_2CHMe$	92.5	387.2	Correlation	2002TUM/KRO
diisopropyl ether $(CH_3)_2CHOCH(CH_3)_2$	(1) 93.9 (2) 93.7	392.9 392.2	(1) Re-anal. of pyrolysis data (2) Correlation	(1) 1998BRO/BEC (2) 2002TUM/KRO
diphenylmethyl methyl ether, substituted 				
Y = H Y' = H	84.6	354.1	Correlation	2002TUM/KRO
3-Cl 3-Cl	84.2	352.4		

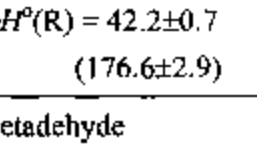
续表

断裂键 (黑体 · 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)		BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	BDEs kJ/mol	方法	文献
4-Br	4-Br	83.7	350.1		
4-Me	4-Me	82.8	346.6		
4-tBu	4-tBu	83.1	347.6		
4-MeO	4-MeO	81.9	342.8		
4-MeC(O) O	4-MeC(O) O	84.5	353.5		
dimethoxyphenylmethane, substituted 					
Y = H		84.6	353.9	Correlation	2002TUM/KRO
4-Cl		84.7	354.3		
4-Br		84.7	354.3		
4-tBu		84.4	353.1		
4-MeC(O) O		84.9	355.2		
oxirane  $\Delta_f H^\circ$(R) = 35.8±1.5 (149.8±6.3)		100.5±1.5	420.5±6.5	Pyrolysis	1984BAL/KEE
2-methyl-oxirane 		89.9	376.0	Correlation	2002TUM/KRO
tetrahydrofuran  $\Delta_f H^\circ$(R) = -4.3±1.5 (-18.0±6.3)		(1) 92±1 (2) **92.1±1.6** (3) 92 (4) 93.6±0.1	384.9±4.2 **385.3±6.7** 384.9 391.6±0.4	(1) Kinetics (2) PAC (3) PAC (4) Correlation	(1) 1982MCM/GOL (2) 1997LAA/MUL (3) 2000KRA/CIR (4) 2002TUM/KRO
2-methyl-tetrahydrofuran 		91.8	384.1	Correlation	2002TUM/KRO
2,5-dimethyl-tetrahydrofuran 		92.6	387.5	Correlation	2002TUM/KRO
2H-3,4,5,6-tetrahydropyran 		96.0	401.7	Correlation	2002TUM/KRO

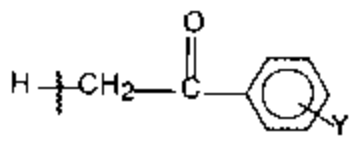
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
formaldehyde HCO–**H** $\Delta_f H^\circ$(R) = 9.96±0.20 (41.67±0.84)	(1) 88.8±0.5 (2) 88.0 (3) **88.04±0.16** (4) 88.15±0.01 (5) 88.64±0.1	371.5±2.1 368.2 **368.40±0.67** 368.80±0.03 370.86±0.28	(1) Electron impact (2) Photolysis (3) Recommended (4) Photolysis (5) Laser flash photolysis	(1) 1985TRA (2) 1987CHU/FOL (3) 1994BER/ELL (4) 1996TER/KAB (5) 1997BEC/CAR
formyl fluoride FCO-**H**	101.1	423.0	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
ethanal or acetadehyde CH_3CO–**H** $\Delta_f H^\circ$(R) = –2.4±0.2 (–10.0±0.8)	(1) 87.1±1.3 (2) 87.3±2.0 (3) 89.3±0.5 (4) **89.4±0.3** (5) 88.7	364.4±5.4 365.3±8.4 373.6±2.1 **374.0±1.3** 371.1	(1) Iodination (2) Electron impact (3) PIMS detect. (4) Recommended (5) SPST	(1) 1973ONE/BEN (2) 1984HOL/LOS (3) 1992NII/GUT (4) 1994BER/ELL (5) 1999TSA
trifluoroacetadehyde CF_3CO–**H**	91±2	380.7±8.4	Bromination	1970AMP/WHI
Propanal C_2H_5CO–**H** $\Delta_f H^\circ$(R) – –7.7±1 (–32.3±4.2)	(1) 87.4±1.0 (2) 89.5 (3) **88.7**	365.7±4.2 374.5 **371.1**	(1) Kinetics (2) Electrochem. (3) Derived	(1) 1973WAT/THO (2) 1995LUN/DAA (3) 2000ATK/BAU
Propenal CH_2=CHCO–**H** $\Delta_f H^\circ$(R) = 15.3±2 (64.0±8.4)	(1) 87±1 (2) **89.1**	364.0±4.2 **372.8**	(1) Iodination (2) Electrochem.	(1) 1973ALF/GOL (2) 1995LUN/DAA
bytanal PrC(O) **H**	88.7	371.2	Correlation	2002TUM/KRO
2-methylpropanal isoPrC(O) **H**	87.1	364.5	Correlation	2002TUM/KRO
pentanal BuC(O) **H**	88.9	372.0	Correlation	2002TUM/KRO
3-methylbytanal $(CH_3)_2CHCH_2C(O)$ **H**	86.6	362.5	Correlation	2002TUM/KRO
2-methylbytanal $C_2H_5CH(CH_3)C(O)$ **H**	86.2	360.8	Correlation	2002TUM/KRO
2,2,-dimethylpropanal tert-BuC(O) **H**	89.7	375 1	Correlation	2002TUM/KRO
2-ethylbutanal $Et_2CHC(O)$ **H**	87.8	367.2	Correlation	2002TUM/KRO
decanal $CH_3(CH_2)_8C(O)$ **H**	89.2	373.3	Correlation	2002TUM/KRO
furfurol 	90.5	378.7	Correlation	2000DEN/DEN

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 - 推荐值; 括号内数字 - 文献编号)		方法	文献
	kcal/mol	kJ/mol		
benzaldehyde C_6H_5CO-**H** $\Delta_f H^\circ$(R) = 27.8±2.6 (116.3±10.9)	(1) 86.9±1.0 (2) **88.7±2.6** (3) 88.9 (4) 83.2	363.6±4.2 **371.1±10.9** 372 0 348.0	(1) Iodination (2) PAC (3) Electrochem. (4) Correlation	(1) 1982MCM/GOL (2) 1989SIM/GRI (3) 1995LUN/DAA (4) 2002TUM/KRO
benzaldehyde, substituted 				
Y = 3-Cl	84.5	353.6	Correlation	2002TUM/KRO
4-Cl	84.2	352.3		
3-Br	84.6	353.8		
3-Me	82.9	347.0		
4-Me	82.6	345.8		
3-Bu	80.6	337.1		
4-Bu	82.6	345.4		
3-MeO	83.9	350.9		
4-MeO	82.8	346.4		
3-NO_2	82.2	343.7		
4-NO_2	81.3	340.4		
4-PhO	83.0	347.1		
2-pyenylethanal $PhCH_2C(O)$ **H**	86.5	362.0	Correlation	2002TUM/KRO
2-methy-2-phenylpropanal $PhC(CH_3)_2C(O)$ **H**	86.7	362.9	Correlation	2002TUM/KRO
ketene **H**–CH=C=O $\Delta_f H^\circ$(R) = 42.2±0.7 (176.6±2.9)	(1) 105.3±2.1 (2) **107.1**	440.6±8.8 **448.1**	(1) Recommended (2) Derived from $\Delta_f H^\circ$(R) in ref.	(1) 1994BER/ELL (2) 2000TRA
acetadehyde $CH_3C(O)$ H $\Delta_f H^\circ$(R) = 2.5±2.2 (10.5±9.2)	(1) 94.3±2.2 (2) 94.2	394.5±9.2 394.3	(1) Recommended (2) Correlation	(1) 1994BER/ELL (2) 2002TUM/KRO
acetyl chloride $CH_3C(O)$ Cl	≤101.2	≤423.4	Infrared chemilu-minescence	1998SRI/ARU

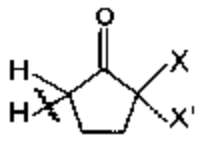
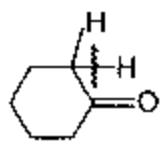
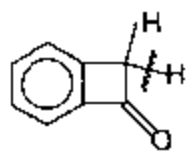
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 -- 文献编号) kcal/mol	kJ/mol	方法	文献
acetone CH_3COCH_3 $\Delta_f H^\circ$(R) = –8.1±0.7 (–33.9±3)	(1) 98.3±1.8 (2) 92±2 (3) **95.9±0.7** (4) 94 (5) 96.0±2.2	411.3±7.5 384.9±8.4 **401.2±2.9** 393.3 401.7±9.2	(1) Bromination (2) AE (3) Derived from $\Delta_f H^\circ$(R) in ref. (4) AOP (5) GPA	(1) 1970KIN/GOL (2) 1984HOL/LOS(b) (3) 2001BOU/CHA (4) 2002ALN/ZHA (5) 2003REE/HAR
ethyl methyl ketone $MeCOCH_2Me$ $\Delta_f H^\circ$(R) = –16.8±1.7 (–70.3±7.1)	(1) 92.3±1.7 (2) 93.8	386.2±7.1 392.6	(1) Iodination (2) Correlation	(1) 1970SOL/GOL (2) 2002TUM/KRO
diethyl ketone $EtCOCH_2Me$	(1) 88 (2) 94.8±0.7	368.2 396.5±2.8	(1) AOP (2) Correlation	(1) 1990BOR/HAR (2) 2002TUM/KRO
dipropyl ketone $CH_3CH_2CH_2C(O)\ CH_2CH_2CH_3$	94.3±0.8	394.6±3.3	Correlation	2002TUM/KRO
dibutyl ketone $CH_3CH_2CH_2CH_2C(O)\ C4H_9$	94.6±0.6	395.8±2.4	Correlation	2002TUM/KRO
isopropyl methyl ketone $MeCOCHMe_2$	91.7	383.8	Correlation	2002TUM/KRO
diisopropyl ketone $(CH_3)_2CHC(O)\ CH(CH_3)_2$	92.6±0.5	387.5±1.9	Correlation	2002TUM/KRO
isobutyl methyl ketone $CH_3C(O)\ CH_2CH(CH_3)_2$	92.9	388.7	Correlation	2002TUM/KRO
methyl tert-butyl ketone CH_3COtBu $\Delta_f H^\circ$(R) = –27.6±3 (–115.5±12.6)	(1) 94 (2) 93.9	393.3 392.9	AOP	(1) 1990BOR/HAR (2) 2002ALN/ZHA
methyl phenyl ketone, substituted 				
Y = H $\Delta_f H^\circ$(R) = 20.2±3 (84.5±12.6)	(1) 93 (2) 93.3 (3) 96.3±0.9	389.1 390.4 402.8±3.6	(1) AOP (2) AOP (3) Correlation	(1) 1990BOR/ZHA (2) 2002ALN/ZHA (3) 2002TUM/KRO
p-NO2	(4) 89	372.4	(4) AOP	(4) 1995ZHA/BOR
p-CN	(5) 93.4	390.8	(5) AOP	(5) 2002ALN/ZHA
p-MeO	(5) 93.3	390.4		
methyl trimethylphenyl ketone $CH_3CO(C_6H_2(Me)_3)$	93.8	392.5	AOP	2002ALN/ZHA

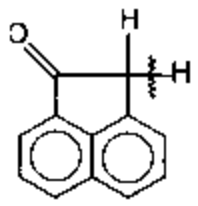
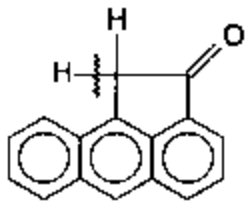
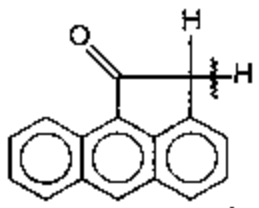
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methyl naphthyl-1 ketone CH_3CO(1-naphthyl)	94	393.3	AOP	2002ALN/ZHA
methyl anthracenyl-9 ketone CH_3CO(9-anthracenyl)	94	393.3	AOP	2002ALN/ZHA
methyl phynel ketone bromide $PhCOCH_2H^+Br$	93.2	390	AOP	1997CHE/LIU
ethyl ethyl ketone $CH_3CH_2COCH_2CH_3$	88.4	369.9	AOP	2002ALN/ZHA
methyl benzyl ketone CH_3COCH_2Ph	83	347.3	AOP	2002ALN/ZHA
ethyl phenyl ketone $MeCH_2COPh$ $\Delta_f H^\circ$(R) = 9.9±5 (41.4±20.9)	(1) 88 (2) 92.9 (3) 94.3	368.2 388.7 394.4	(1) AOP (2) Re-anal. of pyrolysis data (3) Correlation	(1) 1990BOR/HAR (2) 1998BRO/BEC (3) 2002TUM/KRO
propyl phenyl ketone $EtCH_2COPh$	94.2	394.3	Correlation	2002TUM/KRO
nonanyl phenyl ketone $CH_3(CH_2)_7CH_2C(O)$ Ph	94.2	394.3	Correlation	2002TUM/KRO
tert-butyl phenyl ketone $(CH_3)_3CC(O)$ Ph	98.8	413.3	Correlation	2002TUM/KRO
isopropyl phenyl ketone $(CH_3)_2CHC(O)$ Ph	92.1	385.3	Correlation	2002TUM/KRO
sec-butyl phenyl ketone $(CH_3)_2CHCH_2C(O)$ Ph	92.1	385.2	Correlation	2002TUM/KRO
benzyl methyl ketone $PhCH_2COMe$	(1) 82.3 (2) 82.6	344.3 345.6	AOP	(1) 1992BOR/JI (2) 2002ALN/ZHA
benzyl phenyl ketone $PhCH_2COPh$	(1) 82.5 (2) 82.7	345.2 346 0	AOP	(1) 1990BOR/HAR (2) 2002ALN/ZHA
dibenzyl ketone $PhCH_2COCH_2Ph$ $\Delta_f H^\circ$(R) = 32.1±3 (134.3±12.6)	(1) 83 (2) 87.1	347.3 364.5	(1) AOP (2) Correlation	(1) 1990BOR/HAR (2) 2000DEN/DEN
propylphenyl phenyl ketone $PhCH_2CH_2COPh$	88.5	370.3	AOP	1990BOR/HAR
anthracenyl-2 phenyl ketone $PhCOCH_2$Anth(2)	81.6	341.4	AOP	2002ALN/ZHA
anthracenyl-9 phenyl ketone $PhCOCH_2$Anth(9)	84.4	353.1	AOP	2002ALN/ZHA
naphthyl-1 phenyl ketone $PhCOCH_2$Naphth(1)	83	347.3	AOP	2002ALN/ZHA
naphthyl-2 phenyl ketone $PhCOCH_2$Naphth(2)	82.7	346.0	AOP	2002ALN/ZHA

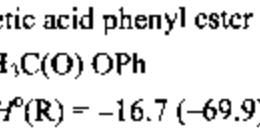
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
phenyl pyrenyl-1 ketone PhCOC**H**$_2$Py(1)	80.7	337.6	AOP	2002ALN/ZHA
phenyl phenathrenyl-2 ketone PhCOC**H**$_2$Phen(2)	83.2	348.1	AOP	2002ALN/ZHA
phenyl phenathrenyl-3 ketone PhCOC**H**$_2$Phen(3)	83.3	348.5	AOP	2002ALN/ZHA
phenyl phenathrenyl-9 ketone PhCOC**H**$_2$Phen(9)	83.9	351.0	AOP	2002ALN/ZHA
phenyl pyridyl ketone PhCOC**H**$_2$Py	85.7	358.6	AOP	2002ALN/ZHA
chromium tricarbonyl complexes PhCOC**H**$_2$Ph(Cr(CO)$_3$)	83.6	349.8	AOP	2002ALN/ZHA
diiso-propyl ketone $Me_2CHCOCHMe_2$ $\Delta_f H^\circ$(R) = –41.5±5 (–173.6±20.9)	(1) 85 (2) 93.6	355.6 391.5	(1) AOP (2) Correlation	(1) 1990BOR/HAR (2) 2000DEN/DEN
iso-propyl phenyl ketone PhCOC**H**Me_2	(1) 86 (2) 87.2 (3) 89.9	359.8 365.0 376.1	(1) AOP (2) Correlation (3) Re-anal. of pyrolysis data	(1) 1990BOR/HAR (2) 2000DEN/DEN (3) 1998BRO/BEC
diphenylmethyl methyl ketone Ph_2C**H**COCH_3	(1) 82 (2) 82.2	343.1 343.9	AOP	(1) 1990BOR/HAR (2) 2002ALN/ZHA
diphenylmethyl phenyl ketone Ph_2C**H**COPh	83	347.3	AOP	1990BOR/HAR
cyclopentanone, substituted  X = H, X′ = H $\Delta_f H^\circ$(cyclopentanonyl) = –10±3 (–41.8±12.6)	(1) 88 (2) 95.9	368.2 401.2	(1) AOP (2) Correlation	(1) 1991BOR/GAL (2) 2002TUM/KRO
Me Me	(1) 89	372.4		
cyclohexanone 	94.2	394.1	Correlation	2002TUM/KRO
2-hydrocyclobuta[2,1-a]-benzen-1-one 	91±3	380.7±12.6	GPA	2002KAS/BRO

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1-acenaphthenone 	82.3	344.3	AOP	2002ALN/ZHA
2-aceanthrenone 	82.5	345.2	AOP	2002ALN/ZHA
1-aceanthrenone 	80	334.7	AOP	2002ALN/ZHA
formic acid **H**–C(O) OH $\Delta_f H^\circ$(R) = –46.5±0.7 (–194.6±2.9)	(1) 98 (2) 93.2 (3) >89.5 (4) **96.6** (5) ≥96.1±0.7	410.0 389.9 >374.5 **404.2** ≥402.1±2.9	(1) Correlation (2) Electron impact (3) Review (4) Review (5) Photoionization, revised	(1) 1973MCK/DUN (2) 1991HOL/LOS (3) 1994BER/ELL (4) 1994BER/ELL (5) 2000RUS/LIT
acetic ion $CH_3C(O)O^-$	(1) 91 9±1 7 (2) 96.1 (3) 93.7±4 (4) ~ **95**	384.5±7.1 402 392.0±16.7 **~397.5**	(1) PAC (2) Derived (3) CID (4) Review	(1) 1989KAM/GRI (2) 1994YU/RAU (3) 1994WEN/SQU(b) (4) 2002REE/KAS
acetic acid $CH_3C(O)OH$ $\Delta_f H^\circ(R) = -60.2\pm2.9$ (–251.9±12.0)	(1) 96.1 (2) 93.9±2 (3) **95.3±2.9** (4) 95.9 (5) 98.7±0.8	402.1 392.9±8.4 **398.7±12.1** 401.3 413.0±3.3	(1) Correlation (2) AE (3) CID (4) Correlation (5) Calorimetry	(1) 1984NON/WAL (2) 1991HOL/LOS (3) 1994WEN/SQU(b) (4) 2000DEN/DEN (5) 2001LAG/DIO
chloroacetic acid $ClCH_2C(O)OH$	(1) 95.3 (2) 91.0±0.9	398.9 380.7±3.9	(1) Correlation (2) Combination	(1) 2002TUM/KRO (2) 2002LAG/DIO
carboxylic acid $CH_3(CH_2)_nCH_2C(O)OH$				
n – 0	95.3	398.8	Correlation	2002TUM/KRO
1	95.3	398.7		
2	95.5	399.4		
3	95.5	399.4		
4	95.4	399.1		
7	95.4	399.1		

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值: 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1-methyl propanoic acid $(CH_3)_2$**C**HC(O) OH	93.0	389.0	Correlation	2000DEN/DEN
2,2-dimethlpropanioc acid $(CH_3)_3$CC(O) OH	99.2	415.2	Correlation	2002TUM/KRO
cyclohexacarboxylic acid 	93.0	389.0	Correlation	2000DEN/DEN
benzenacetic acid Ph**C**H$_2$C(O) OH	87.7	367.0	Correlation	2002TUM/KRO
glycolic acid (OH) **C**H$_2$C(O) OH	95.1	397.8	Correlation	2002TUM/KRO
2-hydroxyacetic acid CH$_3$**C**H(OH) C(O) OH	92.2	385.8	Correlation	2002TUM/KRO
2,2-dimethyl-propanoic acid $(CH_3)_3$CC(O) OH	99.2	415.1	Correlation	2000DEN/DEN
methyl formate **H**–C(O) OCH$_3$ $\Delta_f H^\circ$(R) = –40.5±2 (–169.5±8.4)	(1) 92.7±1 (2) 95.4±2	387.9±4.2 399.2±8.4	(1) Kinetics (2) Electron impact	(1) 1969SOL/BEN (2) 1991HOL/LOS
acetic acid methyl ester CH$_3$**C**(O) OCH$_3$ $\Delta_f H^\circ$(R) = –56 6±2 (–236.8±8.4)	(1) 93.9 (2) 97.1±2.5 (3) 96.6	392.9 406.3±10.5 404.0	(1) Electron impact (2) FT-ICR (3) Correlation	(1) 1991HOL/LOS (2) 2002KAR/JAN (3) 2002TUM/KRO
acetic acid methyl ester CH$_3$C(O) OC**H**$_3$	96.7	404.6	Correlation	2000DEN/DEN
acetic acid ethyl ester CH$_3$**C**(O) OCH$_2$CH$_3$ $\Delta_f H^\circ$(R) = –62.2±3 (–260.2±12.6)	(1) 96 (2) 95.5	401.7 399.5	(1) AOP (2) Correlation	(1) 1995BOR/ZHA (2) 2000DEN/DEN
acetic acid isopropyl ester CH$_3$C(O) OC**H**(CH$_3$)$_2$	93.8	392.3	Correlation	2000DEN/DEN
methyl benzoate PhC(O) OC**H**$_3$	100.0	418.4	Correlation	2002TUM/KRO
acetic acid phenyl ester CH$_3$C(O) OPh $\Delta_f H^\circ$(R) = –16.7 (–69.9)	100.2±1.3	419.2±5.4	Iodination	1973ALF/GOL
oxalic acid dimethyl ester CH$_3$C(O) OC(O) OC**H**$_3$	96.5	403.8	Correlation	2000DEN/DEN
acetic acid anhydride CH$_3$C(O) OC(O) C**H**$_3$	97.0	406.0	Correlation	2000DEN/DEN
ethyl propanoate CH$_3$C**H**$_2$C(O) OEt	95.6	400.0	Re-anal. of pyrolysis data	1998BRO/BEC

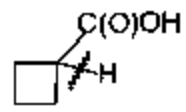
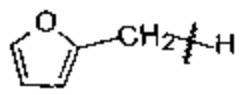
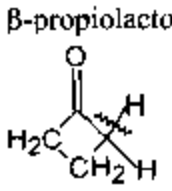
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断裂键 (**黑体** - 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methyl bytanoate $CH_3CH_2CH_2C(O)OCH_3$	94.4	394.9	Correlation	2002TUM/KRO
methyl pebtanoate $CH_3(CH_3)_2CH_2C(O)OCH_3$	94.4	394.9	Correlation	2002TUM/KRO
ethyl pebtanoate $CH_3(CH_3)_4C(O)OCH_2CH_3$	94.1	394.5	Correlation	2002TUM/KRO
propyl pebtanoate $CH_3(CH_3)_4C(O)OCH_2CH_2CH_3$	93.7	392.1	Correlation	2002TUM/KRO
isopropyl pebtanoate $CH_3(CH_3)_4C(O)OCH(CH_3)_2$	92.7	87.9	Correlation	2002TUM/KRO
tert-butyl-2,2-dimethylpropanoate $(CH_3)_3C(O)OC(CH_3)_3$	99.2	415.0	Correlation	2002TUM/KRO
octyl pentanoate $C_4H_9C(O)O\text{-}CH_2C_7H_{15}$	93.7	391.9	Correlation	2002TUM/KRO
ethyl 2-phenylacetate $PhCH_2C(O)OEt$	(1) 84.0 (2) 88.6	351.5 370.7	(1) AOP (2) Re-anal. of pyrolysis data	(1) 1994ZHA/BOR(e) (2) 1998BRO/BEC
2-methoxy-1-phenylethan-1-one $PhCOCH_2OMe$	81	338.9	AOP	1990BOR/HAR
2-ethoxy-1-phenylethan-1-one $PhCOCH_2OEt$	80.6	337.2	AOP	1994BOR/ZHA
1-phenyl-2-phenoxyethan-1-one $PhCOCH_2OPh$	80.6	337.2	AOP	1994BOR/ZHA
butane-2,3-dione $CH_3C(O)C(O)CH_3$	98.4	411.6	Correlation	2002TUM/KRO
pentane-2,4-dione $CH_2(COMe)_2$	(1) 91.6 (2) 87.7 (3) 95.4±0.6	383.3 366.9 399.1±2.7	(1) AOP (2) Re-anal. of pyrolysis data (3) Correlation	(1) 1995BOR/ZHA (2) 1998BRO/BEC (3) 2002TUM/KRO
1,3-diphenylpropane-1,3-dione $CH_2(COPh)_2$	(1) 93 (2) 92	389.1 384.9	AOP	(1) 1990BOR/HAR (2) 1991BOR/HAR
ethyl methyl butane-1,4-dioate $CH_2(COMe)(C(O)OEt)$	92.9	388.7	AOP	1995BOR/ZHA
2-oxoacetic acid $H(O)CC(O)OH$	89.7	375.3	Correlation	2002TUM/KRO
propanedioic acid $CH_2(C(O)OH)_2$	95.6	400.1	Correlation	2002TUM/KRO
butanedioic acid $HO(O)CCH_2CH_2C(O)OH$	95.1	397.8	Correlation	2002TUM/KRO

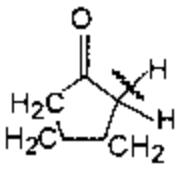
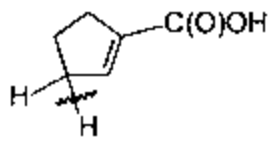
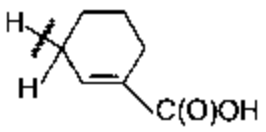
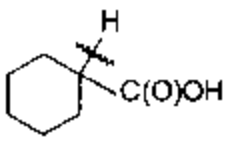
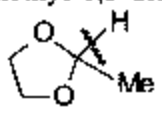
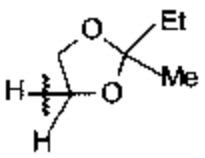
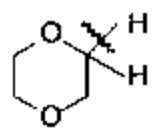
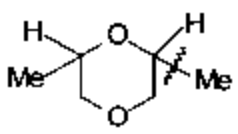
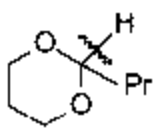
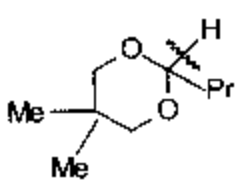
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断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 · 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
carboxylic acid, substituted iPrOC(O) $(CH_2)_n$**C**H_2C(O) OH				
n = 1	94.0	393.1	Correlation	2002TUM/KRO
3	93.6	391.5		
4	93.5	391.3		
7	93.5	391.3		
2-hydroxypropanedioic acid HO(O) CC**H**(OH) C(O) OH	93.9	392.7	Correlation	2002TUM/KRO
diethyl ethane-1,2-dioate $CH_3CH_2OC(O)$ C(O) O**C**H_2CH_3	94.7	396.2	Correlation	2002TUM/KRO
malonic acid dimethyl ester CH_2(MeOC(O))$_2$	(1) 90.5 (2) 93.6	378.7 391.7	(1) AOP (2) Correlation	(1) 1991BAU/FAS(c) (2) 2002TUM/KRO
ethyl 3-oxobutanoate **C**H_2(C(O) Me) (C(O) OEt)	94.8	396.5	Correlation	2002TUM/KRO
ethyl methyl propane-1,3-dioate **C**H_2(C(O) OEt) (C(O) OMe)	92.3	386.2	AOP	1996ZHA/BOR
oxilic axcid diethyl ester **C**H_2(C(O) OEt)$_2$	(1) 95 (2) 94.8	397.5 396.5	(1) AOP (2) Correlation	(1) 1993ZHA/BOR (2) 2000DEN/DEN
dimethyl bytane-1,4-dioate (**C**H_2C(O) OCH_3)$_2$	96.7	404.8	Correlation	2002TUM/KRO
dimethyl pentane-1,5-dioate CH_2(**C**H_2C(O) OCH_3)$_2$	94.0	393.1	Correlation	2002TUM/KRO
dimethyl heptane-1,7-dioate $CH_2(CH_2$**C**H_2C(O) OCH_3)$_2$	94.0	393.2	Correlation	2002TUM/KRO
dimethyl nonane-1,9-dioate $CH_2(CH_2CH_2$**C**H_2C(O) OCH_3)$_2$	93.8	392.6	Correlation	2002TUM/KRO
1-phenylbutane-1,3-dione PhCOC**H**$_2$COMe	92	384.9	AOP	1990BOR/HAR
3-methylpentane-2,4-dione (Me) C**H**(COMe)$_2$	84.7	354.4	Re-anal. of pyrolysis data	1998BRO/BEC
dimethyl 2-methyl propane-1,3-dioate MeC**H**(C(O) OMe)$_2$	(1) 90.5 (2) 90.8	378.7 379.9	AOP	(1) 1994ZHA/BOR(e) (2) 1996ZHA/BOR
ethyl 2-methylpropanoate Me_2C**H**C(O) OEt	92.6	387.4	Re-anal. of pyrolysis data	1998BRO/BEC
ethyl methyl 2-ethyl propane-1,3-dioate EtC**H**(C(O) OEt) (C(O) OMe)	89.6	374.9	AOP	1996ZHA/BOR
diethyl 2-ethyl propane-1,3-dioate EtC**H**(C(O) OEt)$_2$	91.5	382.8	AOP	1996ZHA/BOR

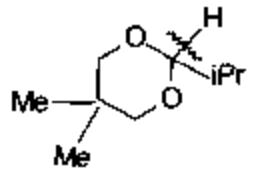
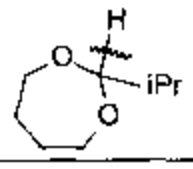
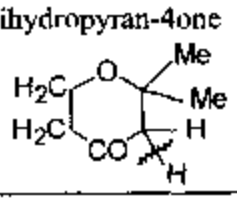
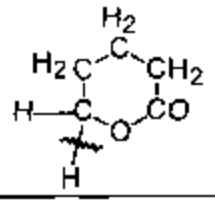
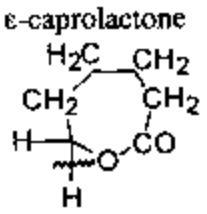
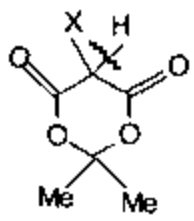
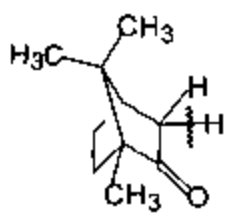
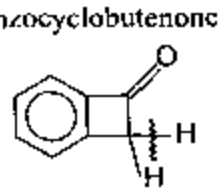
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H°$(R) /kcal (kJ)	BDEs (**黑体** 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
dimethylethyl ethane-1,2-dioate $(Me_2CHOC(O))_2$	94.7	396.2	Correlation	2002TUM/KRO
dimethylethyl butane 1,4-dioate $(Me_2CHOC(O)CH_2)_2$	94.5	395.5	Correlation	2002TUM/KRO
dimethylethyl pentane 1,5-dioate $CH_2(Me_2CHOC(O)CH_2)_2$	93.6	391.7	Correlation	2002TUM/KRO
dimethylethyl heptane 1,7-dioate $CH_2(Me_2CHOC(O)CH_2CH_2)_2$	93.5	391.2	Correlation	2002TUM/KRO
dimethylethyl decane 1,10-dioate $(Me_2CHOC(O)(CH_2)_4)_2$	93.5	391.1	Correlation	2002TUM/KRO
diethoxy 2-phenylpropane-1,3-dione $PhCH(C(O)OEt)_2$	85.3	356.9	AOP	1993ZHA/BOR
ethyl 2-phenylpropanoate PhCHMe(C(O)OEt)	85.6	358.2	Re-anal. of pyrolysis data	1998BRO/BEC
dimethyl ethane-1,2-dioate $CH_3OC(O)C(O)OCH_3$	96.5	404.0	Correlation	2000DEN/DEN
2,3,4,5-tetrahydroxypentanal $CH_2(OH)(CHOH)_3C(O)$ **H**	88.4	370.0	Correlation	2002TUM/KRO
2,3,4,5,6-penta-hydroxyhexanal $CH_2(OH)(CHOH)_4C(O)$ **H**	88.7	371.1	Correlation	2002TUM/KRO
diethyl 2-(1,1-dimethyl-1silaethyl) propane-1,3-dioate $Me_3SiCH_2CH(CO_2Et)_2$	87.3	365.3	AOP	1996ZHA/BOR
ethyl methyl 2-(1,1-dimethyl-1silaethyl) propane-1,3-dioate $Me_3SiCH(CO_2Et)(CO_2Me)$	85.2	365.5	AOP	1996ZHA/BOR
cyclobutacarboxylic acid 	93.2	390.0	Correlation	2002TUM/KRO
2-methyl furan 	86.5±2	361.9±8.4	VLPP	1981STE
β-propiolactone 	99.4±2.3	415.9±9.6	FT-ICR	2002KAR/JAN

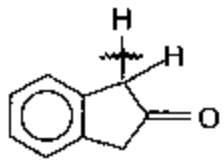
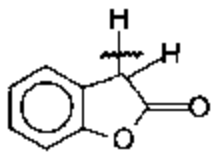
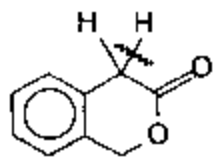
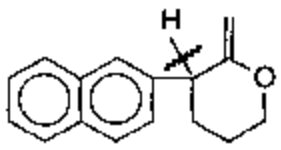
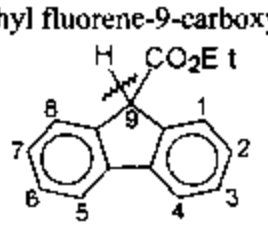
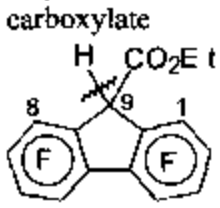
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
γ-butyrolactone 	94.8±2.3	396.6±9.6	FT-ICR	2002KAR/JAN
cyclopen-1-enecarboxylic acid 	86.0	359.8	Correlation	2002TUM/KRO
cyclohex-1-enecarboxylic acid 	88.4	370.0	Correlation	2002TUM/KRO
cyclohexanecaroxylic acid 	92.8	388.2	Correlation	2002TUM/KRO
2-methyl-1,3-dioxolate 	90.1	377.1	Correlation	2002TUM/KRO
2-(methylethyl) -1,3-dioxolate 	91.2	381.7	Correlation	2002TUM/KRO
1,4-dioxane  $\Delta_f H^\circ$(R) = - 31.5±3 (–131 8±12.6)	(1) 96 (2) 96.9±0.2	401.7 405.4±0.7	(1) PAC (2) Correlation	(1) 2000KRA/CIR (2) 2002TUM/KRO
2,5-dimethyl- 1,4-dioxane 	89.2	373.0	Correlation	2002TUM/KRO
2-propyl-1,3-dioxane 	90.2	377.7	Correlation	2002TUM/KRO
5,5-dimethyl-2-(propyl) -1,3-dioxane 	91.3	382.0	Correlation	2002TUM/KRO

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
5,5-dimethyl-2-(methylethyl) -1,3-dioxane 	91.3	382.0	Correlation	2002TUM/KRO
2,2-methylethyl-1,3-dioxepane 	90.4	378.2	Correlation	2002TUM/KRO
2,2-dimethyl-2H-3,5,6-trihydropyran-4one 	93.1	389.6	Correlation	2002TUM/KRO
δ-valerolactone 	89.2±2.3	373.2±9.6	FT-ICR	2002KAR/JAN
ε-caprolactone 	92.8±2.4	388.3±10.0	FT-ICR	2002KAR/JAN
2,2-dimethyl-1,3-dioxane-4,6-dione 				
X = H	92.6	387.4	AOP	1994ZHA/BOR(e)
Me	87.5	366.1		
1,7,7-trimethyl bicyclo(2.2.1) heptane-2-one 	95	397.5	AOP	1991BOR/JI
benzocyclobutenone 	90.5±3.1	378.7±13.0	FT-MS	1999BRO/KAS

续表

断裂键 (**黑体** 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
indan-2-one 	79.1	331.0	AOP	1994ZHA/BOR(e)
3-hydrobenzo(b) furan-2-one 	80.1	335.1	AOP	1994ZHA/BOR(e)
isochroman-3-one 	83.4	348.9	AOP	1994ZHA/BOR(e)
3-(2-naphthyl) -3H-4,5,6,-trihydropyran-2-one 	81.8	342.3	AOP	1994ZHA/BOR(e)
ethyl fluorene-9-carboxylate 	76.1	318.4	AOP	1993BOR/ZHA(b)
ethyl octafluoro-fluorene-9-carboxylate 	80.7	337.6	AOP	1993BOR/ZHA(b)

4.6.2 α位是—N、—CN、—NO、—NO_2、—NN的C—H键

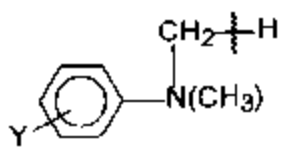
表 4.6.2 α位是—N、—CN、—NO、—NO_2、—NN 的碳氢化合物内的 C—H BDEs

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
methylamine CH_3NH_2 $\Delta_f H^\circ$(R) = 36.3±2 (151.9±8.4)	(1) 93±2.5 (2) 96.6 (3) **93.9±2** (4) 88.7	389.1±10.5 404.2 **392.9±8.4** 371.1	(1) VLPP (2) SPST (3) Electron impact (4) VLPP	(1) 1975KIN/GOD (2) 1981TSA (3) 1983BUR/CAS (4) 1984GRE/COL
2-azaprop-1-ene $CH_3N{=}CH_2$	97.5±3.5	407.9±14.6	VLPP	1993LAZ/PAP

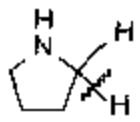
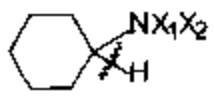
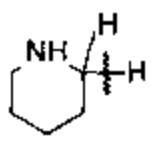
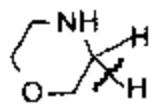
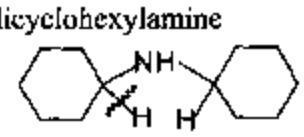
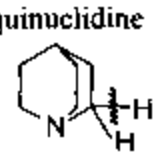
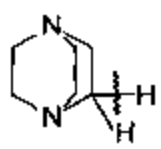
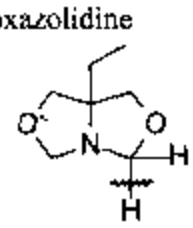
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
ethylamine $CH_3C\mathbf{H}_2NH_2$ $\Delta_f H^\circ$(R) = 26.7±2 (111.7±8.4)	(1) 94.0 (2) **90.1±2** (3) 97.1	393.3 **377.0±8.4** 406.3	(1) SPST (2) Electron impact (3) Re-anal. of pyrolysis data	(1) 1981TSA (2) 1983BUR/CAS (3) 1998BRO/BEC
propylamine $C_2H_5C\mathbf{H}_2NH_2$	(1) **91±2** (2) 93.1±2	**380.7±8.4** 389.5±8.4	PAC	2002LAL/ALL
butylamine $nC_3H_7C\mathbf{H}_2NH_2$	94±2	393.3±8.4	PAC	2002LAL/ALL
pentylamine $nC_4H_9C\mathbf{H}_2NH_2$	(1) **90.5±2** (2) 95.5±2	**387.7±8.4** 399.6±8.4	PAC	2002LAL/ALL
ethanolamine $HOCH_2C\mathbf{H}_2NH_2$	90.7±2	379.5±8.4	PAC	2002LAL/ALL
diethylamine $(CH_3C\mathbf{H}_2)_2NH$	(1) 87±2 (2) 88.6±2	364.0±8.4 370.7±8.4	PAC	2002LAL/ALL
dibutylamine $(nC_3H_7CH_2)_2NH$	(1) **90.8±2** (2) 88.9±2	**379.9±8.4** 372.0±8.4	PAC	2002LAL/ALL
dipentylamine $(nC_4H_9CH_2)_2NH$	91.9±2	384.5±8.4	PAC	2002LAL/ALL
triethylamine $(C_2H_5)_2NC\mathbf{H}_2CH_3$ $\Delta_f H^\circ$(R) = 16.4±0.5 (68.6±2.1)	(1) 85.0 (2) 91.1±2.4 (3) **90.7±0.4** (4) 89 (5) 91.2±2	355.6 381±10 **379.5±1.7** 372.4 381.6±8.4	(1) SPST (2) PAC (3) PAC (4) PAC (5) PAC	(1) 1981TSA (2) 1997WAY/CLA (3) 1999DOM/DIN (4) 2000KRA/CIR (5) 2002LAL/ALL
tripropylamine $(C_2H_5CH_2)_3N$	(1) 89±2 (2) **90±2**	372.4±8.4 **376.6±8.4**	PAC	2002LAL/ALL
triisobytulamine $((CH_3)_2CCH_2)_3N$	92.8±2	388.3±8.4	PAC	2002LAL/ALL
tributylamine $(nBu)_2NCH_2(nPr)$	(1) **91.1±2.4** (2) 89.5±2	**381±10.0** 374.5±8.4	PAC	(1) 1997WAY/CLA (2) 2002LAL/ALL
triisopropylamine $((CH_3)_2CH)_3N$	92.5±2	387.0±8.4	PAC	2002LAL/ALL
iso-propylamine $(CH_3)_2CHNH_2$ $\Delta_f H^\circ$(R) = 16.7±2 (69.9±8.4)	(1) 95.2 (2) **88.9±2** (3) 94.2	398 3 **372.0±8.4** 394.1	(1) SPST (2) Electron impact (3) Re-anal. of pyrolysis data	(1) 1981TSA (2) 1983BUR/CAS (3) 1998BRO/BEC
dimethylamine CH_3NHCH_3 $\Delta_f H^\circ$(R) = 30.5±2 (127.6±8.4)	87±2	364.0±8.4	Electron impact	1981GRI/LOS
trimethylamine $(CH_3)_3N$ $\Delta_f H^\circ$(R) = 33.2±2 (138.9±8.4)	(1) 84±2 (2) 87.0±1.0 (3) 87.5 (4) 88.9±2.4 (5) **91±2**	351.5±8.4 364.0±4.2 366.1 372±10.0 **380.7±8.4**	(1) Electron impact (2) VLPP (3) PAC (4) PAC (5) PAC, revised	(1) 1981GRI/LOS (2) 1984GRE/COL (3) 1993CLA/WAY (4) 1997WAY/CLA (5) 1999LAA/MUL

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
tert-butyldimethylamine t-BuN(CH_3)$_2$	90.0±2	376.6±8.4	PAC	1999DOM/DIN
methyldiethanolamine ((HOCH_2CH_2)$_2$(CH_3)) N	87.1±2	364.4±8.4	PAC	2002LAL/ALL
triethanolamine (HOCH_2CH_2)$_3$N	90.8±2	379.9±8.4	PAC	2002LAL/ALL
triisopropanolamine ((HOCH_2)C**H**(CH_3))$_3$N	(1) **90.8±2** (2) 93.2±2	**379.9±8.4** 389.9±8.4	PAC	2002LAL/ALL
phynelmethylamine PhCH_2NH_2	88.0	368.2	Correlation	2000DEN/KHU
dimethylbenzylamine PhCH_2N(CH_3)$_2$	84.9	355.3	Correlation	2000DEN/KHU
phenyldiethylamine PhN(C**H**$_2$$CH_3$)$_2$	91.6±1.0	383.3±4.2	PAC	1999DOM/DIN
diphenylmethylamine Ph_2NC**H**$_3$	90.7±0.4	379.5±1.7	PAC	1999DOM/DIN
phenyldibenzylamine PhN(CH_2Ph)$_2$	85.4±2.1	357.3±8.8	PAC	1999DOM/DIN
tribenzylamine N(CH_2Ph)$_3$	(1) 89.1±0.6 (2) 86.3	372.8±2.5 361.1	(1) PAC (2) Correlation	(1) 1999DOM/DIN (2) 2000DEN/KHU
phenyldiallylamine PhN(C**H**$_2$CH=CH_2)$_2$	81.1±0.7	339.3±2.9	PAC	1999DOM/DIN
triallylamine N(CH_2CH=CH_2)$_3$	82.6±0.8	345.6±3.3	PAC	1999DOM/DIN
methylhydrazine H_2NNH(CH_3)	98	410	Pyrolysis	1964EBE
1,1-dimethylhydrazine HNN(CH_3)$_2$	98	410	Pyrolysis	1964EBE
N,N-dimethylaniline, substituted  				
Y = H $\Delta_f H^\circ$(R, for Y = H) = 63.6±3 (266.1±12.6)	(1) 91.7±1.3 (2) 85.7	383.7±5.4 358.4	(1) PAC (2) Correlation	(1) 1999DOM/DIN (2) 2000DEN/KHU
4-Cl	(1) 89.8±1.4	375.7±5.9		
4-Me	(1) 89.9±2.5	376.1±10.5		
4-CF_3	(1) 92.2±1.7	385.8±7.1		

续表

断裂键 (**黑体**　离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
2-tBu	(1) 94.7±1.3	396.2±5.4		
2,2-Me_2	(1) 90.2±1.5	377.4±6.5		
pyrrolidine  $\Delta_f H^\circ$(R) = 34.1±3 (142.7±12.6)	(1) 90.1±2.4 (2) 87	377±10.0 364.0	PAC	(1) 1997WAY/CLA (2) 2000KRA/CIR
cyclohexalamine, substituted 				
X_1 = H　X_2 = H	94.6	395.9	Correlation	2000DEN/KHU
H　Me	89.8	375.9		
Me　Me	88.1	368.6		
piperidine  $\Delta_f H^\circ$(R) = 28.6 (119.7)	(1) 89.5 (2) 92.0±2.4 (3) 90.7	374.5 385±10.0 379.6	(1) PAC (2) PAC (3) Correlation	(1) 1993CLA/WAY (2) 1997WAY/CLA (3) 2000DEN/KHU
morpholine 	(1) 90.8 (2) 93.0±2.4 (3) 94 (3) **92±2**	379.9 389±10.0 393.3 **384.9±8.4**	PAC	(1) 1993CLA/WAY (2) 1997WAY/CLA (3) 1999LAA/MUL (3) 2002LAL/ALL
dicyclohexylamine 	89.6	374.9	Correlation	2000DEN/KHU
quinuclidine 	96.2±2	402.5±8.4	PAC	2002LAL/ALL
1,4-diazabicyclo(2.2.2) octane 	(1) 93 (2) 93.8±2	389.1 392.5±8.4	(1) Electrochem. (2) PAC	(1) 2000ZHE/EVE (2) 2002LAL/ALL
7a-ethyl-1H,3H,5H,7H-1,3-oxazolidino-(3,4-C) 1,3-oxazolidine 	89.3±4	373.6±16.7	PAC	2002LAL/ALL

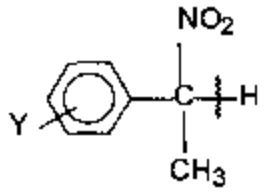
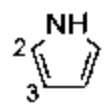
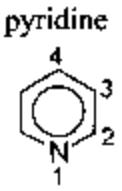
续表

断裂键 (黑体 = 离解原子) Δ_fH°(R) /kcal (kJ)	BDEs (黑体 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
methyl isocyanide **H**–CH_2NC Δ_fH°(R) = 78.0±2.7 (326.4±11.3)	91.0±2.1	380.7±8.8	PES	1987MOR/ELL(b)
methanenitrile **H**–CN Δ_fH°(R) = 105.5±1.1 (441.4±4.6)	(1) 126.1±0.4 (2) **126.3±0.2**	527.6±1.7 **528.5±0.8**	(1) Recommend. (2) Photolysis	(1) 1994BER/ELL (2) 2000COO/LAN
acetonitrile CH_3**C**N Δ_fH°(R) = 60.4±1 (252.6±4.2)	(1) 93±2.5 (2) 94.8±2.1 (3) **96** (4) 97.0±1 (5) 94.8±2.1	389.1±10.5 396.6±8.8 **401.7** 405.8±4.2 396.6±8.8	(1) Review (2) PES (3) PAC (4) Negative ion cycle (5) GPA	(1) 1982MCM/GOL (2) 1987MOR/ELL(b) (3) 1995WAY/LUS (4) 2000LAF/SZA (5) 2003REE/HAR
propanenitrile CH_3CH_2**C**N Δ_fH°(R) = 54.2±3 (226.7±12.6)	(1) 89.8±2.3 (2) **94.0±3** (3) 90±2 (4) 94.9	375.7±9.6 **393.3±12.6** 376.6±8.4 397.1	(1) VLPP (2) Derived from Δ_fH° in ref. (3) AP (4) Re-anal. of pyrolysis data	(1) 1975KIN/GOD (2) 1986PED/NAY (3) 1993HOL/LOS (4) 1998BRO/BEC
phenylacetonitrile PhCH_2CN	82.3	344.3	AOP	1993BOR/ZHA(b)
pentafluorophenyl acetonitrile $C_6F_5CH_2$CN	83.8	350.6	AOP	1993BOR/ZHA(b)
methae-1,1-dicarbonitrile $CH_2(CN)_2$	(1) 90 (2) 87.6	376.6 366.5	(1) AOP (2) Re-anal. of pyrolysis data	(1) 1991BOR/CHE (2) 1998BRO/BEC
2-aminoethanenitrile CH_2(CN) (NH_2)	84.9	355.2	Re-anal. of pyrolysis data	1998BRO/BEC
2-methylpropanenitrile $(CH_3)_2$**C**HCN Δ_fH°(R) = 45.5±3 (190.4±12.6)	(1) 86.5±2 (2) 91.9	361.9±8.4 384.5	(1) VLPP (2) Re-anal. of pyrolysis data	(1) 1976KIN/GOD (2) 1998BRO/BEC
diphenylacetonitrile Ph_2**C**HCN	(1) 77.5 (2) 76.8	324.3 321.3	AOP	(1) 1988BOR/CHE(b) (2) 1993BOR/ZHA(b)
di(pentafluorophenyl) - acetonitrile $(C_6F_5)_2$**C**HCN	81.7	341.8	AOP	1993BOR/ZHA(b)
methylmethane-1,1-dicarbonitrile Me**C**H(CN)$_2$	84.6	354.0	Re-anal. of pyrolysis data	1998BRO/BEC
2-cyclohexyl-2-phenyl-ethanenitrile c-C_6H_{11}**C**H(Ph) CN	81	338.9	AOP	1992BOR/ZHA

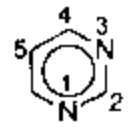
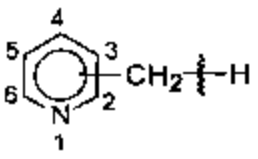
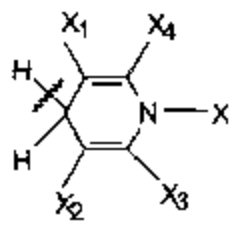
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 - 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
2-phenyl-propanenitrile MeC**H**(Ph) CN	80	334.7	AOP	1992BOR/ZHA
phenylmethane-1,1-dicarbonitrile CNC**H**(Ph) CN	77	322.2	AOP	1992BOR/ZHA
2-phenyl-2-(2-pyridyl) - ethanenitrile c-PyNC**H**(Ph) CN	76	318.0	AOP	1992BOR/ZHA
isocyanomethane CH_3NC $\Delta_f H^\circ$(R) = 80±4 (334.7±16.7)	93±3	389.1±12.6	PES	2002NIM/DAV
diazomethyl radical **H**–HCNN	97±2	405.8±8.4	PES	1998CLI/WEN(b)
diazocarbene **H**–CNN	79.1±4	331±17	PES	1998CLI/WEN(b)
nitromethane CH_3NO_2 $\Delta_f H^\circ$(R) = 27.5±3 (115.1±12.6)	(1) 97.4 (2) 105.1 (3) 96.3	407.5 439.7 402.9	(1) AOP (2) Derived from $\Delta_f H^\circ$ in ref. (3) Derived	(1) 1994BOR/SAT (2) 2003NASA/JPL (3) 2000MIR/VOR
nitroethane $CH_3CH_2NO_2$ $\Delta_f H^\circ$(R) = 14.8±3 (61.9±12.6)	(1) 91.4 (2) 98.1	382.4 410.5	(1) AOP (2) Derived	(1) 1994BOR/SAT (2) 2000MIR/VOR(b)
nitropropane $C_2H_5CH_2NO_2$	98.1	410.5	Derived	2000MIR/VOR(b)
nitrobutane $C_3H_7CH_2NO_2$	97.3	407.1	Derived	2000MIR/VOR(b)
nitropentane $C_4H_9CH_2NO_2$	96.2	402.5	Derived	2000MIR/VOR(b)
2-nitropropane Me_2CHNO_2 $\Delta_f H^\circ$(R) = 1.5±3 (6.3±12.6)	(1) 86.8 (2) 94.7	363.2 396.2	(1) AOP (2) Derived	(1) 1994BOR/SAT (2) 2000MIR/VOR(b)
1,1-dinitroethane (CH_3) C**H**$(NO_2)_2$	98.2	410.9	Derived	2000MIR/VOR(b)
1,1-dinitropropane (C_2H_5) C**H**$(NO_2)_2$	97.8	409.2	Derived	2000MIR/VOR(b)
1,1-dinitrobutane (C_3H_7) C**H**$(NO_2)_2$	98.3	411.3	Derived	2000MIR/VOR(b)
1,1-dinitropentane (C_4H_9) C**H**$(NO_2)_2$	96.9	405.4	Derived	2000MIR/VOR(b)
nitrocyclopropane c-C_3**H**$_5NO_2$	88.4	369.9	AOP	1994BOR/SAT

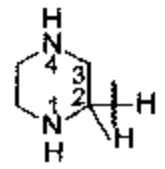
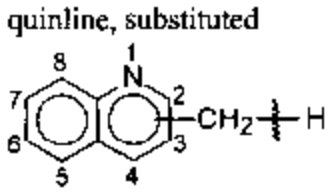
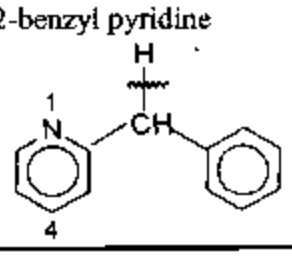
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
nitrocyclopentane c-$C_5H_9NO_2$	86.8	363.2	AOP	1994BOR/SAT
nitrocyclohexane c-$C_6H_{11}NO_2$	88.6	370.7	AOP	1994BOR/SAT
1-phenylnitroethane, substituted  				
Y = H $\Delta_f H^\circ$(R) = 40.4±3 (169.0±12.6)	85.4	357.3	AOP	1995BOR/ZHA(c)
4-F	86.1	360.2		
4-Me	85.6	358.2		
3-MeO	86.9	363.6		
4-MeO	84.9	355.2		
3-NO_2	86.1	360.2		
4-NO_2	86.9	363.6		
3,5-$(NO_2)_2$	88.7	371.1		
nitro(phenylmethoxy) methane $PhCH_2OCH_2NO_2$	86.1	360.2	AOP	1994BOR/SAT
dinitromethane $CH_2(NO_2)_2$	89.7	375.5	Derived	2000MIR/VOR
trinitromethane $CH(NO_2)_3$	86.3	361.0	Derived	2000MIR/VOR
1-aza-1-methyoxy-3-phenyl-2-benzylpro-1-ene $(PhCH_2)_2C=NOMe$	82.9	346.9	AOP	1992ZHA/BOR
pyrrole  				
C–H bond at 2 and 3 site $\Delta_f H^\circ$(pyrrol-2-yl) = 92.2 (385.8) $\Delta_f H^\circ$(pyrrol-3-yl) = 92.2 (385.8)	(1) **118.4±1** (2) 112.3±1	**495.4±4.2** 469.9±4.2	(1) Shock tube (2) Photoionization	(1) 1991MAC/COL (2) 1994BLA/NOR
pyridine  				

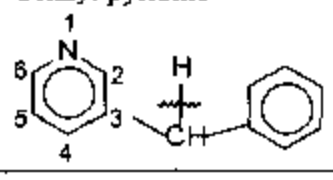
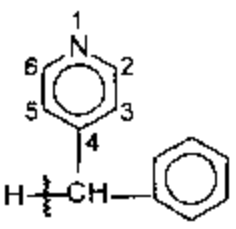
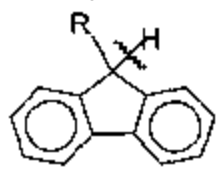
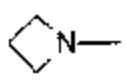
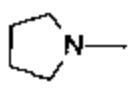
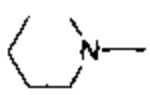
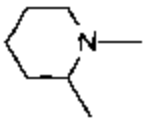
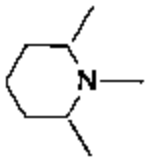
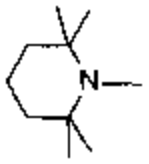
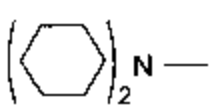
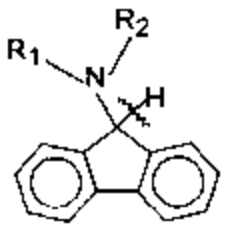
续表

断裂键 （**黑体**：离解原子） $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs （**黑体** = 推荐值； 括号内数字 = 文献编号） kcal/mol	 kJ/mol	方法	文献
C–H bond at 2 site	(1) **105±0.2** (2) 102.7	**439.3±0.8** 429.7	Shock tube	(1) 1997KIE/ZHA (2) 1992DOU/MAC
at 3 site	(1) 112±2	468.6±8.4		
at 4 site	(1) 112±2	468.6±8.4		
$\Delta_f H^\circ$(pyrid-2-yl) = 86.5 (361.9) $\Delta_f H^\circ$(pyrid-3-yl) = 93.5 (391.2) $\Delta_f H^\circ$(pyrid-4-yl) = 93.5 (391.2)				
pyrimidine  C–H bond at 2 site	(1) 98±2 (2) 95.8	410.0±8.4 400.8	Shock tube	(1) 1997KIE/ZHA (2) 1992DOU/MAC
at 4 site	(1) 103±2 (2) 102.8	431.0±8.4 430.1		
at 5 site	(1) 112±2 (2) 111.2	468.6±8.4 465.3		
$\Delta_f H^\circ$(pyrimid-2-yl) = 92.7±2 (387.9±8.4) $\Delta_f H^\circ$(pyrimid-4-yl) = 97.7±2 (408.4±8.4) $\Delta_f H^\circ$(pyrimid-5-yl) = 106.7±2 (446.4±8.4)				
pyridine, substituted 				
2-CH_3	87.2	365.0	Correlation	2002KRO/TUM
3-CH_3	90.4	378.2		
4-CH_3	86.5	362.1		
2,4,6-$(CH_3)_3$	87.7	366.9		
1,4-dihydropyridines, substituted 				

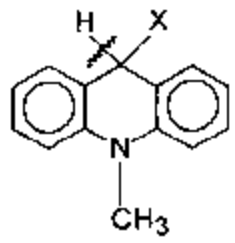
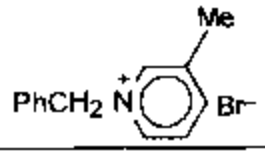
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^0$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值， 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
X_1 = C(O) NH_2, X_2 = X_3 = X_4 = H			AOP	2003ZHU/LI
X = Ph	69.2	289.5		
$PhCH_2$	67.9	284.1		
4-Cl-C_6H_4	69.1	289.1		
4-Br-C_6H_4	69.2	285.5		
4-CH_3-C_6H_4	69.2	285.5		
4-CF_3-C_6H_4	69.5	290.8		
4-MeO-C_6H_4	69.4	290.4		
X_1 = X_2 = C(O) NH_2, X_3 = X_4 = Me				
X = H	69.4	290.4		
Me	68.8	287.9		
piperazine 	(1) 90 (2) 93	376.6 389.1	(1) PAC (2) PAC, revised	(1) 1993CLA/WAY (2) 1999LAA/MUL
quinline, substituted 				
2-CH_3	87.6	366.6	Correlation	2002KRO/TUM
3-CH_3	88.9	372.1		
4-CH_3	86.1	360.1		
5-CH_3	87.5	366.3		
6-CH_3	88.7	371.0		
7-CH_3	88.7	371.0		
8-CH_3	90.3	377.8		
2-benzyl pyridine 	(1) 82.3 (2) 82	344.3 343.1	(1) VLPP (2) AOP	(1) 1984ROS/MCM (2) 1992ZHA/BOR

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^0$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
3-benzyl pyridine 	84	351.5	AOP	1992ZHA/BOR
4-benzyl pyridine 	(1) 82.3 (2) 83	344.3 347.3	(1) VLPP (2) AOP	(1) 1984ROS/MCM (2) 1992ZHA/BOR
fluorene, substituted 				
R = 	66	276.1	AOP	1992ZHA/BOR(b)
	68	284.5		
	72	301.2		
	71.5	299.2		
	72	301.2		
	71	297.1		
	73	305.4		
fluorene, substituted 				
R_1 = Me R_2 = Me	71.5	299.2	AOP	1992ZHA/BOR(b)
Et Et	70.5	295.0		
iPr iPr	73	305.4		

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nBu Me	72	301.2		
$PhCH_2$ Me	72.5	303.3		
10-methyl-9,10-dihydro-acridine, substituted 				
X = H	(1) 72.0±1.6 (2) 73.7	301.2±6.7 308.4	Electrochemical	(1) 1998ANN/FRA (2) 2003ZHU/LI
CN	(1) 71.3±1.5	298.3±6.3		
benzyl trimethylammonium chloride $PhC\mathbf{H}_2{}^+NMe_3\ Cl^-$	90.5	378.7	AOP	1993ZHA/BOR
benzyl trimethylammonium bromide $PhC\mathbf{H}_2{}^+NMe_3\ Br^-$	90.8	380	AOP	1997CHE/LIU
3-methyl-1-benzylpyridinium bromide 	84.7	354.4	AOP	1993ZHA/BOR
1-benzyl pyridinium chloride $PhC\mathbf{H}_2{}^+NPy\ Cl^-$	84.7	354.4	AOP	1993ZHA/BOR
1-acetonitrile trimethyl-ammonium chloride $Me_3{}^+NC\mathbf{H}_2CN\ Cl^-$	95.3	398.7	AOP	1990BOR/ZHA
1-acetonitrile pyridinium chloride $PyN^+C\mathbf{H}_2CN\ Cl^-$	87.6	366.5	AOP	1990BOR/ZHA
fluorenyl trimethylammonium bromide $FLH^+NMe_3\ Br^-$	84.9	355.2	AOP	1997LIU/HUA

4.6.3 α位含有—O和—N两个原子团

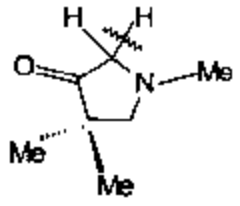
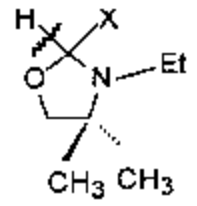
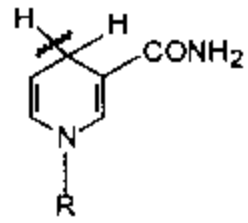
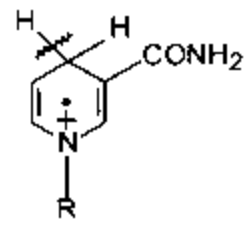
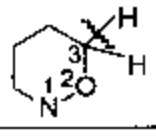
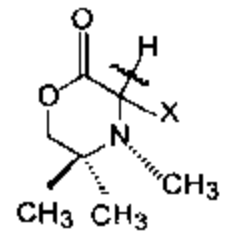
表 4.6.3 α位含有—O 和—N 两个原子团的碳氢化合物内的 C—H BDEs

断裂键 (**黑体** 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 文献编号)		方法	文献
	kcal/mol	kJ/mol		
(1Z) -2-aza-2-methoxy-1,1-phenylvinylamine $PhC(\mathbf{N}H_2)=NOCH_3$	94.9	397.1	AOP	1992BOR/JI

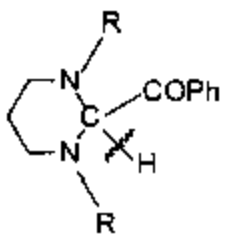
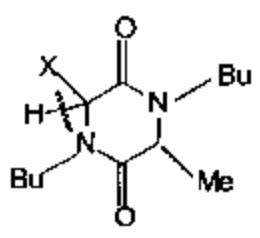
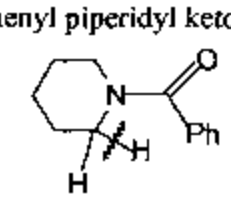
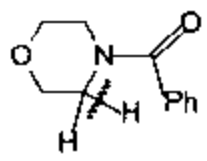
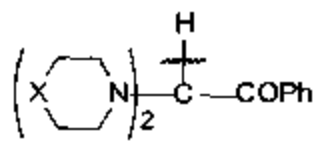
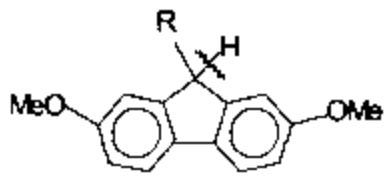
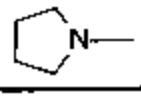
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)，kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
2-methoxyethanenitrile (CN) CH_2OMe	90.3	377.8	Re-anal. of pyrolysis data	1998BRO/BEC
N,N-dimethylacetamide $Me_2NC(O)$ CH_3	91.0	380.9	Correlation	2000DEN/KHU
methyl 2-(dimethylamino) - acetate $Me_2NCH_2C(O)$ Me	77	322.2	PAC	1993CLA/WAY
N-iso-propylacetamide $(CH_3)_2CHNHC(O)$ Me	93.1	389.5	Correlation	2000DEN/KHU
glycine ion $NH_2CH_2C(O)$ O^-	≤82.0	≤343	Electrochem.	1997ZHA/LIN
glycine $NH_2CH_2C(O)$ OH	≤78.6	≤329	Electrochem.	1997ZHA/LIN
methyl-2-aminoacetate $NH_2CH_2C(O)$ OMe	84.3	352.7	Re-anal. of pyrolysis data	1998BRO/BEC
ethyl 2-aminoacetate $NH_2CH_2C(O)$ OEt	79-83	331-347	PAC	1993CLA/WAY
ethyl 3-(dimethylamino) prooanoate $Me_2N(CH_2)_2C(O)$ OEt	88.0	368.0	Correlation	2000DEN/KHU
2-(dimethylamino) -1-phenylethan-1-one $N(CH_3)_2CH_2C(O)$ Ph	78.3	327.6	Re-anal. of pyrolysis data	1998BRO/BEC
phenyl methylene ketone trimethylammonium bromide $PhC(O)$ $CH_2{}^+NMe_3$ Br^-	96.8	405	AOP	1997CHE/LIU
glycine anhydride $NH_2CH_2C(O)$ OCH_2NH_2	81.3±3.6	340±15	PAC	1998JON/WAY
tert-butyl-2-aminopropanoate $NH_2CHMeC(O)$ OtBu	81.3	340.2	Re-anal. of pyrolysis data	1998BRO/BEC
2-hydroxypropanenitrile (CN) $CHMe(OH)$	87.3	365.3	Re-anal. of pyrolysis data	1998BRO/BEC
alanine anhydride $Me(NH_2)$ $CHC(O)$ $OCHNH_2Me$	77.7±3.6	325±15	PAC	1998JON/WAY
2-methoxy-2-phenylethane-nitrile $MeOCH(Ph)$ CN	77.5	324.3	AOP	1992BOR/ZHA
2-phenyl-2-phenoxyethane-nitrile $PhOCH(Ph)$ CN	79.5	332.6	AOP	1992BOR/ZHA
2-cyanoacetic acid (CN) $CH_2C(O)$ OH	95.2	398.4	Correlation	2002TUM/KRO
2-(acetylamino) acetic acid $CH_3C(O)$ $NHCH_2C(O)$ OH	96.1	402.2	Correlation	2002TUM/KRO
2-(acetylamino) propanioc acid $CH_3C(O)$ $NHCH(CH_3)$ C(O) OH	93.9	393.0	Correlation	2002TUM/KRO

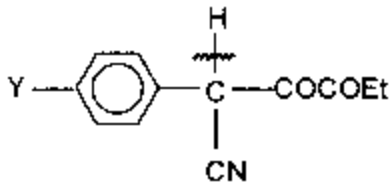
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) , kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ethyl 2-cyano-2-phenyl-acetate C_6H_5**CH**(CN) C(O) OEt	80.9	338.5	AOP	1993BOR/ZHA(b)
ethyl 2-cyano-2-pentafluoro-phenyl-acetate C_6F_5**CH**(CN) C(O) OEt	85.2	356.5	AOP	1993BOR/ZHA(b)
4,4-dimethyl pyrrolidin-3-one 	78	326.4	PAC	1993CLA/WAY
3-ethyl-4,4-dimethyl-1,3-oxazolidine  X = Me C(O) OMe	82.1 84.1	343.5 351.9	PAC	1993CLA/WAY
NADH  R = adenosine diphosphoribosyl	79.3	331.8	Electrochemical	2003ZHU/YAN
$NADH^{\bullet}$  R = adenosine diphosphoribosyl	36.3	151.9	Electrochemical	2003ZHU/YAN
2-oxomorpholine 	(1) 75 (2) 78	313.8 326.4	(1) PAC (2) PAC, revised	(1) 1993CLA/WAY (2) 1999LAA/MUL
4,5,5-trimethyl morpholin-2-one  X = H CH_3	75.3 77.5	315.1 324.3	PAC	1993CLA/WAY

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R), kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/*mol*	 kJ/*mol*	方法	文献
phenyl piperazin-2-yl ketone, substituted 				
R = Me	73	305.4	AOP	1992ZHA/BOR(b)
Et	72	301.2		
1,4-diazaperhydroine-2,5-dione, substituted 				
X = H	92.4	386.6	Re-anal. of pyrolysis data	1998BRO/BEC
Me	89.4	374.0		
phenyl piperidyl ketone 	94.4	395.0	Correlation	2000DEN/KHU
morpholin-4-yl phenyl ketone 	83.3	348.6	Correlation	2000DEN/KHU
1-phenyl 2,2-dipiperidylethan-1-one, analogues 				
X = CH_2	74	309.6	AOP	1992ZHA/BOR(b)
O	75	313.8		
fluorene, substituted 			AOP	1992ZHA/BOR(b)
R = 	69	288.7		

续表

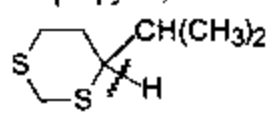
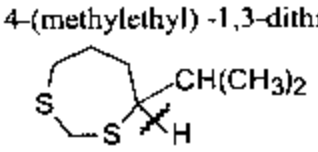
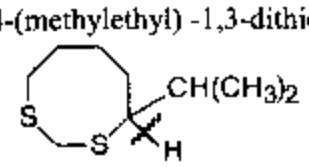
断裂键 (**黑体** 离解原子) $\Delta_f H^\circ$(R), kcal (kJ)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
ethyl-2-cyano-2-phenylacetate, substituted  				
Y = H	80.3	336.0	AOP	2000CHE/LIU
F	80.3	336.0		
Cl	80.8	338.1		
Me	80.0	334.7		
MeO	78.3	327.6		
$MeCO_2$	82.0	343.1		
CF_3	82.2	343.9		
CN	83.2	348.1		
benzoylmethyl trimethylammonium bromide $PhC(O)\,CH_2{}^{+}NMe_3\,Br^-$	96.8	405.0	AOP	1997LIU/HUA
nitrozoamines				
$(NO_2)_3CCH_2N(NO_2)\,CH_2CH_2$– $CH_2N(NO_2)\,CH_2C(NO_2)_3$	72.3	302.5	Derived	2001MIR/KOS
$(NO_2)_2CHCH_2N(NO_2)\,CH_2CH_2$– $CH_2N(NO_2)\,CH_2CH(NO_2)_2$	77.6	324.7		
$(NO_2)_3CCH_2N(NO)\,CH_2CH_2$– $CH_2N(NO)\,CH_2C(NO_2)_3$	72.3	302.5		

4.6.4 α位是—C(S)、—S、—SO、—SO_2的C—H键

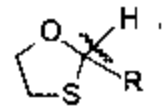
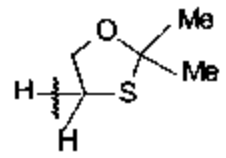
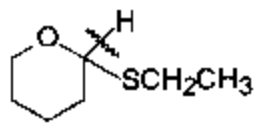
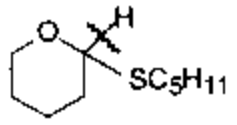
表 4.6.4 α位是—C(S)、—S、—SO、—SO_2的碳氢化合物内的 C—H BDEs

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
thioformaldehyde **H**–C(S) H $\Delta_f H^\circ$(R) = 71.8±2 (300.4±8.4)	95.5±1.2	399.6±5.0	Recommended	1994BER/ELL

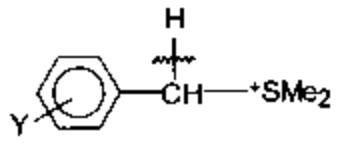
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 - 推荐值; 括号内数字 - 文献编号) kcal/mol	kJ/mol	方法	文献
methanethiol CH_3SH $\Delta_f H^\circ$(R) = 36.3±2 (151.9±8.4)	(1) 92.4±2.0 (2) **93.9±2.0**	386.6±8.4 **392.9±8.4**	(1) PIMS (2) Recommend.	(1) 1992RUS/BER (2) 1994BER/ELL
dimethyl sulphide CH_3SCH_3 $\Delta_f H^\circ$(R) = 32.7±1.4 (136.8±5.9)	93.7±1 4	392.0±5.9	Resonance fluorescence	1994JEF/NIC
diethyl disulfide $CH_3CH_2SCH_2CH_2CH_3$	93.3	390.2	Correlation	2003TUM/DEN
1,1-diethylthio-3-methylbutane $(CH_3CH_2S)_2CHCH(CH3)_2$	93.0	389.0	Correlation	2003TUM/DEN
1,1-dibutylthio-3-methylbutane $(CH_3CH_2CH_2CH_2S)_2CHCH(CH3)_2$	92.1	385.6	Correlation	2003TUM/DEN
Adduct $H_3BS(CH_3)_2$	95.8±3	400.8±12.6	CID	1998REN/WOR
4-methyl-1,3-dithiane 	91.0	380.9	Correlation	2003TUM/DEN
4-iso-propyl-1,3-thiane 	87.2	365.0	Correlation	2003TUM/DEN
4-(methylethyl) -1,3-dithiepane 	92.7	388.0	Correlation	2003TUM/DEN
4-(methylethyl) -1,3-dithiocane 	91.9	384.7	Correlation	2003TUM/DEN
phenyl methyl sulphide $PhSCH_3$ $\Delta_f H^\circ$(R) = 64.2±3 (268.6±12.6)	93.0	389.1	AOP	1993ZHA/BOR
benzyl phenyl sulphide $PhCH_2SPh$ $\Delta_f H^\circ$(R) = 104.1±3 (435.6±12.6)	(1) 84.2 (2) 82.2	352.3 343.9	AOP	(1) 1993ZHA/BOR (2) 1998BOR/LIU
di(phenylthio) phenyl methane $(PhS)_2CHPh$	81.5	341.0	AOP	1992BOR/ZHA
phenyl diphenylmethyl sulphide $PhSCHPh_2$	82.4	344.8	AOP	1992BOR/ZHA

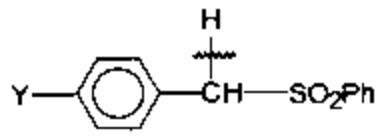
续表

断裂键 (黑体　离解原子) Δ_fH°(R) /kcal (kJ)	BDEs (黑体 = 推荐值, 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1,3-oxathiolane, substituted 				
R = H	91.0	380.9	Correlation	2002TUM/KRO
Me	90.3	377.8		
Et	90.3	377.8		
iPr	90.3	377.8		
2,2-dimeyl-oxathiolane 	94.2	394.3	Correlation	2002TUM/KRO
2-ethythio-2H-3,4,5,6-tetrahydropyran 	87.4	365.5	Correlation	2002TUM/KRO
2-butylthio-2H-3,4,5,6-tetrahydropyran 	87.1	364.4	Correlation	2002TUM/KRO
dimethyl sulphoxide CH_3SOCH_3 Δ_fH°(R) = 5.7±3 (23.8±12.6)	94	393.3	AOP	1998BOR/LIU
dimethyl sulphone $CH_3SO_2CH_3$ Δ_fH°(R) = –42 3±3 (–177.0±12.6)	99	414.2	AOP	1991BOR/HAR
methyl trofluoromethyl sulphone $CH_3SO_2CF_3$	103	431.0	AOP	1991BOR/HAR
methyl phenyl sulphone CH_3SO_2Ph Δ_fH°(R) = –13.7±3 (–57.3±12.6)	99	414.2	AOP	1991BOR/HAR
methyl p-NO_2-phenyl sulphone CH_3SO_2(p-NO_2-C_6H_4)	95	397.5	AOP	1995ZHA/BOR
benzyl methyl sulphone $PhCH_2SO_2Me$ Δ_fH°(R) = –26.1±3 (–109.2±12.6)	91	380.7	AOP	1992ZHA/BOR

续表

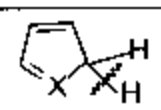
断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (**黑体** – 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
benzyl trifluoromethyl sulphone $PhCH_2SO_2CF_3$	89	372.4	AOP	1992ZHA/BOR
benzyl tert-butyl sulphone $PhCH_2SO_2tBu$	90	376.6	AOP	1992ZHA/BOR
benzyl phenyl sulphone $PhCH_2SO_2Ph$ $\Delta_f H^\circ$(R) = 1.7±3 (7.1±12.6)	(1) 89.7 (2) **90.2**	375.3 **377.4**	AOP	(1) 1998BOR/LIU (2) 1992ZHA/BOR
di(methyl sulphonyl) methane $CH_2(CH_3SO_2)_2$	101.4	424.3	AOP	1994BOR/ZHA
di(trifluoromethyl sulphonyl) methane $CH_2(CF_3SO_2)_2$	113	472.8	AOP	1991BOR/HAR
di(ethyl sulphonyl) methane $CH_2(EtSO_2)_2$	101.3	423.8	AOP	1994BOR/ZHA
di(isopropyl sulphonyl) methane $CH_2(iPrSO_2)_2$	100.1	418.8	AOP	1994BOR/ZHA
di(t-butyl sulphonyl) methane $CH_2(tBuSO_2)_2$	99.7	417.1	AOP	1994BOR/ZHA
di(phenyl sulphonyl) methane $CH_2(PhSO_2)_2$	98	410.0	AOP	1994BOR/ZHA
((diphenylmethyl) sulfonyl) - benzene Ph_2CHSO_2Ph $\Delta_f H^\circ$(R) = 24.4±3 (–102.1±12.6)	87.3	365.3	AOP	1991BOR/ZHA
di(phenylthio) methane $CH_2(SPh)_2$	89	372.4	AOP	1995ALN/ZHA
benzyl dimethylsulfonium bromide $PhCH_2^+SMe_2\ Br^-$	83.2	348	AOP	1997CHE/LIU
benzyl dibutylsulfonium bromide $PhCH_2^+S(nBu)_2\ Br^-$	(1) 84 1 (2) 83.8	352 350.6	AOP	(1) 1997CHE/LIU (2) 1998CHE/LIU
phenyl methylene ketone dibutylsulfonium bromide $PhC(O)\ CH_2^+S(Bu)_2Br^-$	94.9	397	AOP	1997CHE/LIU
benzyl dibutylsulfonium, substituted 			AOP	(1) 1998CHE/LIU

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Y = H	(2) 83.1	347.7		(2) 2000CHE/LIU
p-Me	(2) 82.5	345.2		
p-CN	(2) 86.0	359.8		
p-MeO	(1) 84.6	354.0		
p-MCO_2	(2) 92.0	384.9		
phenyl phenylsulphonyl methane, substituted 				
Y = H	90.3	377.8	AOP	1998BOR/LIU
Me	89.1	372.8		
Cl	91.8	384.1		
Br	90.4	378.2		

4.6.5 α位是其他杂原子的C—H键

表 4.6.5 α位是其他杂原子的碳氢化合物内的 C—H BDEs

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
				
X = P (phosphole)	≤76.7	≤320.9	GPA	1994SUN/PAN
As (arsole)	≤76.7	≤320.9		
ylide bromides				
$PhCH_2{}^+P(Bu)_3Br^-$	89.1	373	AOP	1997CHE/LIU
$PhCH_2{}^+P(Ph)_3Br^-$	88.7	371		
$PhCH_2{}^+As(Bu)_3Br$	91.8	384		
$PhCH_2{}^+Se(Me)_2Br^-$	88.4	370		
$PhCH_2{}^+P(Bu)_2Br^-$	88.9	372		
$PhCH_2{}^+Te(Bu)_2Br$	89.9	376		

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^0$(R) /kcal (kJ)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
PhC(O) CH_2 $^-P(Bu)_3Br^-$	93.2	390		
PhC(O) CH_2 $^-P(Ph)_3Br^-$	96.6	404		
PhC(O) CH_2 $^-As(Ph)_3Br^-$	95.8	401		
PhC(O) CH_2 $^-Se(Me)_2Br$	98.0	410		
PhC(O) CH_2 $^-Te(Bu)_2Br^-$	97.3	407		
ylide bromides FL**H** $^-P(Bu)_3Br$	81.5	340.8	AOP	1997LIU/HUA
PhCH_2 $^-P(Ph)_3Br^-$	81.6	341.5		
PhCH_2 $^-As(Ph)_3Br^-$ FL = fluorenyl	82.6	345.6		
2,2-dimethyl-2-silapropane **H**–CH_2SiMe_3 $\Delta_f H^0$(R) = −7.6±1.5 (−32±6)	100±1.5	418±6.3	Iodination	1998BEC/WAL
2,2,3,3-tetramethyl-2-silabutane **H**–$CH_2C(CH_3)_2SiMe_3$ $\Delta_f H^0$(R) = −29.8 (−125)	97.8±1.2	409±5	Iodination	1998BEC/WAL
phenyl-trimethyl-silane **H**–CH_2SiMe_2Ph	98.0	410.1	Correlation	2002TUM/KRO
bis(trimethylsilyl) methane **H**–$CH((CH_3)_3Si)_2$	95±3	397±13	Electron photodetach.	1998ROM/GAT
alkyldioxaborolanes **H**–$CH_2B(RO)_2$	98.6	412.5	EPR	2000WAL/MCC
bis(dimethylphosphino) methane **H**–$CH((CH_3)_2P)_2$	92±3	385±13	Electron photodetach.	1998ROM/GAT
organoferric species, Fe^{II} **H**–C bonds				
$Fe^{II}(C_5H_5)(\eta^6\text{-}C_6Me_6)^+PF_6$	86.5±1.5	362±6	Electrochemical	1999TRU/CAS
$Fe^{II}(C_5Me_5)(\eta^6\text{-}C_6Me_6)^+PF_6$	85.5±2	358±8		
$Fe^{II}(C_5H_5)(\eta^6\text{-}$ $C_6H_5CH_2C_6H_5)^+PF_6$	84±2	351±8		

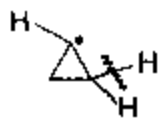
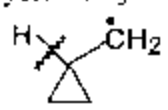
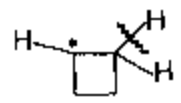
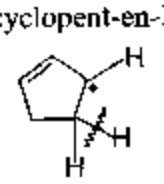
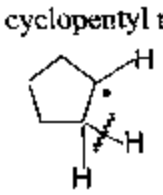
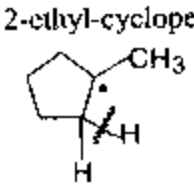
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^0$(R) /kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
$Fe^{II}(C_5H_5)$ (η^6 $C_6H_5CHPh_2$) $^+PF_6^-$	82.6±2	346±8		
$Fe^{II}(C_5H_5)$ (η^6-fluorene) $^+PF_6^-$	81±2	339±8		
$Fe^{II}(C_5H_5)$ (η^6-C_6Me)	67.5±1.5	282±6		
organoferric species, Fe^I				
H–C bonds				
$Fe^I(C_5Me_5)$ (η^6-C_6Me_6)	65.1±2	272±8	Electrochemical	1999TRU/CAS
$Fe^{II}(C_5H_5)$ (η^6-$C_6H_5CH_2C_6H_5$)	59.4±1.5	249±6		
$Fe^{II}(C_5H_5)$ (η^6-$C_6H_5CHPh_2$)	58±1.5	243±6		
$Fe^{II}(C_5H_5)$ (η^6-fluorene)	52.6±1.5	220±6		
organoferric species, Fe^0				
H- C bonds				
$Fe^0(C_5H_5)$ (η^6-C_6Me_6) $^-$	68.2±2	285±8	Electrochemical	1999TRU/CAS
$Fe^0(C_5Me_5)$ (η^6-C_6Me_6)	67.5±2	282±8		
$Fe^0(C_5H_5)$ (η^6-$C_6H_5CH_2C_6H_5$)	59.6±2	249±8		
$Fe^0(C_5H_5)$ (η^6-$C_6H_5CHPh_2$)	59.3±2	248±8		
$Fe^0(C_5H_5)$ (η^6-fluorene)	44.1±2	185±8		
organoferric species, Fe^{III}				
H–C bonds				
$Fe^{III}(C_5H_5)$ (η^6-C_6Me_6) $^{2+}$	48.2±3	202±12	Electrochemical	1999TRU/CAS
$Fe^{III}(C_5Me_5)$ (η^6-C_6Me_6) $^{2+}$	48.1±3	201±12		
$Fe^{III}(C_5H_5)$ (η^6-$C_6H_5CH_2C_6H_5$) $^{2+}$	48.5±3	203±12		
$Fe^{III}(C_5H_5)$ (η^6-$C_6H_5CHPh_2$) $^{2+}$	47±3	197±12		
$Fe^{III}(C_5H_5)$ (η^6-fluorene) $^{2+}$	51±3	213±12		

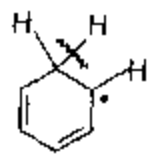
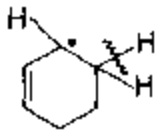
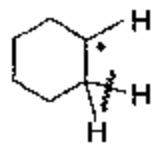
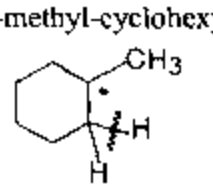
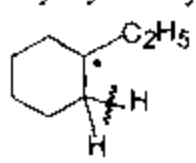
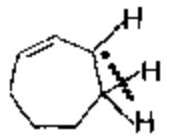
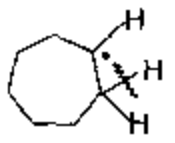
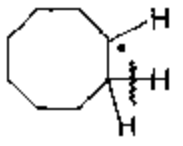
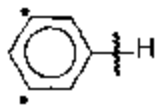
4.7 自由基中的C—H键能

表 4.7 自由基中的 C—H BDES

断裂键 (**黑体** = 离解原子)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methylidyne C–**H**	80.9	338.5	Spectroscopy	2002CRC
methylene CH–**H**	100.8	421.7	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
methyl radical CH_2–**H**	110.35±0.20	461.70±0.84	Recommended	1999RUS/LIT
ethyl radical $C^{\bullet}H_2CH_3$	36.2±0.4	151.5±1.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
n-propyl radical $C^{\bullet}H_2CH_2CH_3$	33.0±0.6	138.1±2.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
i-propyl radical $CH_3C^{\bullet}HCH_3$	35.9±0.8	150.2±3.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
n-butyl radical $C^{\bullet}H_2CH_2CH_2CH_3$	33.5±0.6	140.2±2.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
i-butyl radical $(CH_3)_2CHC^{\bullet}H_2$	31.4±1.0	131.4±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
s-butyl radical $CH_3C^{\bullet}HCH_2CH_3$	35.9±0.6	150.2±2.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
t-butyl radical $(CH_3)_2C^{\bullet}CH_3$	36.6±0.8	153.1±3.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
n-pentyl radical $C^{\bullet}H_2CH_2CH_2CH_2CH_3$	34.0±1.0	142.3±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pentyl-2 radical $CH_3CH_2CH_2C^{\bullet}HCH_3$	32.5±1.0	136.0±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyl-butyl-2 radical $CH_3CH_2C^{\bullet}(CH_3)_2$	35.1±1.0	146.9±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
n-hexyl radical $C^{\bullet}H_2CH_2CH_2CH_2CH_2CH_3$	33.7±1.0	141.0±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
hex-2-yl radical $CH_3C^{\bullet}HCH_2CH_2CH_2CH_3$	32.2±1.2	134.7±5.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyl pent-2-yl radical $C_2H_5CH_2C^{\bullet}(CH_3)_2$	36.3±2	151.9±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-methyl pent-3-yl radical $CH_3CH_2C^{\bullet}(CH_3)(C_2H_5)$	35.1±2.5	146.9±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
acetenyl radical $^{\bullet}C{\equiv}C$–**H**	111.8±2.1	467.6±8.8	Derived from $\Delta_f H^\circ$ in ref.	1994GIN/FIN
propargyl radical $H_2CCC^{\bullet}$–**H**	100±5	418±21	GPA	1999WEN/LIN

断裂键 (黑体 = 离解原子)	BDEs (黑体 推荐值， 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
carbene $^{\bullet}C$–CH–**H**	87.3±4	365.3±16 7	Derived from $\Delta_f H^\circ$ in ref.	1999AHM/PET
vinyl radical C$^{\bullet}$H–CH_2	35.0±0.9	146.4±3.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
vinyl radical $CH_2C^{\bullet}$–**H**	(1) 80.0±5 (2) 80.8±4	334.7±21 338.1±16.7	Derived	(1) 1989ERV/HO (2) This volume
allyl radical CH_2–CH–$C^{\bullet}H_2$	56.8±0.8	237 7±3.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-propen-1-yl CH_3**C**H–$C^{\bullet}$H	32.5±1.5	136.0±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-propen-2-yl CH_3–$C^{\bullet}$–CH_2	42.3±2	177 0±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-buten-4-yl radical CH_2CH$CH_2C^{\bullet}H_2$	32.4±2.5	135.6±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-buten-3-yl radical CH_2–CH$C^{\bullet}$HCH_3	46.6±2	195.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
allyl radical CH_2CH$C^{\bullet}$H–**H**	104 0±3.4	435.1±14.2	Derived	1997POU/NAS
2-methylallyl radical $CH_2C(CH_3)$ $C^{\bullet}H_2$	90±2	377±8	Derived	1999WEN/HU
cyclopropyl radical 	51.4±2.6	215.1±10.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclomethyl radical 	48.9±2	204.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclo-butyl radical 	38.2±1.5	159 8±6.3	Derived from $\Delta_f H^\circ$ in ref	1986PED/NAY
cyclopent-en-3-yl radical 	45.8±1.5	191.6±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclopentyl radical 	34.9±1.5	146.0±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-ethyl-cyclopentyl radical 	36.2±1.5	151.5±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (黑体 = 离解原子)	BDEs (黑体 - 推荐值， 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
cyclohexa-1,3-dien-5-yl radical 	24.2±1.5	101.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclohexa-1-en-3-yl radical 	48.9±1.5	204.6±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclohexyl radical 	32.9±1.5	137.7±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-methyl-cyclohexyl radical 	36.3±1.5	151.9±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-ethyl-cyclohexyl radical 	34.5±1.5	144.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cycloheptenyl radical 	46.1±1.5	192.9±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cycloheptyl radical 	37.8±1.5	158.2±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclooctanyl radical 	31.4±1.5	131.4±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3,5-didehydrophenyl radical 	109.2±5.6	456.9±23.4	CID	2002LAR/NAS
phenyl radical C_6H_4–**H**	78.3	327.6	Derived	1992GRA
benzyl radical $C_6H_5C^{\bullet}H$–**H**	105.2±3.5	440.2±14.6	Derived	1997POU/NAS
α-methylbenzyl radical **H**–$CH_3C^{\bullet}HPh$	47.9	200.4	Kinetics	2003TAN/PAP

续表

断裂键 (黑体 = 离解原子)	BDEs (黑体 = 推荐值， 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
fluoromethylene CF–**H**	78.9±3.8	330.1±15.9	Derived from $\Delta_f H^\circ$ in ref.	1997POU/PAU
chloromethylene CCl **H**	80.0±3.8	334.7±15.9	Derived from $\Delta_f H^\circ$ in ref.	1997POU/PAU
difluoromethyl radical CF_2–**H**	65.7±2	274.9±8.4	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
dichloromethyl radical CCl_2–**H**	83.8±2	350.6±8.4	Derived	This volume
chlorofluoromethyl radical CClF–**H**	74.0±4	309.6±16.7	Derived	This volume
dibromomethyl radical CBr_2–**H**	84.5±2.5	353.5±10.5	Derived	This volume
bromochloromethyl radical CClBr–**H**	81.7±2	341.8±8.4	Derived	This volume
diiodomethyl radical CI_2–**H**	84.3±14	352.7±60	Derived	This volume
fluoromethyl radical CHF–**H**	93.9±3.2	392.9+13 4	Derived from $\Delta_f H^\circ$ in ref.	This volume
chloromethyl radical CHCl–**H**	102.1±2.5	427.2±10.5	Derived	This volume
1,2-difluoro-vin-1-yl radical CHF=C$^\bullet$F	69.2±2.5	289.5±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1,2-dichloro-vin-1-yl radical CHCl=C$^\bullet$Cl	46.1±2.5	192.9±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1-chloro-vin-1-yl radical CH_2=C$^\bullet$Cl	43.2<	181<	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1,1,2,2-tetrafluoro-eth-1-yl radical $CHF_2C^\bullet F_2$	53.1±2.5	222.2±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1,1,2-trifluoro-eth-1-yl radical $CH_2FC^\bullet F_2$	46.3±2.5	193.7±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1,1-difluoro-eth-1-yl radical $CH_3C^\bullet F_2$	44.8±3	187.4±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1,2,2-trifluoro-eth-1-yl radical $CHF_2C^\bullet HF$	47.8±2.5	200.0±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1-fluoro-eth-1-yl radical $CH_3C^\bullet HF$	36.5±3	152.7±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
2,2-difluoro-eth-1-yl radical $CHF_2C^\bullet H_2$	40.6±3	169.9±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
2-fluoro-eth-1-yl radical $CH_2FC^\bullet H_2$	33.9±3	141.8±12 6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1,1,2,2-tetrachloro-eth-1-yl radical $CHCl_2C^\bullet Cl_2$	43.5±3	182.0±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST

续表

断裂键 (**黑体** = 离解原子)	BDEs (**黑体** = 推荐值， 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1,1,2-trichloro-eth-1-yl radical $CH_2ClC^{\bullet}Cl_2$	41.2±3	172.4±12.6	Derived from Δ_fH° in ref.	1998NIST
1,1-dichloro-eth-1-yl radical $CH_3C^{\bullet}Cl_2$	37.3±3	156.1±12.6	Derived from Δ_fH° in ref.	1998NIST
1,2,2-trichloro-eth-1-yl radical $CHCl_2C^{\bullet}HCl$	36.4±3	152.3±12.6	Derived from Δ_fH° in ref.	1998NIST
1,2-dichloro-eth-1-yl radical $CH_2ClC^{\bullet}HCl$	36.9±3	154.4±12.6	Derived from Δ_fH° in ref.	1998NIST
1-chloro-eth-1-yl radical $CH_3C^{\bullet}HCl$	38.8±3	162.3±12.6	Derived from Δ_fH° in ref.	1998NIST
2,2-dichloro-eth-1-yl radical $CHCl_2C^{\bullet}H_2$	31.1±2	130.1±8.4	Derived from Δ_fH° in ref.	1998NIST
2-chloro-eth-1-yl radical $CH_2ClC^{\bullet}H_2$	34.9±2	146.0±8.4	Derived from Δ_fH° in ref.	1998NIST
1-bromo-eth-1-yl radical $CH_3C^{\bullet}HBr$	40.7±2	170.3±8.4	Derived from Δ_fH° in ref.	1998NIST
2-bromo-eth-1-yl radical $CH_2BrC^{\bullet}H_2$	38.7±2	161.9±8.4	Derived from Δ_fH° in ref.	1998NIST
1-chloro-pro-1-yl radical $CH_3CH_2C^{\bullet}HCl$	35.8±2	149.8±8.4	Derived from Δ_fH° in ref.	1998NIST
2-chloro-pro-2-yl radical $CH_3CC^{\bullet}ClCH_3$	39.1±2	163.6±8.4	Derived from Δ_fH° in ref.	1998NIST
$C^{\bullet}H_2CH_2CH_2Br$	34.8±2	145.6±8.4	Derived from Δ_fH° in ref.	1998NIST
$CH_3C^{\bullet}HCH_2Br$	40.4±2.5	169.0±10.5		
$CH_3C^{\bullet}HCH_2Br$	39.5±2.5	165.3±10.5		
$HOCH_2C^{\bullet}H_2$	29.3±2.5	122.6±10.5	Derived from Δ_fH° in ref.	1998NIST
$CH_3C^{\bullet}HOH$	35.6±2.5	149.0±10.5	Derived from Δ_fH° in ref.	1998NIST
$C^{\bullet}H_2CH_2OH$	31.0±2.5	129.7±10.5		
$CH_3CH_2C^{\bullet}HOH$	31.1±2.5	130.1±10.5		
$CH_3C^{\bullet}HCH_2OH$	30.5±2.5	127.6±10.5		
$C^{\bullet}H_2CH_2CH_2OH$	38.6±3	161.5±12.6		
$(CH_3)C^{\bullet}(CH_3)OH$	36.6±3	153.1±12.6		
$C^{\bullet}H_2CH(OH)CH_3$	25.0±3	104.6±12.6		

续表

断裂键 (黑体 = 离解原子)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
$C_7H_5OC^{\bullet}HCH_3$	38.0±3	159.0±12.6		
$HOCH_2C^{\bullet}HOH$	29.2±3	122.2±12.6		
$HC^{\bullet}(O)$	10 5±0.2	43 9±0.8	Derived	This volume
$CH_3C^{\bullet}(O)$	33.7±2	141.0±8.4	Derived from Δ_fH° in ref.	1998NIST
$C^{\bullet}H_2C(O)$ **H**	28.8±2	120.5±8.4	Derived from Δ_fH° in ref.	1998NIST
$CH_3C^{\bullet}HC(O)$ OH	41.6±3	174 1±12.6		
$CH_3O^{\bullet}$	21.6±1	90.4±4	Derived from Δ_fH° in ref.	1998NIST
$CHCl_2O^{\bullet}$	7.2±2.4	30.1±10		
CH_2=$CHO^{\bullet}$	26.8±0.5	112.1±2		
$CH_3CH_2O^{\bullet}$	14.9±1	62.3±4		
$CH_3CH_2CH_2O^{\bullet}$	14.2±2	59.4±8	Derived from Δ_fH° in ref.	1998NIST
$(CH_3)_2CHO^{\bullet}$	11.8±1	49.4	Derived from Δ_fH° in ref.	1986PED/NAY
$CH_3CH_2CH_2CH_2O^{\bullet}$	16.5±2	69.0±8	Derived from Δ_fH° in ref.	1998NIST
C_2H_5C**H**(CH_3) $O^{\bullet}$	11.7±1	49.0±4	Derived from Δ_fH° in ref.	1986PED/NAY
$C_6H_5CH_2O^{\bullet}$	17.7±3	74.1±12.6		
H–C(O) $O^{\bullet}$	–12.0±3	–50 2±12.6	Derived from Δ_fH° in ref.	2003BLA/ELL
H $CH_2C^{\bullet}(CH_3)$ C(O) OCH_3	45.6	190.8	Kinetics	2003TAN/PAP
H–CH(R) $C^{\bullet}(CH_3)$ C(O) OCH_3	46.1	192.9		
H· CHN	23±6, at 0 K	96±25	PES	1991COW/TRA
H-HCNN	97±2	405.8±8.4	PES	1998CLI/WEN(b)
$CH_3C^{\bullet}HNH_2$	36.6±3	153.1±12.6	Derived from Δ_fH° in ref.	1998NIST
$CH_3C^{\bullet}HCN$	40.9±3	171.1±12.6		
$C^{\bullet}H_2CH_2CN$	36.4±3	152.3±12.6		
$NCC^{\bullet}HCH_2CN$	42.1±4	176.1±16.7		

第 5 章　C—C键能

5.1　饱和碳氢化合物

表 5.1　饱和碳氢化合物内的 C—C BDEs

断裂键 (黑体 = 离解原子团)	BDEs (黑体 = 推荐值， 括号内数字 - 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ethane **CH_3**–CH_3	90.2±0.2	377.4±0.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
propane **CH_3**–C_2H_5	88.5±0.5	370.3±2.1	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
butane **CH_3**–nC_3H_7	88.9±0.7	372.0±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
isobutane **CH_3**–iC_3H_7	88.2±0.9	369 0±3 8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pentane **CH_3**–nC_4H_9	88.8±0.7	371.5±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-methylbutane **CH_3**–iC_4H_9	88.5±1.1	370.3±4.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylbutane **CH_3**–sC_4H_9	88.0±0.7	368.2±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2-dimethylpropane **CH_3**–tC_4H_9	86.9±0.7	363.6±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylpentane **CH_3**–$CH(CH_3)C_3H_7$	88.9±1.0	372.0±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-methylpentane **CH_3**–$CH(C_2H_5)_2$	87.4±1.0	365.7±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
butane **C_2H_5**–C_2H_5	86.8±0.6	363.2±2.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pentane **C_2H_5**–nC_3H_7	87.3±0.7	365.3±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
isopentane **C_2H_5**–iC_3H_7	86.1±0.9	360.2±3.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
Hexane **C_2H_5** nC_4H_9	86.9±0.8	363.6±3.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylpentane **C_2H_5**-iC_4H_9	86.9±1.3	363.6±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-methylpentane **C_2H_5**–sC_4H_9	85.7±0.8	358.6±3.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2-dimethylbutane **C_2H_5**–tC_4H_9	84.5±0.9	353.5±3.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylpentane **C_3H_7**–iC_3H_7	86.6±1.3	362.3±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
hexane **nC_3H_7**–nC_3H_7	87.5±0.8	366.1±3.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylpentane **nC_3H_7**–iC_3H_7	86.6±1.0	362.3±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
heptane **nC_3H_7**–nC_4H_9	87.3±0.9	365.3±3.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylhexane **nC_3H_7**–iC_4H_9	84.2±1.3	352.3±5.4	Derived from $\Delta_f H^\circ$ in ref	1986PED/NAY
3-methylhexane **nC_3H_7**–sC_4H_9	85.7±0.9	358.6±3.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2-dimethylpentane **nC_3H_7**–tC_4H_9	84.6±1.0	354.0±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,3-dimethylbutane **iC_3H_7**–iC_3H_7	84.5±1.1	353.5±4.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylhexane **iC_3H_7** nC_4H_9	86.1±1.1	360.2±4.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,4-dimethylpentane **iC_3H_7**–iC_4H_9	85.9±1.3	359.4±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,3-dimethylpentane **iC_3H_7**–sC_4H_9	84.7±1.0	354.4±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2,3-trimethylbutane **iC_3H_7**–tC_4H_9	81.5±1.1	341.0±4.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
Octane **nC_4H_9**–nC_4H_9	87.0±0.9	364.0±3.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylheptane **nC_4H_9**–iC_4H_9	86.8±1.3	363.2±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-methylheptane **nC_4H_9**–sC_4H_9	85.6±0.9	358.2±3.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2-dimethylhexane **nC_4H_9**–tC_4H_9	83.9±1.0	351.0±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,5-dimethylhexane **iC_4H_9** iC_4H_9	86.6±1.5	362.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,4-dimethylhexane **iC_4H_9**–sC_4H_9	85.3±1.3	356.9±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,3,4-trimethylpentane **iC_4H_9**–tC_4H_9	81.3±1.3	340.2±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3,4-dimethylhexane **sC_4H_9**–sC_4H_9	83.3±0.8	348.5±3.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2,3-trimethylpentane **s-C_4H_9**–tC_4H_9	80.4±1.0	336.4±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2,3,3-tetramethylbutane **tC_4H_9**–tC_4H_9	77.1±1.0	322.6±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,3-trimethylpentane lC_3H_7 $C(CH_3)_2C_2H_5$	79.7±1.5	333.5±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (黑体 = 离解原子团)	BDEs (黑体 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nonane $\mathbf{nC_4H_9}$–nC_5H_{11}	86.1±2.0	360.2±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
2,2-dimethylheptane $\mathbf{nC_4H_9}$–$neoC_5H_{11}$	81.8±2.0	342.3±8.4	Derived from Δ_fH° in ref.	1994PED
2,2,5-trimethylhexane $\mathbf{iC_4H_9}$–$neoC_5H_{11}$	85.9±2.0	359.4±8.4	Derived from Δ_fH° in ref	1994PED
2,2,3,3,-tetramethylpentane $\mathbf{tC_4H_9}$–$C(CH_3)_2C_2H_5$	75.3±1.5	315.1±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
2,2,4,4-tetramethypentane $\mathbf{tC_4H_9}$ $neoC_5H_{11}$	78±2.2	326.4±9.2	Derived from Δ_fH° in ref.	1986PED/NAY
2-methylnonane $\mathbf{nC_6H_{13}}$–iC_4H_9	86.8±2.0	363.2±8 4	Derived from Δ_fH° in ref.	1986PED/NAY
5-methylnonane $\mathbf{nC_4H_9}$–$CH(CH_3)(nC_4H_9)$	87.4±2.0	365.7±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
dodecane $\mathbf{nC_6H_{13}}$–nC_6H_{13}	85.0±2.0	355.6±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
methylcyclopentane $\mathbf{CH_3}$–c-C_5H_9	85.6±1.2	358.2±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
methylcyclohexane $\mathbf{CH_3}$–c-C_6H_{11}	90.1±1.8	377.0±7.5	Derived from Δ_fH° in ref.	1986PED/NAY
ethylcyclobutane $\mathbf{C_2H_5}$–c-C_4H_7	86.1±1.3	360.2±5 4	Derived from Δ_fH° in ref.	1986PED/NAY
ethylcyclopentane $\mathbf{C_2H_5}$–c-C_5H_9	84.0±1.3	351.5±5.4	Derived from Δ_fH° in ref.	1986PED/NAY
ethylcyclohexane $\mathbf{C_2H_5}$–c-C_6H_{11}	87.4±1.3	365.7±5.4	Derived from Δ_fH° in ref.	1986PED/NAY
propylcyclopentane $\mathbf{nC_3H_7}$- c-C_5H_9	84.4±1.3	353.1±5.4	Derived from Δ_fH° in ref.	1986PED/NAY
propylcyclohexane $\mathbf{nC_3H_7}$–c-C_6H_{11}	87.8±2.0	367.4±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
butylcyclohexane $\mathbf{nC_4H_9}$–c-C_6H_{11}	85.3±1.5	356.9±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
cyclohexaxylcyclohexane c-$\mathbf{C_6H_{11}}$–c-C_6H_{11}	88.2±2.0	369.0±8.4	Derived from Δ_fH° in ref.	1988LIA/BAR
adamantyl compounds 				
R = 1-Me	(1) **89.2±3** (2) 82.5	**373.2±12.6** 345.3	(f) Derived from Δ_fH° in ref. (2) Derived	(1) 2000MEL/PIM (2) 2002MIR/LEB
2-Me	(1) **87.3±3**	**365.3±12.6**		
1-Et	(1) **86.1±3** (2) 80.3	**335.9±12.6** 336.0		

5.2 链状非饱和碳氢化合物

表 5.2 链状非饱和碳氢化合物内的 C—C BDEs

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 文献编号)		方法	文献
	kcal/mol	kJ/mol		
acetylene **CH**≡CH	228.0±1.0	954.0±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethylene **CH_2**=CH_2	174.1±1.5	728.4±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
propyne **CH_3**–C≡CH	126.5±1.0	529.3±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
buta-1,3-diyne **HC**≡**C** C≡CH	160.2±2.0	670.3±8.4	Derived from $\Delta_f H^\circ$ in ref	1998NIST
but-1-en-3-yne **H_2C**=**C**–C≡CH	136 8±2.5	572.4±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1-butyne **C_2H_5**–C≡CH	124.5±1.0	520.9±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-butyne **CH_3**–CH_2C≡CH	(1) 76.0±2 (2) **76.6±1.2**	318.0±8.4 320.5±5.0	(1) VLPP (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1978KIN (2) 1986PED/NAY
2-butyne **CH_3**–C≡CCH	121.8±3 2	509.6±13.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-pentyne **CH_3**–CH_2C≡CCH_3	73.7±1.5	308.4±6.3	VLPP	1982NGU/KIN
2-methy-1-butyne **CH_3**–CH(CH_3)C≡CH	73±2	305.4±8.4	VLPP	1981NGU/KIN
2-methy-1-pentyne **CH_3**–CH(CH_3)C≡CCH_3	76.7±1 5	320.9±6.3	VLPP	1981KIN/NGU
2,2-dimethy-1-butyne **CH_3**–C(CH_3)$_2$C≡CH	70.7±1.5	295.8±6.3	VLPP	1977KIN
2,2-dimethy-1-pentyne **CH_3**–C(CH_3)$_2$C≡CCH_3	72.5±1.5	303.3±6.3	VLPP	1981KIN/NGU
1-hexyne **nC_3H_7**–CH_2C≡CH	73 2±1 5	306.3±6.3	VLPP	1981KIN
2-ethyl-1-pentyne **sC_4H_9**–CH$_3$C≡CH	71.7±1.5	300.0±6.3	SPTS	1978TSA
propene **CH_3**–CHCH_2	101.9±1.5	426.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1,2-butadiene **CH_3**–CH=CCH_2	86.0±1.4	359.8±5.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1,3-butadiene **C_2H_3**–CH=CH_2	116.9±1.5	489.1±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

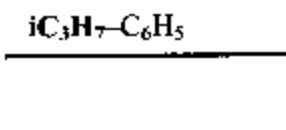
断裂键 (**黑体** 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1-methylcyclopropene **CH_3**–cyclopro-en-1-yl	81 4±5	340.6±20.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-butene **CH_3** $CH_2CH=CH_2$	(1) 76.5±2.2 (2) **75.9±0.9**	320.1±9.2 **317.6±3.8**	(1) VLPP (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1981NGU/KIN (2) 1986PED/NAY
1-butene **C_2H_5**–$CH=CH_2$	100.0±1.0	418.4±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
(E)-2-butene (E)-**CH_3**–$CH=CHCH_3$	101.6±2.0	425.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
(Z)-2-butene (Z)-**CH_3**–$CH=CHCH_3$	102.6±2.0	429.3±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1,2-pentadiene **C_2H_5**–$CH–C=CH_2$	80.6±1.5	337.2±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1,4-pentadiene **C_2H_3** $CH_2CH–CH_2$	87.2±1.2	364.8±5.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
(E)-1,3-pentadiene (E)-**CH_2=CH**–$CH=CHCH_3$	117.2±2.0	490.4±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
(Z)-1,3-pentadiene (Z)-**CH_2=CH**–$CH=CHCH_3$	118.5±2.0	495.8±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-pentene **C_2H_5**–$CH_2CH=CH_2$	74.3±1.5	310.9±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
(E)-2-pentene (E)-**CH_3**–$CH_2CH=CHCH_3$	77.6±2.2	324.7±9.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
(Z)-2-pentene (Z)-**CH_3**–$CH_2CH=CHCH_3$	78.6±2.2	328.9±9.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-pentene **C_2H_5**–$CH=CHCH_3$	99.8±2.0	417.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyl-1-butene **CH_3** $CH_2C(CH_3)–CH_2$	(1) 72.0±2 (2) **74.1±1.0**	301.2±8.4 **310.0±4.2**	(1) Kinetics (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1981STE/ROW (2) 1986PED/NAY
3-methyl-1-butene **CH_3**–$CH(CH_3)CH–CH_2$	72.3±1.5	302.5±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3,3-dimethyl-1-butene **CH_3**–$C(CH_3)_2CH=CH_2$	(1) 68.1±1.5 (2) **67.5±1.5**	284.9±6.3 **282.4±6.3**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1982MCM/GOL (2) 1986PED/NAY
3-methyl-1-butene **iC_3H_7**–$CH–CH_2$	99.2±1.5	415.1±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1,5-hexadiene **C_3H_5**–C_3H_5	61.5±1.0	257.3±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-hexene **nC_3H_7**–$CH_2CH=CH_2$	(1) 70.7±2 (2) **75.0±1.0**	295.8±8.4 **313.8±4.2**	(1) SPST (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1976TSA(b) (2) 1986PED/NAY
1-hexene **nC_4H_9**–$CH=CH_2$	100.6±1.3	420.9±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值， 括号内数字 文献编号)		方法	文献
	kcal/mol	kJ/mol		
(E)-2-hexene (E)-$\mathbf{C_2H_5}$-CH_2CH=$CHCH_3$	76.2±2.4	318.8±10.0	Derived from Δ_fH° in ref.	1986PED/NAY
(Z)-2-hexene (Z)-$\mathbf{C_2H_5}$–CH_2CH=$CHCH_3$	76.6±2.4	320.5±10.0	Derived from Δ_fH° in ref.	1986PED/NAY
2-hexene $\mathbf{C_3H_7}$ CH=$CHCH_3$	100.5±2.0	420.5±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
2-methyl-1-pentene $\mathbf{C_2H_5}$–$CH_2C(CH_3)$=CH_2	73.2±1.0	306.3±4.2	Derived from Δ_fH° in ref.	1986PED/NAY
3-methyl-1-pentene $\mathbf{C_2H_5}$–$CH(CH_3)CH$=CH_2	70.8±1.5	296.2±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
3-methyl-1-pentene $\mathbf{sC_4H_9}$–CH–CH_2	99.6±1.0	416.7±4.2	Derived from Δ_fH° in ref	1986PED/NAY
4-methyl-1-pentene $\mathbf{iC_3H_7}$–CH_2CH=CH_2	74.1±1.0	310.0±4.2	Derived from Δ_fH° in ref.	1986PED/NAY
4-methyl-1-pentene $\mathbf{iC_4H_9}$–CH=CH_2	100.6±1.5	420.9±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
(E)-4-methyl-2-pentene (E)-$\mathbf{iC_3H_7}$–CH $CHCH_3$	99.5±2.0	416.3±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
(Z)-4-methyl-2-pentene (Z)-$\mathbf{iC_3H_7}$ CH=$CHCH_3$	100.5±2.0	420.5±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
3,3-dimethyl-1-butene $\mathbf{tC_4H_9}$ CH=CH_2	97.7±1.3	408.8±5.4	Derived from Δ_fH° in ref.	1986PED/NAY
1-heptene $\mathbf{nC_4H_9}$ CH_2CH–CH_2	74.3±1.0	310.9±4.2	Derived from Δ_fH° in ref.	1986PED/NAY
5-methyl-1-hexene $\mathbf{iC_4H_9}$–CH_2CH=CH_2	73.2±1.5	306.3±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
5-methyl-1-hexene $\mathbf{nC_3H_7}$–$CH_2C(CH_3)$=CH_2	70.1±1.6	293.3±6.7	Derived from Δ_fH° in ref.	1986PED/NAY
2,4-dimethyl-1-pentene $\mathbf{iC_3H_7}$–$CH_2C(CH_3)$–CH_2	71.6±1.5	299.6±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
4,4-dimethyl-1-pentene $\mathbf{tC_4H_9}$–CH_2CH=CH_2	71.9±1.5	300.8±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
(E)-4,4-dimethyl-2-pentene (E)-$\mathbf{tC_4H_9}$–CH=$CHCH_3$	96.6±2.0	404.2±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
(Z)-4,4-dimethyl-2-pentene (Z)-$\mathbf{tC_4H_9}$ CH=$CHCH_3$	100.5±2.0	420.5±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
2,4,4-trimethyl-1-pentene $\mathbf{tC_4H_9}$–$CH_2C(CH_3)$=CH_2	68.6±2.0	287.0±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
1-octene $\mathbf{nC_5H_{11}}$–CH_2CH=CH_2	73.3±1.5	306.7±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
3-cyclopentylpropene **c-pentyl**–CH_2CHCH_2	71.9±1.5	300.8±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
vinylcyclohexane **c-hexayl**-$CHCH_2$	91.3±2.0	382.0±8.4	Derived from Δ_fH° in ref.	1986PED/NAY

5.3 芳香碳氢化合物

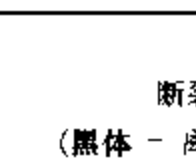
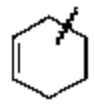
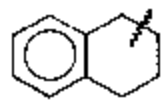
表 5.3 芳香碳氢化合物内的 C—C BDEs

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methylbenzene **CH_3–C_6H_5**	102.0±1.0	426.8±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
phenylacetylene **HCC–C_6H_5**	141.2±1.4	590.8±5.9	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
vinylbenzene **C_2H_3–C_6H_5**	115.2±1.3	482.0±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethylbenzene, substituted  Y = H	(1) 74.1 (2) 75 8±1 (3) **76.4±1.7**	310.0 317.1 **319.7±7.1**	(1) VLPP (2) Derived (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1980BAR/STE (2) 1982MCM/GOL (3) 1986PED/NAY
2-Me	(1) 72.9	305.0		
3-Me	(1) 73.8	308.8		
4-CH_2=CH	(4) 70.6	295.4	(4) VLPP	(4) 1986ROB/STE
2,6-Me_2	(1) 71.2	297.9		
3,6-Me_2	(1) 72.5	303.3		
3,5-Me_2	(1) 73.5	307.5		
ethylbenzene **C_2H_5–C_6H_5**	100.2±1.0	419.2±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclopropylbenzene **c-C_3H_5–C_6H_5**	109.8±1.2	459.4±5.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
prop-2-enylbenzene **C_2H_3–$CH_2C_6H_5$**	87.9	367.8	Derived from $\Delta_f H^\circ$ in ref.	1999VER(c)
propylbenzene **C_2H_5–$CH_2C_6H_5$**	74.9±1.7	313.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
prop-2-enylbenzene **$C_2H_3CH_2$–C_6H_5**	87.6	366.5	Derived from $\Delta_f H^\circ$ in ref.	1999VER(c)
propylbenzene **nC_3H_7–C_6H_5**	100.8±1.0	421.7±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
iso-propylbenzene **CH_3-$CH(CH_3)C_6H_5$**	(1) 73.8 (2) **74.6±1.5**	308.8 **312.1±6.3**	(1) VLPP (2) Rc-cal.	(1) 1981ROB/STE (2) 1984ROS/MCM
iso-propylbenzene **iC_3H_7–C_6H_5**	98.9±1.2	413 8±5.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 - 文献编号)		方法	文献
	kcal/mol	kJ/mol		
butylbenzene **nC_4H_9**–C_6H_5	100.6±1.0	420.9±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
butylbenzene **nC_3H_7**–$CH_2C_6H_5$	75.3±1.7	315.1±7.1	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
4-phenyl-1-butene **CH_2=CHCH_2** -$CH_2C_6H_5$	61.4±2	256.9±8.4	VLPP	1979KIN/NGU
2-methyl-1-phenylpropane **iC_3H_7**–$CH_2C_6H_5$	74.5±1.7	311.7±7.1	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylpropylbenzene **iC_4H_9**–C_6H_5	100.7±1.5	421.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
tert-butylbenzene **tC_4H_9**–C_6H_5	95.8±1.5	400.8±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
4-phenyl-1-butyne **$C_6H_5CH_2$**–$CH_2C{\equiv}CH$	61.4±2	256.9±8.4	VLPP	1979KIN/NGU
2-phenyl-propane **CH_3**–$CH(CH_3)C_6H_5$	74.6±1.5	312.1±6.3	VLPP	1981ROB/STE
2-phenylbutane **C_2H_9**–$CH(CH_3)C_6H_5$	73.7±1.5	308.4±6.3	VLPP	1981ROB/STE
tert-butylbenzene **CH_3**–$C(CH_3)_2C_6H_5$	72.5±2.0	303.3±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
((1Z)-prop-1-enyl)benzene **CH_3**–$CH_2CHCHPh$	70.6	295.4	VLPP	1986ROB/STE
1,1-diphenylethane **CH_3**–$CH(C_6H_5)_2$	(1) 71.3 (2) **75.5±1.5**	298.3 **315.9±6.3**	(1) VLPP (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1984ROS/MCM (2) 1999VER(d)
2-methyl-1,1-diphenylpropane **iC_3H_7**-$CH(C_6H_5)_2$	73.6±1.5	307.9±6.3	Derived from $\Delta_f H^\circ$ in ref.	1999VER(d)
2,2-diphenylpropane **CH_3**–$C(CH_3)(C_6H_5)_2$	69.5±2	290.8±8.4	VLPP	1981STE
biphenyl **C_6H_5**–C_6H_5	114.4±1.5	478.6±6 3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
diphenylmethane **C_6H_5**–$CH_2C_6H_5$	90.4±2.0	378.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
bibenzyl **$C_6H_5CH_2$**–$CH_2C_6H_5$	62.6±2.2	261.9±9.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
triphenylmethane **C_6H_5**–$CH(C_6H_5)_2$	86.3±2 0	361.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
tetraphenylmethane **C_6H_5** -$C(C_6H_5)_3$	77.5±3	324.3±12.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1,1,2,2-tetraphenylethane **Ph_2CH**–$CHPh_2$	59.1±2	247.3±8.4	Derived from $\Delta_f H^\circ$ *in ref.*	1990BEC/DOG

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1,2,2,2-tetraphenylethane **PhCH$_2$**–CPh$_3$	54.8±3.5	229.3±14.6	Derived from $\Delta_f H^\circ$ in ref.	1990BEC/DOG
1-methylindene 	72.4	302.9	VLPP	1986ROB/STE
1-methylnaphthalene **CH$_3$**–naphth-1-yl	103.8±2.0	434.3±8.4	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
2-methylnaphthalene **CH$_3$**–naphth-2-yl	105.3±2.0	440.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclohexylbenzene c-**C$_6$H$_{11}$**–C$_6$H$_5$	98.7±2.0	413.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl-1-naphthalene **CH$_3$**–1-naphthymethyl	72.9±1.5	305.0±6.3	VLPP	1980MCM/TRE
ethyl-9-anthracene **CH$_3$**–9-anthracenylmethyl	67.6±1.5	282.8±6.3	VLPP	1980MCM/TRE
ethyl-9-phenanthrene **CH$_3$**–9-phenanthrenylmethyl	72.9±1.5	305.0±6.3	VLPP	1980MCM/TRE
phenalenyl dimer C–C bond	11.34±0.11	47.4±0.5	ESR	2003ZHE/SAE
cyclohexene 	74.8	313	Derived	1997DOR/PUG
tetralin 	72.9	305	SPST	1995TSA/CUI

5.4 卤代碳氢化合物

表 5.4 卤代碳氢化合物内的 C—C BDEs

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
tetrafluoroethylene **CF$_2$**=CF$_2$	(1) 76.3 (2) 79.1±3.8 (3) 68.7	319.2 331±16 287.4	(1) Pyrolysis, MS detect. (2) Derived (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1968ZMB/UY (2) 1991PAU/SQU (3) 2002CRC

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 - 文献编号) kcal/mol	 kJ/mol	方法	文献
tetrachloroethylene **CCl_2**=CCl_2	(1) 106.3±4.9 (2) 110.6	445±21 462.8	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1991PAU/SUQ (2) 1986PED/NAY
perfluoroethane **CF_3**–CF_3	(1) 93±2 (2) 98.7±2.5 (3) **98.7±1.2** (4) 96.4±5.2	389.1±8.4 413.0±10.5 **413.0±5.0** 403 3±21.8	(1) Pyrolysis (2) Kinetics (3) Derived (4) Review	(1) 1965TSC (2) 1967COO/WHI (3) 1998RUS/MIC (4) 2001LAZ/PRO
pentafluoroethane **CF_3**–CHF_2	95.5±2	399.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	1975CHE/ROD
chloropentafluoroethane **CF_3**–$CClF_2$	89.3±3	373.6±12.5	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
1,1,1,2-tetrafluoroethane **CF_3**–CH_2F	95±2	397.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	1975CHE/ROD
1-bromo-1-chloro-2,2,2-trifluoroethane **CF_3**–CHBrCl	90.1±2	377.0±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1-bromo-2,2,2-trifluoroethane **CF_3**–CH_2Br	95.5±2	399.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
1,1,1-trifluoro-2-iodoethane **CF_3**–CH_2I	97.6±2.5	408.4±10.5	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
1,1,1-trifluoroethane **CF_3**–CH_3	(1) 101.2±1.1 (2) 102.6±1.2	423.4±4.6 429.3±5.0	(1) Kinetics (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1973ROD/FOR (2) 1998NIST
1,1,2,2-tetrafluoroethane **CHF_2**–CHF_2	91.4±3.7	382.4±15.5	SPST	1971MIL/HAR
1,2-dichlorotetrafluoroethane **$CClF_2$**–$CClF_2$	90.5±3	378.7±12.6	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
1,1,2-trifluoroethane **CHF_2**–CH_2F	94.2±4	394.1±16.7	Derived from $\Delta_f H^\circ$ in ref.	1968LAC/SKI
1,2-difluoroethane **CH_2F**–CH_2F	88±2	368.2±8.4	Thermal elimination	1971KER/TIM
1,1-difluoroethane **CHF_2**–CH_3	96.8±2	405.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
fluoroethane **CH_2F**–CH_3	(1) 90.4±3 (2) **93.2±2**	378 2±12.6 **389.9±8.4**	Derived from $\Delta_f H^\circ$ in ref.	(1) 1975CHE/ROD (2) 1998SMI
1-chloro-1-fluoroethane **CHClF**–CH_3	95.5±3	399.6±12.6	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
perchloroethane **CCl_3**–CCl_3	(1) 70.1±3.5 (2) **68.3±1.5**	293.3±14.6 **285.8±6.3**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1997CIO/LIU (2) 2002CRC
1,1,1,2-tetrachloro-2,2-difluoroethane **CCl_3**–$CClF_2$	67.4±3	282.0±12.6	Derived from $\Delta_f H^\circ$ in ref.	2002CRC

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
pentachloroethane **CCl_3–$CHCl_2$**	(1) 75 4±3.9 (2) **73.2±2**	315.5±16.3 **306.3±8.4**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1997CIO/LIU (2) 2002CRC
1,1,1,2-tetrachloroethane **CCl_3–CH_2Cl**	(1) 82.3±3.0 (2) **77.4±2**	344.3±12.6 **323.8±8.4**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1997CIO/LIU (2) 1998NIST
1,1,1-trichloroethane **CCl_3–CH_3**	(1) 87.6±2.0 (2) **86.6±1.5**	366.5±8.4 **362.3±6.3**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1997CIO/LIU (2) 2002CRC
1,1,2,2-tetrachloroethane **$CHCl_2$–$CHCl_2$**	(1) 84.0±4.7 (2) 80.3±2 (3) **81.8**±2	351.5±19.7 336.0±8.4 342.3±8.4	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref. (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1997CIO/LIU (2) 2002CRC (3) 1998NIST
1,1,2-trichloroethane **$CHCl_2$–CH_2Cl**	(1) 86.5±4.0 (2) **85.7±2**	361.9±16 7 **358.6±8.4**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1997CIO/LIU (2) 1998NIST
1,1-dichloroethane **$CHCl_2$–CH_3**	(1) 89.8±3 3 (2) **87.3±0.8**	375.7±13.8 **365.1±3.3**	Derived	(1) 1997CIO/LIU (2) 1998SEE
1,1-bromochloroethane **CHBrCl–CH_3**	89.3	384.5	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
1,2-dibromo-1,2-dichloro-ethane **CHClBr–CHClBr**	77.2±3	323.0±12.6	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
1,2-dichloroethane **CH_2Cl–CH_2Cl**	(1) 87 2±3 3 (2) **86.2±2** (3) 87.1±1.3	364.8±13.8 **360.7±8.4** 364.6±5.3	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref. (3) Derived	(1) 1997CIO/LIU (2) 2002CRC (3) 2002LAG/DIO
1,1-dibromoethane **$CHBr_2$–CH_3**	89.1	372.8	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
1-bromo-2-chloroethane **CH_2Br–CH_2Cl**	90.4	378.2	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
1,2-dibromoethane **CH_2Br–CH_2Br**	90.8±2	379.9±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1,2-diiodoethane **CH_2I–CH_2I**	92.5±2.5	387.0±10.5	Derived from $\Delta_f H^\circ$ in ref.	1994CAR/LAY
chloroethane **CH_3–CH_2Cl**	89.8±2.2	375 7±9 2	Derived	1997CIO/LIU
bromoethane **CH_3–CH_2Br**	91.2±2	381 6±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
iodoethane **CH_3–CH_2I**	91.9±2	384 5±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
perfluoropropane **CF_3–CF_2CF_3**	101.4±3	424.3±13.6	Derived from $\Delta_f H^\circ$ in ref.	2002CRC

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
3,3,3-trifluoroprop-1-yne **CF_3**-C≡CH	123.2	515.5	Derived from Δ_fH° in ref.	1988LIA/BAR
3,3,3-trifluoropropene **CF_3**–CH=CH_2	107±3	447.7±12.6	Derived from Δ_fH° in ref.	2002CRC
perfluoropronene **CF_3**–CF=CF_2	85±2.5	355.6±10.5	SPST	1995HE
fluoropropane **CH_3**–CH_2CH_2F	91.6±3	383.3±12.6	Derived from Δ_fH° in ref.	1998SMI
fluoropropane **CH_3CH_2**–CH_2F	101.5±3	424.7±12.6	Derived from Δ_fH° in ref.	1998SMI
1-chloropropane **CH_3**–CH_2CH_2Cl	88.8±0.6	371.4±2.8	Derived	1998SEE
2-chloropropane **CH_3**–$CHClCH_3$	87.8±0.5	367.5±2.0	Derived	1998SEE
1,2-dichloropropane **CH_2Cl**–$CHClCH_3$	85.2±2	356.5±8.4	Derived from Δ_fH° in ref.	2002CRC
1,3-dichloropropane **CH_2Cl**–CH_2CClH_2	88.2±2	369.0±8.4	Derived from Δ_fH° in ref.	2002CRC
2,2-dichlororopane **CH_3**–CCl_2CH_3	86.7±2	362.8±8.4	Derived from Δ_fH° in ref.	2002CRC
1,2-dibromopropane **CH_2Br**–$CHBrCH_3$	88.3±2	369.4±8.4	Derived from Δ_fH° in ref.	2002CRC
1,3-dichlorobutane **CH_2ClCH_2**–$CHClCH_3$	87.1±2	364.4±8.4	Derived from Δ_fH° in ref.	2002CRC
1,4-dichlorobutane **CH_2ClCH_2** CH_2CClCH_2	88.2±2	369.0±8.4	Derived from Δ_fH° in ref.	2002CRC
2,3-dibromobutane **CH_3CHBr**–$CHBrCH_3$	85.0±2	355.6±8.4	Derived from Δ_fH° in ref	2002CRC
1-bromobutane **CH_2Br**–C_3H_7	90.3±2	377.8±8.4	Derived from Δ_fH° in ref.	2002CRC
2-bromobutane **CH_3CHBr**–C_2H_5	87.5±2	366.1±8.4	Derived from Δ_fH° in ref.	2002CRC
1-chlorobutane **CH_2Cl**–C_3H_7	88.7±2	371.1±8.4	Derived from Δ_fH° in ref.	2002CRC
2-chlorobutane **CH_3CHCl**–C_2H_5	85.2±2	356.5±8.4	Derived from Δ_fH° in ref.	2002CRC
1-chlorobutane **CH_2Cl**–iC_3H_7	87.1±2	364.4±8.4	Derived from Δ_fH° in ref.	2002CRC
1-bromopentane **CH_2Br**–nC_4H_9	90.3±2	377.8±8.4	Derived from Δ_fH° in ref.	2002CRC
1-chloropentane **CH_2Cl**–nC_4H_9	88.4±2	369.9±8.4	Derived from Δ_fH° in ref.	2002CRC

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1-chloropentane **CH_2ClCH_2**–C_3H_7	87.8±2	367.4±8.4	Derived from Δ_fH° in ref.	2002CRC
2-chloro-3-methyl-butane **CH_2Cl**–iC_4H_9	87.6±2	366.5±8.4	Derived from Δ_fH° in ref.	2002CRC
2-chloro-3-methyl-butane **CH_2ClCH_2**–iC_3H_7	86.1±2	360.2±8.4	Derived from Δ_fH° in ref.	2002CRC
1-bromohexane **CH_2Cl**–nC_5H_{11}	88.8±2	371.5±8.4	Derived from Δ_fH° in ref.	2002CRC
2-chlorohexane **CH_2ClCH_2** nC_4H_9	85.7±2	358 6±8.4	Derived from Δ_fH° in ref.	2002CRC
fluorononane **CH_2FCH_2**–nC_7H_{13}	90.0±3	376.6±12.6	Derived from Δ_fH° in ref.	1997SCH/VER
2,2-difluorononane **CH_3CF_2**–nC_7H_{13}	91.2±3	381.6±12.6	Derived from Δ_fH° in ref.	1997SCH/VER
(chloromethyl)benzene **CH_2Cl**–C_6H_5	102.7	429.7	Derived from Δ_fH° in ref.	2002VER/KRA
(bromomethyl)benzene **CH_2Br**–C_6H_5	100.8	421.7	Derived from Δ_fH° in ref.	2002VER/KRA
(iodomethyl)benzene **CH_2I**–C_6H_5	103.4	432.6	Derived from Δ_fH° in ref.	2002VER/KRA
(trifluoromethyl)benzene **CF_3**–C_6H_5	110.7±3	463 2±12.6	Derived from Δ_fH° in ref.	1994PED
pentafluorophenylmethane **CH_3**–C_6F_5	105	439.3	Derived	1975CHO/GOL
pentafluorophenyl trifluoromethane **CF_3**–C_6F_5	104	435.1	Derived	1975CHO/GOL
(2,2,2-trifluoroethyl)benzene **CF_3**–$CH_2C_6H_5$	86.1±3	360.2±12.6	Derived from Δ_fH° in ref.	1997SCH/VER
(3,3-difluoropropyl)benzene **CHF_2**–$CH_2CH_2C_6H_5$	97.8±4	409.2±16.7	Derived from Δ_fH° in ref.	1997SCH/VER
(3,3-difluoropropyl)benzene **CHF_2CH_2**–$CH_2C_6H_5$	79.1±3	331.0	Derived from Δ_fH° in ref.	1997SCH/VER
bipentafluorophenyl **C_6F_5**–C_6F_5	116.7	488.3	Combustion	1979PRI/SAP
(2,2,2-trifluoro-1-phenyl-ethyl)benzene **CF_3**–$CHPh_2$	84.2±4	352.3±16.7	Derived from Δ_fH° in ref.	1997SCH/VER
(2,2,2-trifluoro-1,1-diphenyl-ethyl)benzene **CF_3**–CPh_3	69.5±4	290.8±16 7	Derived from Δ_fH° in ref.	1997SCH/VER

续表

断裂键 (黑体　离解原子团)	BDEs (黑体 = 推荐值; 括号内数字 - 文献编号)		方法	文献
	kcal/mol	kJ/mol		
(3-fluoro-1,1-diphenyl-propyl)benzene **CH_2FCH_2–CPh_3**	65.7±4	274.9±16.7	Derived from $\Delta_f H^\circ$ in ref.	1997SCH/VER
(3,3-difluoro-1,1-diphenyl-propyl)benzene **CHF_2CH_2–CPh_3**	63.1±4	264.0±16.7	Derived from $\Delta_f H^\circ$ in ref.	1997SCH/VER

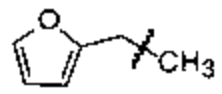
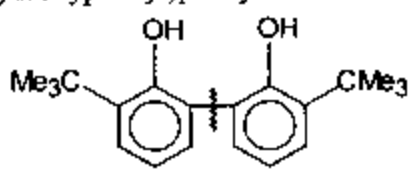
5.5　含杂原子的碳氢化合物

5.5.1　含氧原子的碳氢化合物

表 5.5.1　含氧原子的碳氢化合物内的 C—C BDEs

断裂键 (黑体 = 离解原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ethanol **CH_3–CH_2OH**	87.2±1.0	364.8±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2,2-trifluoroethanol **CF_3–CH_2OH**	96.9±1.5	405.4±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
allyl alcohol **C_2H_3–CH_2OH**	97.1±1.2	406.3±5.0	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1-propanol **C_2H_5–CH_2OH**	85.3±1.2	356.9±5.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2,3,3-tetrafluoro-1-propanol **CHF_2CF_2–CH_2OH**	90.7±2	379.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
1-butanol **C_3H_7–CH_2OH**	85.4±0.8	357.3±3.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyl-1-propanol **iC_3H_7–CH_2OH**	84.8±1.0	354.8±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-pentanol **C_4H_9–CH_2OH**	85.0±1.0	355.6±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyl-1-butanol **sC_4H_9–CH_2OH**	84.3±1.0	352.7±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-methyl-1-butanol **iC_4H_9–CH_2OH**	84.6±1.3	354.0±5 4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
hexanol **nC_5H_{11}–CH_2OH**	84.4±1.3	353.1±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
benzyl alcohol **C_6H_5–CH_2OH**	98.8±1.3	413.4±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
2-propanol **CH_3**–$CH(CH_3)OH$	87.9±1.2	367.8±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
2-butanol **C_2H_5**–$CH(CH_3)OH$	86.0±1.2	359.8±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
2-pentanol **C_3H_7**–$CH(CH_3)OH$	86.1+1.2	360.2+5.0	Derived from Δ_fH° in ref.	1986PED/NAY
3-methyl-2-butanol **iC_3H_7**–$CH(CH_3)OH$	83.9+1.3	351.0+5.4	Derived from Δ_fH° in ref.	1986PED/NAY
tert-butyl alcohol **CH_3**–$C(CH_3)_2OH$	83.5±1.2	349.4±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
2-methyl-2-butanol **C_2H_5**–$C(CH_3)_2OH$	81.2±1.2	339.7±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
3-pentanol **C_2H_5**–$CH(C_2H_5)OH$	84.8±1.2	354.8±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
ethylene glycol **HOH_2C**–CH_2OH	85.6±1.5	358.2±6.3	Derived from Δ_fH° in ref.	2002CRC
1,2-propylene glycol **$CH_3CH(OH)$** –CH_2OH	86.2±1.8	360.7±7.5	Derived from Δ_fH° in ref.	2002CRC
1,2-propanediol **$HOCH_2$**–$CH(CH_3)OH$	84.2±1.3	352.3±5.4	Derived from Δ_fH° in ref.	1986PED/NAY
2,3-butanediol **$OH(CH_3)CH$**–$CH(CH_3)OH$	90.5±1.5	378.7±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
2-aminoethan-1-ol **NH_2CH_2**–CH_2OH	80.2±2.5	335.6±10.5	Derived from Δ_fH° in ref.	1988LIA/BAR
ethyl methyl ether **CH_3**–CH_2OCH_3	86.8±1.2	363.2±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
ethyl propyl ether **C_2H_5**–CH_2OCH_3	85.3±1.2	356.9±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
1,2-methyloxyethane **CH_3OCH_2**–CH_2OCH_3	(1) 81±2.5 (2) 68.7	338.9±10.5 287.5	(1) Derived from Δ_fH° in ref. (2) UV Photoioniz.	(1) 1988LIA/BAR (2) 2003WAN/WU
2-ethyl furan 	75±2	313.8±8.4	VLPP	1981STE
6-(tert-butyl)-2-(3-(tert-butyl)-2-hydroxyphenyl)phenyl 	83.1	347.7	EPR	2001LUC/PED
ketenylidene C=CO	52.8±4.6	220.9±19.3	Derived	1996ZEN/PER

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ethanal **H_2C**=CO	78.73±0.02	329.41±0.08	GPA, revised	1999RUS/LIT
acetaldehyde **CH_3**–C(O)H	84.8±0.4	354.8±1.7	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
trichloroacetaldehyde **CCl_3**–C(O)H	73.9±1.2	309.2±5.0	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
acetyl fluoride **CH_3**–C(O)F	99.8±1.5	417.6±6.3	Derived from $\Delta_f H^\circ$ in ref	2002CRC
acetyl chloride **CH_3**–C(O)Cl	87.9±1.5	367.8±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
trichloroacetyl chloride **CCl_3**–C(O)Cl	69.1±1.5	289.1±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
dichloroacetyl chloride **$CHCl_2$**–C(O)Cl	74.7±2	312.5±8.4	Derived from $\Delta_f H^\circ$ in ref	2002CRC
chloroacetyl chloride **$CClH_2$**–C(O)Cl	81.3±2	340.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
propanal **C_2H_5**–C(O)H	82.7±0.5	346.0±2.1	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
(*Z*) 2 butenal **CH_3CH**=CH C(O)H	97.8±2.0	409.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
butanal **C_3H_7**–C(O)H	82.7±1.0	346.0±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methylpropanal **iC_3H_7**–C(O)H	82.5±1.2	345.2±5.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pentanal **nC_4H_9**–C(O)H	83.2±0.7	348.1±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
heptanal **nC_6H_{13}**–C(O)H	81±2.0	338.9±8.4	Derived from $\Delta_f H^\circ$ in ref.	1994PED
benzaldehyde **C_6H_5**–C(O)H	97.6±1.0	408.4±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
propanal **CH_3**–CH_2C(O)H	82.0±2.4	343.1±10.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
butanal **C_2H_5**–CH_2C(O)H	79.8±2.5	333.9±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pentanal **C_3H_7**–CH_2C(O)H	80.9±2.5	338.5±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
heptanal **C_5H_{11}**–CH_2C(O)H	78.5±3.0	328.4±12.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-phenylpropanone **$C_6H_5CH_2$**–CH_2C(O)H	67.9±1.5	284.1±6.3	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
dimethyl ketone **CH_3**–C(O)CH_3	84.1±0.5	351.9±2.1	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值， 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
bromoacetone **CH_2Br**–C(O)CH_3	85 9±1.5	359.4±6.3	Derived from Δ_fH° in ref.	2002CRC
chloroacetone **CH_2I**–C(O)CH_3	83.5±2.5	349.4±10.5	Derived from Δ_fH° in ref.	1086PED/NAY
ethyl methyl ketone **CH_3**–C(O)C_2H_5	84.3±0.5	352.7±2.1	Derived from Δ_fH° in ref.	1986PED/NAY
ethyl methyl ketone **C_2H_5**–C(O)CH_3	83.0±0.7	347.3±2.9	Derived from Δ_fH° in ref.	1986PED/NAY
diethyl ketone **C_2H_5**–C(O)C_2H_5	82.3±1.2	344.3±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
methyl propyl ketone **C_3H_7**–C(O)CH_3	83.3±0.7	348.5±2.9	Derived from Δ_fH° in ref.	1986PED/NAY
ethyl propyl ketone **C_3H_7**–C(O)C_2H_5	82.3±1.3	344.3±5.4	Derived from Δ_fH° in ref.	1994PED
iso-propyl methyl ketone **iC_3H_7**–C(O)CH_3	81.3±0.9	340.2±3.8	Derived from Δ_fH° in ref.	1986PED/NAY
iso-propyl ethyl ketone **iC_3H_7**–C(O)C_2H_5	81.6±1.5	341.4±6.3	Derived from Δ_fH° in ref.	1994PED
butyl methyl ketone **nC_4H_7**–C(O)CH_3	82.9±1.3	346.9±5.4	Derived from Δ_fH° in ref.	1986PED/NAY
tert-butyl methyl ketone **tC_4H_9**–C(O)CH_3	78.7±1.0	329.3+4 2	Derived from Δ_fH° in ref.	1986PED/NAY
tert-butyl ethyl ketone **tC_4H_9**–C(O)C_2H_5	78.8±1.0	329 7±4.2	Derived from Δ_fH° in ref.	1994PED
benzyl methyl ketone **$C_6H_5CH_2$**–C(O)CH_3	70.1±2	293.3±8.4	Derived from Δ_fH° in ref.	1994PED
benzyl phenyl ketone **$C_6H_5CH_2$** -C(O)C_6H_5	71.2±3	297.9±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
ethyl methyl ketone **CH_3**–CH_2C(O)CH_3	86.5±3	361.9±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
butyl methyl ketone **C_3H_7**–CH_2C(O)CH_3	82.4±1.5	344.8±6.3	Derived from Δ_fH° in ref.	2002CRC
methyl phenyl ketone **CH_3**–C(O)C_6H_5	85.0	355.6	Photolysis	1997ZHA/CHE
trifluoromethyl phenyl ketone **CF_3**–C(O)C_6H_5	73.8±2	308.8±8.4	VLPP	1977COL/ZAB
ethyl phenyl ketone **C_2H_5**–C(O)C_6H_5	82.2±2.8	343.9±11.7	Derived from Δ_fH° in ref.	1986PED/NAY
diphenyl ketone **C_6H_5**-C(O)C_6H_5	94.7±4	396.2±16.7	Derived from Δ_fH° in ref.	1988LIA/BAR
benzyl phenyl ketone **PhCH_2**–C(O)Ph	71.2±3.5	297.9±14.6	Derived from Δ_fH° in ref.	1986PED/NAY

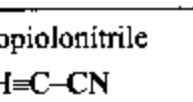
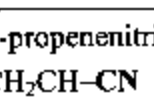
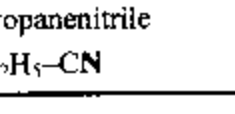
续表

断裂键 （**黑体** = 离解原子团）	BDEs （**黑体** – 推荐值， 括号内数字 = 文献编号）		方法	文献
	kcal/mol	kJ/mol		
bibenzyl ketone **PhCH$_2$**–C(O)CH$_2$Ph	65.4	273.6	Review	1982MCM/GOL
ethane-1,2-dial **HC(O)** –C(O)H	70.7±1.5	295.8±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
oxalyl chloride **ClC(O)**–C(O)Cl	69.9±2	292.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
1,2-propanedione **CH$_3$C(O)** –C(O)H	72.3±2	302.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
biacetyl **CH$_3$C(O)** –C(O)CH$_3$	73.4±1	307.1±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
bibenzoyl **C$_6$H$_5$C(O)** –C(O)C$_6$H$_5$	68.9±4	288.3±16.7	Review	1982MCM/GOL
2,4-pentanedione **CH$_3$C(O)** –CH$_2$C(O)CH$_3$	80.8±2	338.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1994PED
acetic acid **CH$_3$**–C(O)OH	92.0±2	384.9±8.4	Derived from $\Delta_f H^\circ$ in ref	1986PED/NAY
trifluoroacetic acid **CF$_3$**–C(O)OH	88.6±2	370.7±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
chloroacetic acid **CClH$_2$**–C(O)OH	85.5±2	357.7±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
bromoacetic acid **CH$_2$Br**–C(O)OH	85.6±2	358.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	2001DOR/NOV
glycine **NH$_2$CH$_2$**–C(O)OH	83.5±2	349.4±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
N-methylglycine **CH$_3$NHCH$_2$**–C(O)OH	71.8±2	300.4±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
propenoic acid **C$_2$H$_3$**- C(O)OH	104.1±2	435.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
propanoic acid **C$_2$H$_5$**–C(O)OH	90.8±1.5	379.9±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-chloropropanoinc acid **CH$_3$CHCl**- C(O)OH	85.5±2	357.7±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
butanoic acid **C$_3$H$_7$**–C(O)OH	91.0±1.5	380.7±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pentanoic acid **C$_4$H$_9$**–C(O)OH	89.7±1.5	375.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1994PED
3-methylbutanoic acid **sC$_4$H$_9$**–C(O)OH	91.6±3	383.3±12.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2-dimethylpropanoic acid **tC$_4$H$_9$**–C(O)OH	82.5±4	345.2±16.7	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
hexanoic acid **C$_5$H$_{11}$**–C(O)OH	88.8±1.5	371.5±6.3	Derived from $\Delta_f H^\circ$ in ref.	1994PED

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
heptanoic acid **C_6H_{13}**–C(O)OH	89.7±1.5	375.3±6.3	Derived from Δ_fH^o in ref.	1994PED
benzoic acid **Ph**–C(O)OH	102.7±2	429.7±8.4	Derived from Δ_fH^o in ref.	1994PED
2-phenylacetic acid **$PhCH_2$**–C(O)OH	67	280.3	Review	1970ONE/BEN
diphenylacetic acid **Ph_2CH**–C(O)OH	59.4±3	248.5±12 6	Review	1970ONE/BEN
naphthlene-1-carboxylic acid **$C_{10}H_7$**–1-C(O)OH	102.8±2.0	430.1±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
naphthlene-2-carboxylic acid **$C_{10}H_7$**–2-C(O)OH	104.8±2.0	438.5±8.4	Derived from Δ_fH^o in ref.	1986PED/NAY
glycolic acid **$HOCH_2$**–C(O)OH	88.8±1.3	371.5±5.4	Derived from Δ_fH^o in ref.	2001DOR/NOV
oxalic acid **HOC(O)**–C(O)OH	80.0±1.5	334.7±6.3	Derived from Δ_fH^o in ref.	1994PED
sarcosine **CH_3NHCH_2**–C(O)OH	72.0±4	301.2±16.7	Derived from Δ_fH^o in ref	1988LIA/BAR
L-alanine **$CH_3CH(NH_2)$**–C(O)OH	79.2±4	331.4±16.7	Derived from Δ_fH^o in ref	1988LIA/BAR
acetic acid methyl ester **CH_3**–C(O)OCH_3	92.6±3	387.4±12.5	Derived from Δ_fH^o in ref.	1986PED/NAY
methyl acrylate **C_2H_3** C(O)OCH_3	106.2±2.5	444 3±10.5	Derived from Δ_fH^o in ref.	2002CRC
methyl benzoate **Ph**–C(O)OCH_3	(1) 102.8±3 (2) **104.4±2.5**	430.1±12 6 **436.8±10.5**	Derived from Δ_fH^o in ref.	(1) 1986PED/NAY (2) 2002ROU/TEM
methyl-2-phenyl-propionate **$C_6H_5CH(CH_3)$**–C(O)OCH_3	75.5±1.5	315.9±6.3	Derived from Δ_fH^o in ref.	1999VER(b)
methyl 2-hydroxyacetate **$HOCH_2$**–C(O)OCH_3	88.5±2.5	370.3±10.5	Derived from Δ_fH^o in ref	1998NIST
dimethyl oxalate **$CH_3OC(O)$**–C(O)OCH_3	88.4±2.5	369.9±10.5	Derived from Δ_fH^o in ref.	2002CRC
propanoic acid **CH_3**–CH_2C(O)OH	84.5±3	353.5±12.6	Derived from Δ_fH^o in ref.	2002CRC
butanoic acid **C_2H_5**–CH_2C(O)OH	82.6±3	345.6±12.6	Derived from Δ_fH^o in ref.	1986PED/NAY
β-alanine **NH_2CH_2**–CH_2C(O)OH	77.8±4	325.5±16.7	Derived from Δ_fH^o in ref.	1988LIA/BAR
butanedioic acid **HO(O)CH_2**- CH_2C(O)OH	81.9±1.0	342.7±4.3	Derived	2002LAG/DIO

续表

断裂键 (黑体 = 离解原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methyl ketene **CH_3–CH=C=O**	93.3±1.5	390.4±6.3	Derived from $\Delta_f H^\circ$ in ref	2000TRA
diketene **O=C=CH**–CH=C=O	129.9±2	543.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
2,3-dimethylbutanedioic acid **R**–R, R is $CH(CH_3)C(O)OH$	66.7±1.6	279.1±6.7	Derived	2002LAG/DIO
2-chlorooxirane 	89.8±2.5	375.7±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyoxirane 	93.5±2.5	391.2±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
proline 	74.6±2.5	312.1±10.5	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR

5.5.2 含氮原子的碳氢化合物

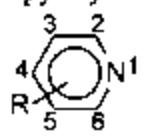
表 5.5.2 含氮原子的碳氢化合物内的 C—C BDEs

断裂键 (黑体 = 离解原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
cyanogen **CN–CN**	(1) **136.7±1.6** (2) 137.1	**571.9±6.7** 573.6	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived	(1) 1986PED/NAY (2) 2002MAT/LEB(a)
formyl cyanide HC(O)–CN	108.8±2	455.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	1996BOR/ING
thioformyl cyanide HC(S)–CN	126.7±2	530.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1996BOR/ING
trifluoroacetonitrile CF_3–CN	(1) 112.6±1.3 (2) **112.1±1.0**	471.1±5.4 **469.0±4.2**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1998RUS/MIC (2) 1998NIST
acetonitrile CH_3–CN	124.7±2.2	521.7±9.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
propiolonitrile CH≡C–CN	(1) 143.9 (2) **155.5±2.5**	(1) 602.1 (2) **650.6±10.5**	(1) Photolysis (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1973OKA/DIB (2) 1998NIST
2-propenenitrile CH_2CH–CN	133.4±1.8	558.1±7.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
propanenitrile C_2H_5–CN	121.1±1.8	506.7±7.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

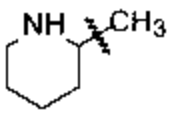
续表

断裂键 (**黑体** · 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
3-butenenitrile CH_2CHCH_2–CN	108.1±2	452.3±8.4	Derived from Δ_fH° in ref.	1998NIST
butanenitrile C_3H_7–CN	120.8±2.0	505.4±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
2-methylpropanenitrile iC_4H_7–CN	120.4±2.0	503.8±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
pentanenitrile nC_4H_9–CN	121.1±2.0	506.7±8 4	Derived from Δ_fH° in ref.	1986PED/NAY
2,2-dimethylpropanenitrile tC_4H_9–CN	117 2±2.0	490.4±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
cyclobutanecarbonitrile c-C_4H_7–CN	122.2±2.0	511.3±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
cyclopentanecarbonitrile c-C_5H_9–CN	120.0±2.0	502.1±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
cyclohexanecarbonitrile c-C_6H_{11}-CN	121.9±2.0	510 0±8 4	Derived from Δ_fH° in ref.	1986PED/NAY
benzonitrile C_6H_5–CN	132.3±2.0	553.5±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
heptanenitrile nC_6H_{13}–CN	120.4±2.0	503.8±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
benzylcyanide $C_6H_5CH_7$–CN	106.1±2	443.9±8.4	Derived from Δ_fH° in ref.	2000VER
α-methyl-benzylcyanide $C_6H_5CH(CH_3)$ –CN	104.6±2	437.6±8.4	Derived from Δ_fH° in ref.	2000VER
α,α-dimethyl-benzylcyanide $C_6H_5C(CH_3)_2$–CN	102.8±2	430.1±8.4	Derived from Δ_fH° in ref.	2000VER
propanenitrile CH_3–CH_2CN	83.2±3	348.1±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
butanenitrile C_2H_5 -CH_2CN	(1) 76.9±1.7 (2) **80.8±2**	321.7±7.1 **338.1±8.4**	(1) VLPP (2) Derived from Δ_fH° in ref.	(1) 1975KIN/GOD (2) 1986PED/NAY
3-butenenitrile C_2H_3–CH_2CN	110.4±2	461.9±8.4	Derived from Δ_fH° in ref.	2002CRC
pentanenitrile nC_3H_7–CH_2CN	81.7±3	341.8±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
2-methylbutanenitrile iC_3H_7–CH_2CN	73±2	305.4±8.4	VLPP	1975KIN/GOD
heptanenitrile nC_5H_{11}–CH_2CN	80.8±3	338.1±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
octanenitrile nC_6H_{13}–CH_2CN	80.5±3	336.8±12.6	Derived from Δ_fH° in ref.	1986PED/NAY

续表

断裂键 （**黑体** = 离解原子团）	BDEs （**黑体** = 推荐值； 括号内数字 = 文献编号） kcal/mol	 kJ/mol	方法	文献
benzylcyanide **C_6H_5**–CH_2CN	92.4±2	386.6±8.4	Derived from Δ_fH° in ref.	2000VER
2-methylpropanenitrile **CH_3**–$CH(CH_3)CN$	(1) 78.8±2 (2) **79.5±2**	329.7±8.4 **332.6±8.4**	(1) VLPP (2) Derived from Δ_fH° in ref.	(1) 1975KIN/GOD (2) 1986PED/NAY
α-methyl-benzylcyanide **C_6H_5**–$CH(CH_3)CN$	92.7±2	387.7±8.4	Derived from Δ_fH° in ref.	2000VER
2,2-dimethyl propanenitrile **CH_3**–$C(CH_3)_2CN$	(1) 74.7±1.6 (2) 81.4±4	312.5±6.7 340.6±16.7	(1) VLPP (2) Derived from Δ_fH° in ref.	(1) 1976KIN/GOD (2) 1998NIST
α,α–dimethyl-benzylcyanide **C_6H_5**–$C(CH_3)_2CN$	90.6±4	379.1±16.7	Derived from Δ_fH° in ref.	2000VER
propanedinitrile $(CN)CH_2$–**CN**	101.9±3	426.3±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
butanedinitrile $(CN)CH_2$–**CH_2CN**	70.7±4	295.8±16.7	Derived from Δ_fH° in ref.	1986PED/NAY
tetramethylbutanedinitrile $(CN)C(CH_3)_2$–**$C(CH_3)_2CN$**	61.2±3	256.1±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
2-methy-2-phenyl-propanenitrile **CH_3**–$C(CH_3)(CN)C_6H_5$	59.9	250.6	Pyrolysis	1982MEO
2-butynedinitrile **NCC≡CCN**	138.5	580	Derived from Δ_fH° in ref.	1998NIST
pyridine, substituted **R**–pyridyl  				
R = 2-Me	(1) 97.9±2	409.6±8.4	(1) Derived from Δ_fH° in ref.	(1) 1986PED/NAY
3-Me	(1) 103.2±2	431.8±8.4		
4-Me	(1) 103.7±2	433.9±8.4		
2-CH_2Ph	(2) 86.7	362.8	(2) VLPP	(2) 1984ROS/MCM
2-methyl-piperidine **CH_3**–pyrerid-2-yl	83.4±2	348.9±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
2-ethylpyridine **CH_3**–2-pyridylmethyl	75.5±2.9	315.9±12.1	VLPP	1981BAR/STE
3-ethylpyridine **CH_3**–3-pyridylmethyl	73.9±2.6	309.2±10.9	VLPP	1981BAR/STE
4-ethylpyridine **CH_3**–4-pyridylmethyl	74.6±2.6	312.1±10.9	VLPP	1981BAR/STE

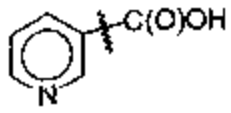
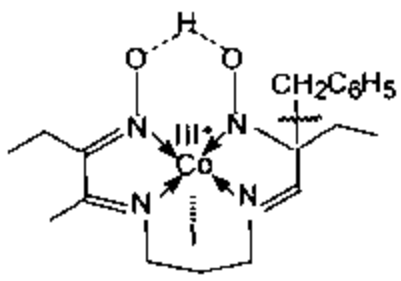
续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ethylamine **CH_3**–CH_2NH_2	82.7±2.3	346.0±9.6	Derived from Δ_fH° in ref.	1986PED/NAY
propylamine **C_2H_5**–CH_2NH_2	81.5±2.3	341.0±9.6	Derived from Δ_fH° in ref.	1986PED/NAY
phenylmethylamine **C_6H_5**–CH_2NH_2	94.2±2.5	394.1±10.5	Derived from Δ_fH° in ref.	1986PED/NAY
benzyl dimethylamine **C_6H_5**–$CH_2N(CH_3)_2$	92.7±2.5	387.9±10.5	Derived from Δ_fH° in ref.	1999VER
benzyl methylamine **$C_6H_5CH_2$**–CH_2NH_2	68.0±2	284.5±8.4	Pyrolysis	1977COL/BEN
2-propylamine **CH_3**–$CH(CH_3)NH_2$	81.8±2.3	342 3±9.6	Derived from Δ_fH° in ref.	1986PED/NAY
2-methylpropylamine **CH_3**–$C(CH_3)_2NH_2$	73.4±2.5	307.1±10.5	Derived from Δ_fH° in ref.	1986PED/NAY
1,2-ethanediamine **NH_2CH_2**–CH_2NH_2	68.4±3	286.2±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
1,2-propanediamine **NH_2CH_2**–$CH(CH_3)NH_2$	75.8±3	317.1±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
2-methyl-1,2-propanediamine **NH_2CH_2**–$C(CH_3)_2NH_2$	74.6±3	312 1+12.6	Derived from Δ_fH° in ref.	1986PED/NAY
2-(2-pyridyl)pyridine **NC_5H_4**-C_5H_4N	103.9±3	434.7+12 6	Derived from Δ_fH° in ref.	1988LIA/BAR
2-methylpiperidine 	83.9±3	351.0±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
methoxyacetonitrile CH_3OCH_2–**CN**	113.5	474.9	Derived from Δ_fH° in ref.	1998NIST
oxopropanedinitrile NCC(O) –**CN**	96.0±2.5	401.7±10 5	Derived from Δ_fH° in ref.	2001DOR/NOV
nitroethane **CH_2**–CH_2NO_2	(1) 94.7 (2) 87.1	369.2 364.4	(1) Derived (2) Derived from Δ_fH° in ref.	(1) 2000MAT/LEB (2) 2002CRC
1-(dimethylamino)-2-propanone **$(CH_3)_2NCH_2$**–$C(O)CH_3$	73.8	308.8	Derived from Δ_fH° in ref.	1998NIST
methyl ester nitrous acid **H_2NCH_2**–C(O)OH	83.1±2.5	347.7±10.5	Derived from Δ_fH° in ref.	1998NIST
alanine **$H_2NC(CH_3)H$** -C(O)OH	79.3±3	331.8±12.6	Derived from Δ_fH° in ref.	1998NIST
1-nitropropane **C_2H_5**–CH_2NO_2	90.7	379.5	Derived	2000MIR/VOR(b)
1-nitrobutane **C_3H_7**–CH_2NO_2	90.8	379 9	Derived	2000MIR/VOR(b)

续表

断裂键 （**黑体** = 离解原子团）	BDEs （**黑体** = 推荐值； 括号内数字 = 文献编号）		方法	文献
	kcal/mol	kJ/mol		
1-nitropentane **C_4H_9**–CH_2NO_2	89.5	374.5	Derived	2000MIR/VOR(b)
2-nitropropane **CH_3**–$CH(NO_2)CH_3$	90.0	376.6	Derived	2000MIR/VOR(b)
2-nitrobutane **CH_3**–$CH(NO_2)C_2H_5$	90.3	377.8	Derived	2000MIR/VOR(b)
1,2-dinitroethane **NO_2CH_2**–CH_2NO_2	93.8	392.5	Derived	2000MAT/LEB
1,1-dinitroethane **CH_3**–$CH(NO_2)_2$	99.3	415.5	Derived	2000MAT/LEB
1,1-dinitropropane **C_2H_5**–$CH(NO_2)_2$	95.1	397.9	Derived	2000MIR/VOR(b)
2,2-dinitropropane **CH_3**–$C(NO_2)_2CH_3$	92.2	385.8	Derived	2000MIR/VOR(b)
1,1-dinitrobutane **C_3H_7**–$CH(NO_2)_2$	95.8	400.8	Derived	2000MIR/VOR(b)
1,1-dinitropentane **C_4H_9**–$CH(NO_2)_2$	94.6	395.8	Derived	2000MIR/VOR(b)
1,1,1-trinitroethane **H_3C**–$C(NO_2)_3$	98.3	411.3	Derived	2002MAT/LEB(a)
1,1,1-trinitropropane **H_2C_2**–$C(NO_2)_3$	93.9	392.9	Derived	2000MIR/VOR(b)
1,1,1-trinitrobutane **H_3C_2**–$C(NO_2)_3$	94.5	395.4	Derived	2000MIR/VOR(b)
1,1,1-trinitropropane **H_4C_3**–$C(NO_2)_3$	93.5	391.2	Derived	2000MIR/VOR(b)
2,3-dimethyl-2,3-dinitrobutane **$(CH_3)_2C(NO_2)$** $C(NO_2)(CH_3)_2$	72.7	304.2	Derived	2000MIR/VOR(b)
2,2,3,3-tetranitrobutane **$CH_3C(NO_2)_2$**–$C(NO_2)_2CH_3$	74.9	313.4	Derived	2000MIR/VOR(b)
pentanitropropane **CH_3** $C(NO_2)C(NO_2)_3$	72.6	303.8	Derived	2000MIR/VOR(b)
hexanitrothane **$(NO_2)_3C$**–$C(NO_2)_3$	73.8	308.8	Derived	2000MAT/LEB
trinitromethancyanide **NC**–$C(NO_2)_3$	101.6	425.1	Derived	2002MAT/LEB(a)
nitro(2-(nitrooxy)ethyl)oxy **O_2NOH_2C**–CH_2ONO_2	91.0	380.7	Derived	2002MAT/LEB(a)
nitro(2-(nitrooxy)ethyl)amine **O_2NNHH_2C**–CH_2NHNO_2	68.2	285.3	Derived	2002MAT/LEB(a)

续表

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitrozoamines				
$(NO_2)_3C$– $CH_2N(NO_2)CH_2C(NO_2)_3$	74.0	309.6	Derived	2001MIR/KOS
$(NO_2)_2CH$– $CH_2N(NO_2)CH_2CH(NO_2)_2$	79.5	332.6		
$(NO_2)_3CCH_2$– $CH_2N(NO_2)CH_2C(NO_2)_3$	70.5	295.0		
$(NO_2)_3C$– $CH_2CH_2N(NO_2)CH_2C(NO_2)_3$	87.3	365.3		
$(NO_2)_3CCH_2N(NO_2)CH_2$– $CH_2N(NO_2)CH_2C(NO_2)_3$	56.3	235.6		
$(NO_2)_3C$–$CH_2N(NO_2)CH_2CH_2$– $N(NO_2)CH_2C(NO_2)_3$	74.5	311.7		
$(NO_2)_2CHCH_2N(NO_2)CH_2$– $CH_2N(NO_2)CH_2CH(NO_2)_2$	61.6	257.7		
$(NO_2)_2CH$– $CH_2N(NO_2)CH_2CH_2$– $N(NO_2)CH_2CH(NO_2)_2$	79.8	333.9		
$(NO_2)_3C$– $CH_2N(NO)CH_2C(NO_2)_3$	73.8	308.8		
$(NO_2)_3CCH_2N(NO)CH_2$– $CH_2N(NO)CH_2C(NO_2)_3$	53.2	222.6		
$(NO_2)_3C$–$CH_2N(NO)CH_2CH_2$– $N(NO)CH_2C(NO_2)_3$	74.5	311.7		
niacin 	99.9	418	Derived from $\Delta_f H°$ in ref.	1998NIST
coenzyme B12, substituted 	25	104.6	Photolysis	1991DAI/FIN

5.5.3 含硫原子的碳氢化合物

表 5.5.3 含硫原子的碳氢化合物内的 C—C BDEs

断裂键 (**黑体** = 离解原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ethylthiol **CH_3**–CH_2SH	82.5±2.2	345.2±9.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-propanethiol **C_2H_5**–CH_2SH	80.9±2.4	338.5±10.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-butanethiol **C_3H_7**–CH_2SH	81.1±2.5	339.3±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyl-1-propanethiol **iC_3H_7**–CH_2SH	80.6±2.5	337.2±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-pentanethiol **C_4H_9**–CH_2SH	81.2±2.5	339.7±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyl-1-butanethiol **sC_4H_9**–CH_2SH	80.0±2.5	334.7±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-methyl-1-butanethiol **iC_4H_9**–CH_2SH	80.5±2.5	336.8±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2-dimethyl-1-propanethiol **tC_4H_9**–CH_2SH	78.7±2.5	329.3±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-hexanethiol **nC_5H_{11}**–CH_2SH	80.3±2.5	336.0±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-heptanethiol **nC_6H_{13}**–CH_2SH	80.2±2.5	335.6±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
phenylmethane-1-thiol **C_6H_5**–CH_2SH	93.2±2.5	389.9±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1,2-ethanethiol **$HSCH_2$**–CH_2SH	74.9±2.8	313.4±11.7	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl methyl sulphide **CH_3**–CH_2SCH_3	82.0±2.0	343.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methyl propyl sulphide **C_2H_5**–CH_2SCH_3	80.8±2.0	338.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl phenyl sulphide **CH_3**–$CH_2SC_6H_5$	80.9±2.0	338.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
dibenzyl sulphide **C_6H_5**–$CH_2SC_6H_5$	97.1±2.0	406.3±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

5.6 自由基中的C—C键能

表 5.6 自由基中的 C—C BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
C–C_x				
x = 1	(1) 143.75	601.45	(1) Spectroscopy	(1) 2002CRC
2	(2) **167.9**	**703**	(2) Derived from $\Delta_f H^\circ$ in ref.	(2) 1994GIN/FIN
	(3) 175.5	734	(3) Derived from $\Delta_f H^\circ$ in ref.	(3) 1998CHA
3	(2) **118.5**	**496**		
	(3) 135.3	566		
4	(2) **164.4**	**688**		
	(3) 169.3	708		
5	(2) 116.1	486		
6	(2) 168.2	704		
C_2–C_2	(1) **139.1**	**582**	Derived from $\Delta_f H^\circ$ in ref.	(1) 1994GIN/FIN
	(2) 168.4	705		(2) 1998CHA
–C_3	(1) **135.5**	**567**		
	(2) 162.2	679		
–C_4	(1) 133.1	557		
C_3–C_3	83.7	350	Derived from $\Delta_f H^\circ$ in ref.	1994GIN/FIN
–C_4	133 4	558		
CH≡**C**$^\bullet$	178.5±0.5	746.8±2.1	Derived	This volume
CH_2=**C**$^{\bullet\bullet}$	164.3±4	687.4±16.7		
CH_2=**C**$^\bullet$**H**	164.5±1	688.3±4.2		
CH_3–**C**$^\bullet H_2$	100.0±0.5	418.4±2.1		
CH_2=CH–**C**$^\bullet H_2$	124.0±1.1	518.8±4.6		
CH_3–**C**$^\bullet$=CH_2	80.1±4	335.1±16.7		
CH_3–CH=**C**$^\bullet$**H**	25.8±1.6	107.9±6.7	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
CH_3–CH_2**C**$^\bullet H_2$	23.7±1	99.2±4.2		

续表

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
CH_3CH_2–$CH_2C^{\bullet}H_2$	22.3±1	93.3±4.2		
CH_3 $C(CH_3)$=$C^{\bullet}H_2$	23.3±1	97.5±4.2		
CH_3–$CH_2C^{\bullet}HCH_3$	23.8±1	99.6±4.2		
$CH_3CH_2CH_2$–$CH_2C^{\bullet}H_2$	23.4±1	97.9±4.2		
CH_3–$CH_2C^{\bullet}HCH_2CH_3$	23.8±1	99.6±4.2		
CH_3CH_2–$CH_2C^{\bullet}HCH_3$	21.3±1.5	89.1±6.3	Derived from Δ_fH° in ref.	1998NIST
CH_3–$C(CH_3)_2C^{\bullet}H_2$	22.1±1.5	92.5±6.3		
CH_3–$CH_2C^{\bullet}(CH_3)_2$	23.9±1.5	100.0±6.3		
$CH_3CH_2CH_2CH_2$–$CH_2C^{\bullet}H_2$	23.1±1.5	96.7±6.3		
$CH_3CH_2CH_2$–$CH_2C^{\bullet}HCH_3$	21.8±2	91.2±8.4		
$CH_3CH_2CH_2CH_2$–$CH_2C^{\bullet}HCH_3$	21.8±2	91.2±8.4		
$CH_3CH_2CH_2CH_2CH_2$–$CH_2C^{\bullet}HCH_3$	21.5±2	90.0±8.4		
$CH_2CHC^{\bullet}HCH_2$–**CH_3**	34.9±2.0	146.0±8.4	Derived from Δ_fH° in ref.	1998NIST
CH_2CHCH_2–$CH_2C^{\bullet}H_2$	10.5±2.0	43.9±8.4		
$CH_2CHC^{\bullet}HCH_2$–**CH_2CH_3**	33.1±2.0	138.5±8.4		
$CH_2CHC^{\bullet}HCH_2$–**$CH_2CH_2CH_2CH_3$**	32.7±3	136 8±12.6		
$C_6H_5C^{\bullet}HCH_2$–**CH_2CH_3**	31.3±3	131 0±12.6		
$C_6H_5CH_2$–CH_2CHCH_3	9.2±2	38.5±8.4		
CH_3–$CH_2C^{\bullet}HCl$	26.6±2	111.3±8.4	Derived from Δ_fH° in ref.	1998NIST
CH_2Br–$CH_2C^{\bullet}H_2$	24.7±2	103.3±8.4		
CH_3–$CH_2C^{\bullet}HBr$	28.3±2	118.4±8.4		
CH–CO	74.2	310.2	Derived from Δ_fH° in ref.	1997OSB/MOR
CH_3–$CH_2C^{\bullet}HOH$	24.7±2.5	103.3±10.5	Derived from Δ_fH° in ref.	1998NIST
$HOCH_2$–$CH_2C^{\bullet}H_2$	24.4±2.5	102.1±10.5		

续表

断裂键 (**黑体** · 离解原子 或原子团)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
CH_3–$CH(OH)C^{\bullet}H_2$	20.3±3	84.9±12.6		
CH_3–$CH_2C^{\bullet}(O)$	22.0±2.5	92.0±10.5		
CH_3–$C(O)C^{\bullet}H_2$	22.3±2.5	93.3±10.5		
tC_4H_9–$C(O)C^{\bullet}H_2$	18.2±3	76.1±12.6		
C_6H_5–$C(O)C^{\bullet}H_2$	37.8±3	158.2±12.6		
$C^{\bullet}H_2CH_2$–**CN**	58.8±3.5	246.0±14.6		
CH_3–$CH_2O^{\bullet}$	12 7±1	53.1±4.2	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
CF_3–$CHFO^{\bullet}$	2 1	8.8		
CH_3CH_2–$CH_2O^{\bullet}$	9.6±2	40.2±8.4		
CH_3–$CH(CH_3)O^{\bullet}$	5.9±1	24.7±4.2		
CH_3–$CCl(CH_3)O^{\bullet}$	2.6±2	10.9±8.4		
$CH_3CH_2CH_2$–$CH_2O^{\bullet}$	12.9±3	54.0±12.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
CH_3CH_2–$CH(CH_3)O^{\bullet}$	4.2±2	17.6±8.4		
CH_3–$C(CH_3)_2O^{\bullet}$	3.4±3	14.2±12.6		
CH_2=CH–$CH_2O^{\bullet}$	24.8±3	103.8±12.6		
C_6H_5–$CH_2O^{\bullet}$	27.3±3	114.2±12.6		
CH_3–$C(O)O^{\bullet}$	–16.0±3	–66.9±12.6	Derived from $\Delta_f H^\circ$ in ref.	2003BLA/ELL
CF_3–$C(O)O^{\bullet}$	–14.8±3	–61.9±12.6	Derived from $\Delta_f H^\circ$ in ref.	1995TAK/PAS
C_6H_5–$C(O)O^{\bullet}$	–3.2±3	–13.4±12.6	Derived from $\Delta_f H^\circ$ in ref.	2003BLA/ELL
C_6H_5–$CH_2N^{\bullet}H$	26.0±3	108.8±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
CH_3–$CH_2S^{\bullet}$	33±5	138±21		
H_3CH_2–$CH_2S^{\bullet}$	31 3±5	131±21		
CH_3–$CH(CH_3)S^{\bullet}$	29.2±5	122±21		
C_6H_5–$CH_2S^{\bullet}$	36.1±5	151±21		

第 6 章　C—X(卤) 键能

6.1　C—F键能

表 6.1　C—F BDEs

断裂键 (黑体 = 离解原 f) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
cyanogen fluoride F-CN	(1) 112.3±1.2 (2) **115.4**	469.9±5.0 **482.8**	(1) AE (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1978DAY/GOW (2) 1998NIST
tetrafluoromethane F CF_3	(1) 130.5 (2) **130.7±0.5**	546.0 546.8±2.1	Derived	(1) 1975CHE/ROD (2) 1998RUS/MIC
trifluoromethane F–CHF_2	(1) 126.0 (2) 127 (3) **127.6±1.4**	527.2 531.4 **533.9±5.9**	(1) Derived (2) Bromination (3) Review	(1) 1975CHE/ROD (2) 1987TSC/PAD (3) 2001LAZ/PRO
difluoromethane F–CH_2F	(1) 119.0 (2) **118.6±2.1**	497.9 **496.2±8.8**	(1) Derived (2) Review	(1) 1975CHE/ROD (2) 2001LAZ/PRO
chlorofluoromethane F–CF_2Cl	(1) 117±6 (2) 123 (3) **122.3**	489.5±25 514.6 **511.7**	(1) Kinetics (2) Derived (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1972FOO/TAI(b) (2) 1975CHE/ROD (3) 1998NIST
trifluorobromomethane F–CF_2Br	120.4±5	504±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
dichlorofluoromethane F–$CFCl_2$	(1) 110±6 (2) **115.2±2.5** (3) 120.4	460±25 **482.0±10.5** 503.4	(1) Kinetics (2) Derived from $\Delta_f H^\circ$ in ref. (3) PIMS	(1) 1972FOO/TAI(b) (2) 1998CHA (3) 1997SHE/QI
chlorodifluoromethane F–CHFCl	110.5±2.4	462.3±10.0	Derived	1987TSC/PAD
trichlorofluoromethane F–CCl_3	(1) 101.9 (2) **105±1**	426.3 **439.3±4**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1975CHE/ROD (2) 1998CHA
dichlorofluoromethane F–$CHCl_2$	108.2±5.5	453±23	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
chlorofluoromethane F–CH_2Cl	111.2±2.3	465.3±9.6	Derived	1987TSC/PAD
bromochlorodifluoromethane F–CFClBr	114.5±4	479±17	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
bromochlorofluoromethane F–CHClBr	108.2±4	453±17	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
bromodichlorofluoromethane F–CCl_2Br	104.7±5	438±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
dibromochlorofluoromethane F–$CClBr_2$	100±5	418±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
tribromofluoromethane F–CBr_3	96.7±5	405±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
dibromofluoromethane F–$CHBr_2$	105.8±5	443±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
bromofluoromethane F–CH_2Br	111.3±4	466±17	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
triiodofluoromethane F–CI_3	109.6±10	459±42	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
diiodofluoromethane F–CHI_2	114±9	477±38	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
fluoroiodomethane F–CH_2I	≤110.0	≤460.2	IR chemiluminescence	2002ARU/VIJ
fluoromethane F–CH_3	(1) 109.9 (2) 112.8 (3) **110.0±2.0** (4) 109.8±1.2	459.8 472.0 **460.2±8.4** 459.4±5.0	(1) Derived (2) Review (3) Derived from $\Delta_f H^\circ$ in ref. (4) Review	(1) 1975CHE/ROD (2) 1988LIA/BAR (3) 1998CHA (4) 2001LAZ/PRO
fluoroethyne F–C≡CH	124.6	521.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
difluoroethyne F–C≡CF	124±5	519±21	Review	1996ZAR/WES
tetrafluoroethylene F–CF=CF_2	130.6±3	546.4±12.6	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
hexafluoroethane F–CF_2CF_3	(1) 126.8±1.8 (2) **127.2±1.5**	530.5±7.5 **532.2±6.3**	(1) Derived (2) Review	(1) 1982MCM/GOL (2) 2001LAZ/PRO
1,1,1,2-tetrafluoroethane F–CH_2CF_3	109.4	457.7	Derived	1975CHE/ROD
1,1,1-trifluoroethane F–CF_2CH_3	124.8±2	522.2±8.4	Derived	1975CHE/ROD
vinyl fluoride F–C_2H_3	123.7±3	517.6±12.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
fluoroethane F–C_2H_5	(1) 107.7 (2) **113.1±2**	450.6 **473.2±8.4**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1975CHE/ROD (2) 1998SMI
1-fluopropane F–C_3H_7	(1) 111.1±3 (2) **113.5±2**	464.8±12.6 **474.9±8.4**	Derived from $\Delta_f H^\circ$ in ref.	(1) 1986PED/NAY (2) 1998SMI
2-fluopropane F–iC_3H_7	(1) 110.1±5 (2) **115.4±2**	460.7±21 **482.8±8.4**	Derived from $\Delta_f H^\circ$ in ref.	(1) 1986PED/NAY (2) 1998SMI
2-fluoro-2-methyl-propane F–tC_4H_9	117.0±2	489.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	1998SMI

续表

断裂键 (**黑体** · 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
fluorobenzene **F**–C_6H_5	125.6±2	525.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
hexafluorobenzene **F**–C_6F_5	(1) 114 (2) **116±6**	477.0 **485±25**	Derived	(1) 1975CHO/GOL (2) 2004CAR/KOY
fluoro-cyclo-hexane **F**–c-C_6H_{11}	117.4±2	491.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	1997SCH/VER
(fluoromethyl)benzene **F**–$CH_2C_6H_5$	98.7±1	412.8±4.2	Derived	2003VER/KRA
formyl fluoride **F**–COH	119.0±2.5	497.9±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
fluoroformyl fluoride **F**–COF	(1) 127.9±3 (2) **129.6±3**	535.1±12.6 **542.2±12.6**	(1) PIMS (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1995BUC/JOH (2) 1996ASH/APP
chloroformyl fluoride **F**–COCl	115.8	484.5	Derived from $\Delta_f H^\circ$ in ref	1998CHA
acetyl fluoride **F**–C(O)CH_3	122.3±3	511.7±12.6	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
F–C	122.8±2.4	513.8±10.0	Derived	This volume
–CF	121.1±3	506.6±12.6		
–CCl	117.5±4.5	491.6±18.8		
–CH	127.6±3.1	533.9±13		
–CF_2	85.8±2	359.0±8.4		
–CCl_2	94.3±3	394.6±1.6		
–CClF	93.1±3.8	389.5±15.9		
–CClBr	91.3±3	382.0±12.6		
–CHF	110.3±3.2	461.5±13.4		
–CHCl	111.5±3	466.5±12.6		
–CH_2	119.9±1.1	501.7±4.6		
F–C$^\bullet$	104±6	435±25	Derived	This volume
F–CFC$^\bullet$F	69.9±3	292.5±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
–CFC$^\bullet$H	71.2±3	297.9±12.6		
–CHC$^\bullet$F	61.7±3	258.2±12.6		
–$CF_2C^\bullet F_2$	75.0±3	313.8±12.6		

续表

断裂键 (**黑体** – 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
–CHFC$^\bullet$F$_2$	64.6±3	270.3±12.6		
–CH$_2$C$^\bullet$F$_2$	44.3±3	185.4±12.6		
–CF$_2$C$^\bullet$HF	68.4±3	286.2±12.6		
–CH$_2$C$^\bullet$HF	43.6±3	182.4±12.6		
–CF$_2$C$^\bullet$H$_2$	60.4±3	252.7±12.6		
–CHFC$^\bullet$H$_2$	54.9±3	229.7±12.6		
–CH$_2$C$^\bullet$H$_2$	45.7±3	191.2±12.6		
–CClFC$^\bullet$F$_2$	62.2±3	260.2±12.6		
F–CF$_2$O$^\bullet$	27±1	113.0±4.2	Re-evaluated	2000REI/PRA
F–C$^\bullet$(O)	31.1±3	130.1±12.6	Derived	This volume

6.2 C—Cl 键能

表 6.2 C—Cl BDEs

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
cyanogen chloride Cl–CN	(1) 100.8±1.2 (2) **101.0±2.0**	421.7±5.0 **422.6±8.4**	(1) AP (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1978DAY/GOW (2) 2002CRC
chlorotrifluoromethane **Cl** CF_3	(1) 86.1±0.8 (2) 86.2±3 (3) 89.1 (4) **87.3±0.9**	360.2±3.3 360.7±12.6 372.8 **365.3±3.8**	(1) Kinetics (2) Kinetics (3) Electron capture detection (4) Derived	(1) 1967COO/WHI (2) 1983MAR/PAR (3) 1989CHE/ALB (4) 1998RUS/MIC
chlorodifluoromethane Cl–CHF_2	87.0±2	364±8	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
chlorofluoromethane Cl–CH_2F	84.7±2.8	354.4±11.7	Derived	1987TSC/PAD
dichlorodifluoromethane Cl–CF_2Cl	(1) 76±2 (2) 73.4±2.5 (3) **79.8±2.5** (4) 83.9±2.3	318.0±8.4 307.1±10.5 **333.9±10.5** 351.2±9.6	(1) Kinetics (2) Electron capture detection (3) Derived from $\Delta_f H^\circ$ in ref. (4) PI MS	(1) 1972FOO/TAI(b) (2) 1989CHE/ALB (3) 1998CHA (4) 1997SHE/QI

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值， 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
trichlorofluoromethane Cl–$CFCl_2$	(1) 72±2 (2) 70.5 (3) **76.7±2**	301.2±8.4 295.0 **320.9±8.4**	(1) Kinetics (2) Electron capture detection (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1972FOO/TAI(b) (2) 1989CHE/ALB (3) 1998CHA
dichlorofluoromethane Cl–CHFCl	(1) **82.7±3.2** (2) 83.4	**346.0±13.4** 348.9	(1) Derived (2) Electron capture detection	(1) 1987TSC/PAD (2) 1989CHE/ALB
tetrachloromethane Cl–CCl_3	(1) 70.4±1 (2) 70.8±1.3 (3) 73.3 (4) 71.0 (5) **70.9**	294.6±4.2 296.2±5.4 306.8 297.2 **296.6**	(1) Bromination (2) Correlation (3) Photoionizat. (4) PIMS (5) Review	(1) 1973MEN/GOL (2) 1978KAT/RAJ (3) 1996LI/RAN(c) (4) 1996LI/RAN (5) 2001LAZ/PRO
trichloromethane Cl-$CHCl_2$	(1) 76.2 (2) 80.9±1 (3) 73.6 (4) **76.6±1.5**	318.8 338.5±4.2 307.9 **320.5±6.3**	(1) Correlation (2) Derived (3) Electron capture detection (4) Review	(1) 1978KAT/RAJ (2) 1987TSC/PAD (3) 1989CHE/ALB (4) 2001LAZ/PRO
dichloromethane Cl–CH_2Cl	(1) 80.9±1.0 (2) 77.9 (3) 79.1 (4) **80.8** (5) 78.5	338.5±4.2 325.9 331.0 **338.1** 328.4	(1) Derived (2) Electron capture detection (3) Photolysis (4) Review (5) Correlation	(1) 1987TSC/PAD (2) 1989CHE/ALB (3) 1994TZE/LEE (4) 2001LAZ/PRO (5) 1995DEN
bromodichlorofluoromethane Cl–CFClBr	76.7±4	321±17	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
bromochloromethane Cl–CHClBr	74.0±4	310±17	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
bromotrichloromethane Cl–$CBrCl_2$	68.6±2.5	287±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
dibromodichloromethane Cl–CBr_2Cl	65.6±4	274±17	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
tribromochloromethane Cl–CBr_3	62.5±2.5	261.5±10.5	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
dibromochloromethane Cl–$CHBr_2$	71.5±5	299±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
bromochloromethane Cl–CH_2Br	74.9	313.4	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
chlorotriiodomethane Cl-CI_3	76.6±10	321±42	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
chlorodiiodomethane Cl–CHI_2	79.5±7.5	333±32	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
chloroiodomethane Cl CH_2I	(1) ≤72.0 (2) 82.7±6.5	≤301.2 346±27	(1) IR chemiluminescence (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 2002ARU/VIJ (2) 1991GUR/VEY

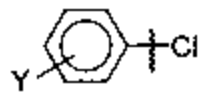
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
chloromethane **Cl**–CH_3	83.7±0.4	350.2±1.7	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
dichloroethyne **Cl**–C≡CCl	106±12	443±50	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
chloroethyne **Cl**–C≡CH	104.1±2	435.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
2-chloroethanenitrile **Cl**–CH_2CN	63.9	267.4	CID	2002POU/UPS
(Z)-1,2-dichloroethylene (Z)-ClCH=CH–**Cl**	88.2	369.0	Electron capture detection	1989CHE/ALB
(E)-1,2-dichloroethylene (E)-ClCH=CH–**Cl**	88.4	369.9	Electron capture detection	1989CHE/ALB
1,2-dichloroethylene g-CH_2=CCl–**Cl**	93.4	390.8	Electron capture detection	1989CHE/ALB
1,1,2-trichloroethylene ClCH=CCl–**Cl**	93.6	391.6	Electron capture detection	1989CHE/ALB
tetrachloroethylene CCl_2=CCl–**Cl**	91.7	383.7	Electron capture detection	1989CHE/ALB
vinyl chloride **Cl**–CH=CH_2	(1) 91.7±1.0 (2) **94.8±1.2** (3) 93.5	383.7±4.2 **396.5±4.8** 391.3	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Photoionizat. (3) Correlation	(1) 1986PED/NAY (2) 1995SHE/QI (3) 2003KRO/TUM
chlorotrifluoroethylene **Cl**–CF=CF_2	103.9±2	434.7±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
chloropentafluoroethane **Cl**–CF_2CF_3	(1) **82.7±1.7** (2) 78±2 (3) 82.0±1.2	**346.0±7.1** 326.4±8.4 343.1±5.0	Kinetics	(1) 1967COO/WHI (2) 1972FOO/TAI(b) (3) 1989TAC/SAL
dichlorotetrafluoroethane **Cl**–CF_2CF_2Cl	(1) 78±2 (2) 79.2±5	326.4±8.4 331.4±20.9	Kinetics	(1) 1972FOO/TAI(b) (2) 1989TAC/SAL
1,1,1-trichloro-2,2,2-trifluoro ethane **Cl**–CCl_2CF_3	(1) 71 (2) 73.6	297.1 307.9	Correlation	(1) 1978KAT/RAJ (2) 1995DEN
hexachloroethane **Cl**–CCl_2CCl_3	(1) **72.6** (2) 71.7 (3) 71.5	**303.8** 300.0 299.2	(1) Photochlorin. (2) Correlation (3) Derived	(1) 1069FRA/HUY (2) 1995DEN (3) 1997CIO/LIU
pentachloroethane **Cl**–CHClCCl_3	79.0±1	330.5±4.2	Pyrolysis	1982BEN/WEI
pentachloroethane **Cl**–CCl_2CHCl_2	(1) 67.8 (2) 74.5	283.7 311.7	(1) Derived (2) Correlation	(1) 1997CIO/LIU (2) 1995DEN
1,1,1,2-tetrachloroethane **Cl**–CCl_2CH_2Cl	76.0	318.0	Correlation	1995DEN
1,1,1-trichloroethane **Cl**–CCl_2CH_3	(1) 70 (2) 78.5	292.9 328.4	Correlation	(1) 1978KAT/RAJ (2) 1995DEN

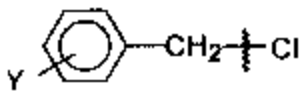
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1,1-dichloroethane Cl-CHClCH$_3$	(1) 79.5±2.1 (2) **78.4±0.4**	332.6±8.8 **327.9±1.8**	Derived	(1) 1997CIO/LIU (2) 1998SEE
1,2-dichloroethane Cl–CH$_2$CH$_2$Cl	(1) 79.1 (2) 83.2±2.3 (3) **82.5±1.2**	331.0 348.1±9.6 **345.1±5.0**	(1) Electron capture detection (2) Derived (3) Derived	(1) 1989CHE/ALB (2) 1997CIO/LIU (3) 1998SEE
1,1-bromochloroethane Cl–CHBrCH$_3$	79 3±2 0	331.8±8.4	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
chlorocthane Cl–CH$_2$CH$_3$	84.2±0.8	352.3±3 3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-chloro-1-propyne Cl-CH$_2$CH=CH$_2$	71.0	297.1	Correlation	2003KRO/TUM
3-chloro-1-propene Cl–CH$_2$CH=CH$_2$	(1) **71.3±1.2** (2) 71.2	**298.3±5.0** 297.9	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
3-chloro-2-methyl-1-propene Cl–CH$_2$C(CH$_3$)=CH$_2$	66.2	277.0	Correlation	1995DEN
1-chloropropene cis-Cl–CH=CHCH$_3$ trans-Cl–CH=CHCH$_3$	95.2 94.5	398.3 395.3	Correlation	003KRO/TUM
1-chloropropane Cl-nC$_3$H$_7$	84.3±1.0	352.7±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1,3-dichloropropane Cl–CH$_2$CH$_2$CH$_2$Cl	83.4	348.9	Electron capture detection	1989CHE/ALB
2-chloropropane Cl–iC$_3$H$_7$	(1) **84.6±1.5** (2) 85.2	**354.0±6.3** 356.3	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
1,4-dichloro-2-butene Cl–CH$_2$CH=CHCH$_2$Cl	67.0	280.3	Correlation	1995DEN
1-chlorobutane Cl-nC$_4$H$_9$	84.5±1.0	353.5±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-chloro-2-methylpropane Cl- iC$_4$H$_9$	(1) **83.8±1.5** (2) 83.7	**350.6±6.3** 350.3	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
2-chlorobutane Cl–sC$_4$H$_9$	(1) **83.7±1.5** (2) 85.3	**350.2±6.3** 357.0	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
2-chloro-2-methylpropane Cl tC$_4$H$_9$	(1) **84.1±1.5** (2) 83.5	**351.9±6.3** 349.2	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
3-chloro-but-1-ene CH$_2$CHCHCl(CH$_3$)	71.1	297.7	Correlation	2003KRO/TUM

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
4-chloro-but-1-ene **Cl**–$CH_2CH_2CH{=}CH_2$	81.9	342.7	Correlation	2003KRO/TUM
1-chloropentane **Cl**–nC_5H_{11}	(1) **83.8±1.5** (2) 84.6	350.6±6.3 354.1	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
1-chloro-2,2-dimethyl-propane **Cl**–$CH_2C(CH_3)_3$	84.2	352.1	Correlation	2003KRO/TUM
1-chloroalkanes **Cl**–C_nH_{2n+1}				
n = 6	83.3	348.5	Correlation	2003KRO/TUM
7	84.3	352.8		
8	85.1	355.9		
12	85.2	356.5		
16	84.3	352.5		
18	85.3	356.7		
2-chloro-2-methylbutane **Cl**–$C(CH_3)_2(C_2H_5)$	(1) **84.3±1.5** (2) 84.1	**352.7±6.3** 352.0	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
2-chloroalkanes **Cl**–$CH(CH_3)(C_nH_{2n+1})$				
n = 3	(2) 84.0	351.3	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1994PED
4	(1) **84.8±1.5** (2) 84.5	**354.8±6.3** 353.6	(2) Correlation	(2) 2003KRO/TUM
5	(2) 83.1	347.9		
6	(2) 83.8	350.5		
chlorocyclohentane **Cl**–cycloC_5H_9	82.4	344.9	Correlation	2003KRO/TUM
chlorocyclohexane **Cl**–cycloC_6H_{11}	(1) **86.1±2** (2) 85.0	**360.2±6.5** 355.5	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
chlorobenzene, substituted  Y = H	(1) **95.5±1.5** (2) 95.1±2.5 (3) 94.5±2.3	**399.6±6.3** 397.9±10.5 395.4	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Electron capture detection (3) Electron capture detection	(1) 1986PED/NAY (2) 1989CHE/ALB (3) 2002CHE/CHE

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** – 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
2-Cl	(2) 92.2	385.8		
3-Cl	(2) 89.9	376.1		
4-Cl	(2) 93.7	392.0		
2-Me	(2) 93.7	392.0		
2-CF_3	(2) 93.0	389.1		
4-CF_3	(2) 93.0	389.1		
3-CH_3CO	(2) 92.2	385.8		
4-CH_3CO	(2) 91.4	382.4		
3-F-4-Cl	(2) 91.6	383.3		
2-CF_3-4-Cl	(2) 90.3	377.8		
3,5-Cl_2	(2) 94.5	395.4		
2,4,5-Cl_3	(2) 94.4	395.0		
chloropentafluorobenzene **Cl**–C_6F_5	91.6±2	383.3±8.4	Derived	1982MCM/GOL
chlorocyclohexane **Cl**–C_6H_{11}	85.1±2	356.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
trichloro-phenyl methane **Cl**–$CCl_2C_6H_5$	66.5	278.2	Correlation	1995DEN
benzyl chloride **Cl**–$CH_2C_6H_5$	(1) 72.9±2	305.0±8.4	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1986PED/NAY
	(2) 71.6	299.6	(2) Electrochem.	(2) 1992AND/GOR
	(3) **71.7±1.1**	**299.9±4.3**	(3) Derived	(3) 2003VER/KRA
benzyl chloride, substituted 				
Y = 3-F	68.5	286.8	Correlation	1998DEN
4-F	69.1	289.0		
3-Cl	69.1	289.0		
3-Me	69.1	289.0		

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
4-Me	69.9	292.5		
3-CF_3	68.4	286.2		
3-MeO	69.2	289.6		
4-tBu	69.8	291.9		
4-CN	67.0	280.3		
3,4-Cl_2	68.3	285.6		
3,5-Cl_2	66.7	279.2		
3,5-$(CF_3)_2$	66.3	277.6		
1-chloroethylbenzene $C_6H_5CH(CH_3)$–**Cl**	69.9±1.1	292.4±4.4	Derived	2003VER/KRA
(1-chloro-isopropyl)benzene $C_6H_5C(CH_3)_2$–**Cl**	70.0±1.5	292 8±6 3	Derived	2003VER/KRA
(2-chloroethyl)benzene **Cl**–$CH_2CH_2C_6H_5$	76.4	319.8	Correlation	2003KRO/TUM
1-chloronaphthalene **Cl**–1-naphthyl	(1) 93.4±3 (2) **96.3±2.7** (3) 95.7	390.8±12.6 **402.9±11.3** 400.4	(1) Electron capture detection (2) Derived from $\Delta_f H^\circ$ in ref. (3) Derived	(1) 1989CHE/ALB (2) 1986PED/NAY (3) 1998GAL/PAU
2-chloronaphthalene **Cl**–2-naphthyl	(1) **91.9±2.7** (2) 93.1	**384.5±11.3** 389.5	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived	(1) 1986PED/NAY (2) 1998GAL/PAU
1-adamantyl chloride **Cl**–1-adamantyl	(1) 83.8±3 (2) **90.4±3**	350.6±12.6 **378.2±12.6**	Derived from $\Delta_f H^\circ$ in ref.	(1) 1999FLO/DAV (2) 2002LI/BAR
2,2,2-trichloroethanenitrile $CNCCl_2$–**Cl**	62.2	260.2	Correlation	1995DEN
2,2-dichloroethanenitrile CNCHCl–**Cl**	70.7	295.8	Correlation	1995DEN
carbonyl chloride **Cl**–C(O)Cl	(1) 76.2±2 (2) 65.0±4.6, at 0 K	318.8±8.4 272.1±19.3	(1) Derived from $\Delta_f H^\circ$ in ref. (2) CID	(1) 2002CRC (2) 2003LIY/STY
chloroformyl fluoride **Cl**–COF	90.0	376.6	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
acetyl chloride **Cl**–C(O)CH_3	84.6±2	354.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
2-chloroacetyl chloride **Cl**–CH_2C(O)Cl	64.7	270.7	Correlation	1995DEN

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** - 推荐值, 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
benzoyl chloride **Cl**–C(O)C_6H_5	81.5±2	341.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
2-chloro-1-phenylethan-1-one **Cl**–CH_2C(O)C_6H_5	73.9	309	VI.PP	1999DOR/HEM
2-chloroacetic acid **Cl**–CH_2C(O)OH	(1) 66.6 (2) **74.3±0.5** (3) 71.0±3	278.7 **310.9±2.2** 297 1±12.6	(1) Correlation (2) Calorimetry (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1995DEN (2) 2001LAG/DIO (3) 2001DOR/NOV
2,2-dichloroacetic acid **Cl**–CClHC(O)OH	67.2	281.2	Correlation	1995DEN
2,2,2-trichloroacetic acid **Cl**–CCl_2C(O)OH	66.3	277.4	Correlation	1995DEN
2-chloropropionic acid CH_3**CH**ClC(O)OH	71.2±0.8	298.0±3 2	Combination	2002LAG/DIO
methyl 2-chloroacetate **Cl**–CH_2C(O)OCH_3	72.1	301.7	Correlation	1995DEN
ethyl 2,2-dichloroacetate **Cl**–CClHC(O)OC_2H_5	68.8	287.9	Correlation	1995DEN
ethyl 2,2,2-trichloroacetate **Cl**–CCl_2C(O)OC_2H_5	66.7	279.1	Correlation	1995DEN
phenyl 2-chloroacetate **Cl**–C(O)OC_6H_5	(1) 81 (2) **87**	338.9 **364.0**	(1) PAC (2) PAC, revised	(1) 1989SIM/GRI (2) 1999LAA/MUL
diethyl 2,2-dichloropropane-1,3-dioate **Cl**–CCl(C(O)OEt)$_2$	67.3	281.6	Correlation	1995DEN
chlorothioformyl chloride **Cl**–C(S)Cl	63.4±0.5	265.3±2.1	Photolysis	1977OKA
Cl–C	94.4±3.2	394.9±13.4	Derived	This volume
–CF	82.6±3.8	345.6±15.9		
–CCl	80.9±3.1	338.5±13.0		
–CBr	87.2±15	364.8±63		
–CH	93.8±2.2	392.3±9.2		
–CF_2	52.2±2.5	218.4±10.5		

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
–CClF	57.7±3.8	241.4±15.9		
$-CCl_2$	66.0±2	276.1±8.4		
$-CBr_2$	67.4±3.5	282.0±14.6		
–CClBr	63.2±4	264.4±16.7		
–CHF	77.7±3.8	325.1±15.9		
–CHCl	84.7±2.5	354 4±10.5		
$-CH_2$	94.3±1	394.6±4.2		
–CC$^\bullet$	89±7	372±29		
Cl–CClC$^\bullet$Cl	33.7±3	141.0±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
$-CF_2C^\bullet F_2$	35.6±3	149.0±12.6		
$-CF_2C^\bullet HF$	23.4±3	97.9±12.6		
$-CF_2C^\bullet H_2$	21.1±3	88.3±12.6		
$-CCl_2C^\bullet Cl_2$	17.6±3	73.6±12.6		
$-CHClC^\bullet Cl_2$	18.8±3	78.7±12.6		
$-CH_2C^\bullet Cl_2$	23.2±3	97.1±12.6		
Cl–$CCl_2C^\bullet HCl$	12.2±3	51.0±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
$-CHClC^\bullet HCl$	18.3±3	76.6±12.6		
$-CH_2C^\bullet HCl$	18.4±3	77.0±12.6		
$-CCl_2C^\bullet H_2$	12.3±3	51.5±12.6		
$-CHClC^\bullet H_2$	12.5±3	52.3±12.6		
$-CH_2C^\bullet H_2$	19.3±2	80.8±8.4		
Cl–C$^\bullet$(O)	(1) 7.8±1 (2) 17.1±4.6	32.6±4 71.4±19.3	(1) Derived (2) CID	(1) This volume (2) 2003LIY/STY

6.3 C—Br 键能

表 6.3 C—Br BDEs

断裂键 (**黑体** – 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
cyanogen bromide **Br**–CN	(1) 87.8±1.2 (2) **87.2±1.0**	367.4±5 0 **364.8±4.2**	(1) AE (2) Derived from $\Delta_f H°$ in ref.	(1) 1978DAY/GOW (2) 1998NIST
bromotrifluoromethane **Br**–CF_3	(1) 70.6±3 (2) 69.6 (3) 71.0 (4) **70.8±0.3** (5) 70.8±0.7	295.4±12.6 291.2 297.1 **296.2±1.3** 296.2±2.9	(1) Kinetics (2) Derived (3) Correlation (4) PIMS (5) Derived	(1) 1972FER/WHI(b) (2) 1983EVA/WEE (3) 1995DEN (4) 1997ASH/RUS (5) 1998RUS/MIC
bromodifluoromethane **Br**–CHF_2	69±2	288.7±8.4	Bromination	1974OKA/WHI
bromofluoromethane **Br**–CH_2F	70.5±4	295±17	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
bromochlorodifluoromethane **Br**–CF_2Cl	(1) 64.5±1.5 (2) 64.1±2	269.9±6.3 268±8	(1) Review (2) Thermolysis	(1) 1982MCM/GOL (2) 1994DEL/LOU
difluorodibromomethane **Br**–CF_2Br	63.8±4	270±17	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
bromodichlorofluoromethane **Br**–CCl_2F	61.6±4	257.7±17	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
bromochlorofluoromethane **Br**–CHFCl	67.2±4	281±17	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
bromotrichloromethane **Br**–CCl_3	55.3±1	231.4±4.2	Bromination	1973MEN/GOL
bromodichloromethane **Br**–$CHCl_2$	59.8±5	250±21	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
bromochloromethane **Br**–CH_2Cl	(1) 65.5±4 (2) **68.0**	274±17 **285**	(1) Derived from $\Delta_f H°$ in ref. (2) Photodissoc.	(1) 1991GUR/VEY (2) 1994TZE/LEE
dibromochlorofluoromethane **Br**–CFClBr	61.4±1.2	257±5	Derived from $\Delta_f H°$ in ref.	2003OWE/NAU
dibromochloromethane **Br**–CHClBr	58.3±5	244±21	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
dibromodichloromethane **Br**–$CBrCl_2$	53.9±4	225.5±17	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
tribromochloromethane **Br**–CBr_2Cl	50.4±2.5	210.9±10.5	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
tetrabromomethane **Br**–CBr_3	(1) 56.2±1.8 (2) **54.7±2.3**	235.1±7.5 **228.9±9.6**	(1) Bromination (2) Review	(1) 1971KIN/GOL (2) 2001LAZ/PRO

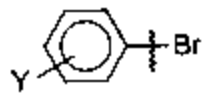
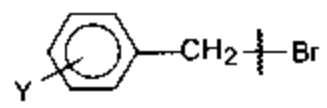
续表

断裂键 (**黑体** – 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (**黑体** – 推荐值; 括号内数字 – 文献编号) kcal/mol	kJ/mol	方法	文献
tribromomethane **Br**–$CHBr_2$	(1) 64.8 (2) **65.7±3.1**	271.1 **274.9±13.0**	(1) Electron capture detection (2) Review	(1) 1989CHE/ALB (2) 2001LAZ/PRO
dibromomethane **Br**–CH_2Br	(1) 69.8±2 (2) 65.8 (3) 60.0 (4) **69.3±2.4**	292.0±8.4 275.3 250.9 **290.0±10.0**	(1) Bromination (2) Electron capture detection (3) Photoionization (4) Review	(1) 1987TSC/PAD (2) 1989CHE/ALB (3) 1996LI/RAN(b) (4) 2001LAZ/PRO
bromotriiodomethane **Br**–CI_3	62.6±11	262±46	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
bromodiiodomethane **Br**–CHI_2	67±9	280±38	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
bromoiodomethane **Br**–CH_2I	67.3±6.5	282±27	Derived from $\Delta_f H°$ in ref.	1991GUR/VEY
bromomethane **Br**–CH_3	70.3±0 5	294.1±2.1	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
bromoethyne **Br**–C≡CH	98.1	410.5	Derived from $\Delta_f H°$ in ref.	1998NIST
(Z)-1,2-dibromoethylene (Z)-CHBr=CH–**Br**	< 83.8	<350.6	Electron capture detection	1989CHE/ALB
(E)-1,2-dibromoethylene (E)-CHBr=CH–**Br**	< 83.3	<348.5	Electron capture detection	1989CHE/ALB
vinyl bromide **Br**–$CH=CH_2$	(1) **79.4±1.5** (2) 77±3 (3) 79.3	**332.2±6.3** 322.2±12.6 331.8	(1) Derived from $\Delta_f H°$ in ref. (2) Photodissociat. (3) Correlation	(1) 1986PED/NAY (2) 1989WOD/HIN (3) 2003KRO/TUM
bromopentafluoroethane **Br**-CF_2CF_3	(1) 68.6±1.5 (2) 68.8 (3) **67.7±1.5**	287.0±6.3 287.9 **283.3±6.3**	(1) Kinetics (2) Derived (3) Derived from $\Delta_f H°$ in ref.	(1) 1972FER/WHI (2) 1983EVA/WEE (3) 2002CRC
1,1-dibromo-1-chloro-2,2,2-trifluoroethane **Br**–$CClBrCF_3$	60.0±1.5	251.0±6.3	Review	1982MCM/GOL
1,2-dibromo-1,1,2,2-tetrafluoroethane **Br**-CF_2CF_2Br	67.6±1.6, at 0 K	282.8±6.7	UV photolysis	1989NAT/MIN
1-bromo-1-chloro-2,2,2-trifluoroethane **Br**–$CHClCF_3$	65.7±1.5	274.9±6.3	Review	1982MCM/GOL
1-bromo-1,1-difluoroethane **Br**–CF_2CH_3	68.6±1.3	287.0±5.4	Kinetics	1977PIC/ROD

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (**黑体** - 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1-bromo-2-chloroethane **Br**–CH_2CH_2Cl	69.9±2.0	292.5±8.4	Derived from $\Delta_f H°$ in ref.	1988LIA/BAR
1,1-bromochloroethane **Br**–$CHClCH_3$	65±2	272.0±8 4	Derived from $\Delta_f H°$ in ref.	1988LIA/BAR
bromoethane **Br**–C_2H_5	(1) **70.0±1.0** (2) 70.4	**292.9±4.2** 294.6	(1) Derived from $\Delta_f H°$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
3-bromo-1-propene **Br** $CH_2CH=CH_2$	(1) **56.7±1.2** (2) 56.4	**237.2±5.0** 235.8	(1) Derived from $\Delta_f H°$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
(E)-1-bromo-1-propene (E)-**Br** $CH=CHCH_3$	(1) **80.0±1.2** (2) 78.9	**334.7±5.0** 330.1	(1) Derived from $\Delta_f H°$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
(Z)-1-bromo-1-propene (Z)-**Br**–$CH=CHCH_3$	(1) **80.7±1.2** (2) 79.6	**337.6±5.0** 332.9	(1) Derived from $\Delta_f H°$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
1-bromopropane **Br**–nC_3H_7	(1) **71.3±1.0** (2) 70.5	**298.3±4.2** 294.9	(1) Derived from $\Delta_f H°$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
2-bromopropane **Br**–iC_3H_7	(1) **71.5±1.5** (2) 71.2	**299.2±6.3** 297.7	(1) Derived from $\Delta_f H°$ in ref. (2) Correlation	(1) 2002CRC (2) 2003KRO/TUM
1,3-dibromopropane **Br** $CH_2CH_2CH_2Br$	77.6	324.7	Electron capture detection	1989CHE/ALB
1-bromo-heptafluoropropane **Br**–$CF_2CF_2CF_3$	66.5±2.5	278.2±10.5	Kinetics	1967COO/WHI
2-bromo-heptafluoropropane CF_3CF**Br**CF_3	(1) 65.5±1.1 (2) 65.4	274.2±4.6 273.6	(1) Review (2) Kinetics	(1) 1982MCM/GOL (2) 1983EVA/WEE
1,1,1-tribromopropane **Br**–$CBr_2CH_2CH_3$	60.8	254.4	Correlation	1995DEN
1-bromobutane **Br** nC_4H_9	(1) **70.9±1** (2) 71.1	**296.6±4.2** 297.4	(1) Derived from $\Delta_f H°$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
1-bromo-2-methyl-propane **Br**–$CH_2CH(CH_3)_2$	70.5	295.0	Correlation	2003KRO/TUM
2-bromobutane **Br**–sC_4H_9	(1) **71.7±1** (2) 71.9	**300.0±4.2** 300.7	(1) Derived from $\Delta_f H°$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
2-bromo-2-methylpropane **Br**–tC_4H_9	(1) **70.0±1.5** (2) 69.9	**292.9±6.3** 292.4	(1) Derived from $\Delta_f H°$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 - 文献编号) kcal/mol	kJ/mol	方法	文献
3-bromo-but-1-nen CH_2=CHCH**Br**CH_3	55.7	233.1	Correlation	2003KRO/TUM
4-bromo-but-1-nen **Br**-CH_2CH_2CH=CH_2	68.1	284.8	Correlation	2003KRO/TUM
2-bromo-alkanes **Br**- $CH(CH_3)(C_nH_{2n-1})$ n = 3	70.9	296.6	Correlation	2003KRO/TUM
4	71.0	296.9		
5	71.1	297.3		
6	70.8	296.3		
1-bromo-2,2-dimethyl-propane **Br**–$CH_2C(CH_3)_3$	71.3	298.2	Correlation	2003KRO/TUM
2-bromo-2-methyl-butane $(CH_3)_2$C**Br**C_2H_5	68.7	287.6	Correlation	2003KRO/TUM
bromocycloheptane **Br**–cyclo-C_7H_9	69.6	291.1	Correlation	2003KRO/TUM
bromocyclohexane **Br**–cyclo-C_6H_{11}	69.9	292.4	Correlation	2003KRO/TUM
bromopentafluorobenzene **Br**–C_6F_5	~78.4	~328	Derived	1996ING/WEI
bromobenzene, substituted  Y = H	(1) 83.5±2.5 (2) **80.4±1.5**	349.4±10.5 **336.4±6.3**	(1) Electron capture detection (2) Derived from $\Delta_f H°$ in ref.	(1) 1989CHE/ALB (2) 1986PED/NAY
2-F	(3) 82.0	343.1	(3) Correlation	(3) 1995DEN
2-Me	(3) 83.9	351.0		
3-CF_3	(3) 79.9	334.3		
bromotoluene, substituted  Y = p-H	(1) 60.0±3 (2) 55.9 (3) 60.7±1 (4) 55.1±2.5 (5) **57.2±1.5**	251.0±12.6 233.9 254±4 230.5±10.5 **239.3±6.3**	(1) Derived from $\Delta_f H°$ in ref. (2) Electrochem. (3) PAC (4) Derived from $\Delta_f H°$ in ref. (5) Derived	(1) 1986PED/NAY (2) 1992AND/GOR (3) 1997LAA/BOR (4) 1998NIST (5) 2003VER/KRA

续表

断裂键 (**黑体** – 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (**黑体** – 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
p-F	(6) 58.9	246.4	(6) AOP	(6) 1993ZHA
p-Br	(6) 57.6	241.0		
p-CN	(1) 60.9±1 (6) **54.4**	255±4 **227.6**		
p-Me	(6) 59.7	249.8		
p-t-Bu	(1) 60.0±1	251±4		
m-CF_3	(1) 60.9±1	255±4		
(1-bromovinyl)benzene CH_2=CH**Br**Ph	63.4	265.3	Correlation	1995DEN
(2-bromovinyl)benzene **Br**–CH=CHPh	65.1	272.4	Correlation	1995DEN
benzyl bromide **Br**–$CH_2C_6F_5$	53.8±1.5	225.1±6.3	Toluene carrier tech	1980KOM/KRE
(1,2,2,2-tetraethyl)benzene **Br**–$CBr_2CHBrPh$	60.3	252.3	Correlation	1995DEN
(2-bromoethyl)benzene **Br**–$CH_2CH_2C_6H_5$	64.1	268.3	Correlation	2003KRO/TUM
1-bromoethylbenzene $C_6H_5CH(CH_3)$ –**Br**	57.4±2	240.1±8.2	Derived	2003VER/KRA
(1-bromo-isopropyl)benzene $C_6H_5C(CH_3)_2$–**Br**	56.6±1.6	236.7±6.9	Derived	2003VER/KRA
1-bromonaphthalene **Br**–$C_{10}H_7$	(1) 79.3 (2) **81.2**	331.8 **339.7**	(1) Electron capture detection (2) Derived	(1) 1989CHE/ALB (2) 1998GAL/PAU
2-bromonaphthalene **Br**–$C_{10}H_7$	81.7	341.8	Derived	1998GAL/PAU
(1,2-dibromo-2-phenylethyl)-benzene $(PhCHBr)_2$	62.9	263.2	Correlation	1995DEN
9-anthracenyl bromide **Br**-anthracenyl	77.1	322.6	Derived	1998GAL/PAU
acetyl bromide **Br**–C(O)CH_3	(1) 64 (2) **69.8±2**	267.8 **292.0±8.4**	(1) Photolysis (2) Derived from $\Delta_f H°$ in ref.	(1) 1995SU/DIB (2) 2002CRC
benzoyl bromide **Br**-C(O)C_6H_5	(1) 64.1 (2) **66.1±2**	268.2 **276.6±8.4**	(1) Review (2) Derived from $\Delta_f H°$ in ref.	(1) 1970ONE/BEN (2) 1994PED

续表

断裂键 (**黑体** = 离解原了) $\Delta_f H°$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1-bromoacetone **Br**–$CH_2C(O)CH_3$	62.5	261.5	VLPP	1978ZAB/BEN
2-bromo-1-phenylethan-1-one **Br**–$CH_2C(O)C_6H_5$	64.8	271	VLPP	1999DOR/HEM
2-bromoacetic acid **Br**–$CH_2C(O)OH$	(1) **61.5±0.9** (2) 58.2±3 (3) 64.3	**257.4±3.7** 243.5±12.6 269.0	(1) Calorimetry (2) Derived from $\Delta_f H°$ in ref. (3) Correlation	(1) 2001LAG/DIO (2) 2001DOR/NOV (3) 2003KRO/TUM
2,2,2-tribromoacetic acid **Br**–$CBr_2C(O)OH$	60.8	254.4	Correlation	1995DEN
2-bromopropanoic acid CH_3CH**Br**$C(O)OH$	61.3	256.3	Correlation	2003KRO/TIM
3-bromopropanoic acid **Br**–$CH_2CH_2C(O)OH$	66.0	276.3	Correlation	2003KRO/TIM
ethyl 2,2-dibromoacetate **Br**–$CHBrC(O)OC_2H_5$	62.9	263.2	Correlation	1995DEN
ethyl 2,2,2-tribromoacetate **Br**–$CBr_2C(O)OC_2H_5$	58.9	246.4	Correlation	1995DEN
diethyl 2-bromopropane-1,3-dioate **Br**–$CH(C(O)OEt)_2$	63.5	265.7	Correlation	1995DEN
diethyl 2,2-dibromopropane-1,3-dioate **Br**–$CBr(C(O)OEt)_2$	61.4	256.9	Correlation	1995DEN
Br–C	76.0±2	318.0±8.4	Derived	This volume
–CBr	71.3±2	298.3±8.4		
$–CF_2$	36.9±3.5	154.4±14.6		
–CClF	42.6±3.5	178.2±14.6		
$-CCl_2$	51.1±2.5	213.8±10.5		
–CClBr	51.5±2.5	215.5±10.5		
$–CBr_2$	55.1±2	230. 5±8.4		
–CHCl	70.5±2.5	295.0±10.5		
$–CH_2$	79 1±0.7	331.0±2.9		
Br–$CH_2C^•H_2$	6.9±2	28.9±8.4	Derived from $\Delta_f H°$ in ref.	1998NIST
$–CH_2C^•HCH_3$	8.5±2	35.6±8.4		

6.4 C—I键能

表 6.4 C—I BDEs

断裂键 (**黑体** - 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
cyanogen iodide **I**–CN	(1) 72.5±1.2 (2) **76.5**	303.3±5.0 **320.1**	(1) AP (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1978DAY/GOW (2) 2002CRC
trifluoroiodomethane **I**–CF_3	(1) 52.6±1.1 (2) 53.5 (3) 54.4±0.5 (4) **54.3±0.3** (5) 54.3±0.7	220.1±4.6 223.8 227.6±2.1 **227.2±1.3** 227.2±2.9	(1) Kinetics (3) Kinetics (2) Kinetics (4) PIMS (5) Derived	(1) 1975OKA/WHI (2) 1984AHO/WHI (3) 1991SKO/DYM (4) 1997ASH/RUS (5) 1998RUS/MIC
difluoroiodomethane **I**- CHF_2	57.3±6	240±25	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
fluoroiodomethane **I**–CH_2F	55.6±6	233±25	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
difluorochloroiodomethane **I**–$CClF_2$	49.6±6.5	208±27	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
difluorobromoiodomethane **I**–CF_2Br	49.5±5	207±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
fluorodichloroiodomethane **I**–CCl_2F	47.2±5.5	197±23	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
fluorochloroiodomethane **I**–CHClF	52.8±5.5	221±23	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
trichloroiodomethane **I**–CCl_3	40.1±10	168±42	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
dichloroiodomethane **I**–$CHCl_2$	46.6±5	195±21	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
chloroiodomethane **I**–CH_2Cl	48.8±0.2	204.2±0.8	Kinetics	1996SKO/DYM
bromochlorofluoroiodomethane **I**–CFClBr	46.9±5.5	196±23	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
bromochloroiodomethane **I**–CHClBr	45.4±5.5	190±23	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
bromodichloroiodomethane **I**-$CBrCl_2$	40.8±5.5	171±23	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
dibromochloroiodomethane **I**–CBr_2Cl	37.0±6.5	155±27	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
tribromoiodomethane **I** CBr_3	34.1±6.5	143±27	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
dibromoiodomethane **I**-$CHBr_2$	44.2±6.5	185±27	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY

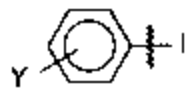
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; · 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
bromoiodomethane I–CH_2Br	52.1±6.5	218+27	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
tetraiodomethane I–CI_3	45.8±12	192+50	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
triiodomethane I–CHI_2	52.7±8	220.5±33	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
diiodomethane I–CH_2I	(1) **51.9±2** (2) 50.6	**217.1±8.4** 211.7	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1993CAR/LAY (2) 1995DEN
iodomethane I–CH_3	57.1±0.5	238.9±2.1	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-iodoethanenitrile I–CH_2CN	44.7±1.5	187.0±6.3	PES	2000LAF/SZA
pentafluoroiodoethane I–CF_2CF_3	(1) 51.2±1 (2) 52.3 (3) **52.4±0.5**	214.2±4.2 218.8 **219.2±2.1**	Kinetics	(1) 1976WU/ROD (2) 1984AHO/WHI (3) 1991SKO/DYM
1,2-diiodo-1,1,2,2-tetrafluoro ethane I–CF_2CF_2I	52±1.6, at 0K	217.6±6.7	UV photolysis	1984KRA/BUT
1,1,1-trifluoro-2-iodoethane I–CH_2CF_3	(1) **56.3±1** (2) 52.9	**235.6±4.2** 221.3	(1) Iodination (2) Correlation	(1) 1973WU/ROD (2) 1995DEN
1-chloro-1,1,2-trifluoro-2-iodo-ethane I–$CHFCClF_2$	48.3±0.5	202±2	Kinetics	1998SKO/DYM
1,1-difluoro-1-iodoethane I–CF_2CH_3	52±1	217.6±4.2	Review	1982MCM/GOL
1-fluoro-1,1-diiodoethane I–$CFICH_3$	52.1±1	218.0±4.2	Iodination	1976PIC/ROD
1-chloro-2-iodo-ethane I–CH_2CH_2Cl	54.2	226.8	Correlation	1995DEN
1-chloro-2-bromoethane I–CH_2CH_2Br	53.0	221.8	Correlation	1995DEN
pentafluoro-2-iodopropane CF_3CFICF_3	51.4	215.1	Kinetics	1984AHO/WHI
iodoethyne I–CCH	78.8	329.9	Correlation	2003KRO/TUM
iodoethylene I–$CH=CH_2$	(1) 61.9±1.0 (2) 66.0	259.0±4.2 276.3	(1) Photofrag-mentation (2) Correlation	(1) 1989CAO/ZHA (2) 2003KRO/TUM
iodoethane I–C_2H_5	55.8±1.5	233.5±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-iodo-prop-1-yne I–CH_2CCH	44.1	184.6	Correlation	2003KRO/TUM

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
3-iodo-1-propene I–$CH_2CH{=}CH_2$	(1) **44.4±1.5** (2) 42.7	**185.8±6.3** 178.5	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
(Z)-1-iodo-1-propene I–$CH{=}CHCH_3$	(1) 68.6±2 (2) 67.5	287.0±8.4 282.3	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
(E)-1-iodo-1-propene I–$CH{=}CHCH_3$	(1) **67.0±2** (2) 65.9	**280.3±8.4** 275.6	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
1-iodopropane I–nC_3H_7	(1) **56.6±1** (2) 56.9	**236.8±4.2** 238.0	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
2-iodopropane I–iC_3H_7	(1) **56.1±1.5** (2) 57.1	**234.7±6.3** 239.0	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
1,3-diiodopropane I–$CH_2CH_2CH_2I$	54.4	227.6	Correlation	1995DEN
1-iodononafluorobutane I–C_4F_9	49.2	205.8	Kinetics	1991SKO/DYM
1-iodo-2-methyl-propane I–$isoC_4H_9$	57.3	239.8	Correlation	2003KRO/TUM
2-iodobutane I–sC_4H_9	54.1	226.4	Correlation	1995DEN
2-iodo-2-methylpropane I–tC_4H_9	(1) **54.3±1.5** (2) 54.3	**227.2±6.3** 227.0	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Correlation	(1) 1986PED/NAY (2) 2003KRO/TUM
3-iodo-but-1-nen $CH_3CHICH{=}CH_2$	40.3	168.7	Correlation	2003KRO/TUM
4-iodo-but-1-nen I–$CH_2CH_2CH{=}CH_2$	55.8	233.7	Correlation	2003KRO/TUM
1-iodo-alkanes I–C_nH_{2n+1}				
n = 4	56.2	235.0	Correlation	2003KRO/TUM
5	56.3	235.7		
6	56.4	236.0		
7	56.2	235.2		
8	56.1	234.9		
12	56.1	234.9		

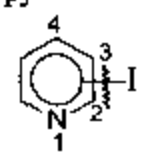
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
16	56.2	234.9		
18	56.1	234.9		
1-iodo-2,2-imethylpropane I–$CH_2C(CH_3)_3$	57.1	239.1	Correlation	2003KRO/TUM
2-iodo-alkanes $CH_3CHIC_nH_{2n+1}$				
n = 3	55.5	232.3	Correlation	2003KRO/TUM
4	55.5	232.4		
5	55.7	233.2		
6	55.4	231.8		
2-iodo-2-methyl-butane $(CH_3)_2CIC_2H_5$	54.3	227.0	Correlation	2003KRO/TUM
iodocycloheptane I–cyclo-C_5H_9	55.4	231.8	Correlation	2003KRO/TUM
iodocyclohexane I–cyclo-C_6H_{11}	(1) **55.5±1.5**	**232.2±6.3**	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1986PED/NAY
	(2) 54.8	229.2	(2) Correlation	(2) 2003KRO/TUM
iodobenzene I–C_6H_5	65.0±1	272.0±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pentafluoroiodobenzene	(1) 65.4±2	273.6±8.4	(1) Toluene carrier tech.	(1) 1976KOM/KRE
I–C_6F_5	(2) <72.1	<301.7	(2) Electron capture detection	(2) 1989CHE/ALB
iodobenzene, substituted 				
Y = 2-F	(1) 65.9	275.7	Correlation	(1) 1995DEN
	(2) 67.4	281.9		(2) 2003KRO/TUM
2-Cl	(1) 65.1	272.4		
2-Br	(1) 64.2	268.6		
	(2) 65.5	273.9		
2-I	(1) 63.6	266.1		
	(2) 67.3	281.6		
2-Me	(1) 65.7	274.9		
	(2) 67.2	281.0		
2-CF_3	(1) 63.2	264.4		

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
2-NH_2	(1) 66.7 (2) 70.3	279.1 294.3		
2-NO_2	(1) 65.6	274.5		
2-MeO	(1) 66.6 (2) 68.0	278.7 284.7		
2-Et	(1) 65.5 (2) 67.0	274.1 280.2		
2-EtO	(1) 66.7 (2) 68.0	279.1 284.6		
2-Ph	(1) 64.8 (2) 66.2	271.1 276.8		
2,6-Me_2	(1) 65.9 (2) 67.4	275.7 281.8		
benzyl iodide I–$CH_2C_6H_5$	(1) 45.4 (2) 43.9±2 (3) **44.9±1.1**	190.0 183.7±8.4 **187.8±4.8**	(1) Shock wave (2) Derived from $\Delta_f H^\circ$ in ref. (3) Derived	(1) 1990HIP/TRO (2) 1998NIST (3) 2003VER/KRA
(2-iodoethyl)benzene I–$CH_2CH_2C_6H_5$	54.9	229.7	Correlation	1995DEN
1-iodoethylbenzene $C_6H_5CH(CH_3)$–I	42.1±1	176.1±4.3	Derived	2003VER/KRA
(1-iodo-isopropyl)benzene $C_6H_5C(CH_3)_2$–I	42.1±1	176.1±4.3	Derived	2003VER/KRA
1-iodonaphthalene I–1-naphthyl	(1) **65.6±2.5** (2) 65.0 (3) 66.8	**274.5±10.5** 272.0 279.5	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived (3) Correlation	(1) 1986PED/NAY (2) 1998GAL/PAU (3) 2003KRO/TUM
2-iodonaphthalene I–2-naphthyl	(1) **65.0±2.5** (2) 66.3 (3) 67.1	**272.0±10.5** 277.4 280.9	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived (3) Correlation	(1) 1986PED/NAY (2) 1998GAL/PAU (3) 2003KRO/TUM
1-adamantyl iodide I–1-adamantyl	53.7	224.7	Correlation	1995DEN
iodoacetonitrile I–CH_2CN	44.7±2.0	187.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	2000LAF/SZA
acetyl iodide I–$C(O)CH_3$	53.3±2	223.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
benzoyl iodide I–$C(O)C_6H_5$	50.7±2	212.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1994PED

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值， 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
iodoacetic acid I–$CH_2C(O)OH$	(1) 51.2 (2) **47.2±0.6**	214.2 **197.5±2.7**	(1) Correlation (2) Calorimetry	(1) 1995DEN (2) 2001LAG/DIO
3-iodopropanioc acid I–$CH_2CH_2C(O)OH$	54.5	228.0	Correlation	1995DEN
ethyl 2-iodoacetate I–$CH_2C(O)OC_2H_5$	51.9	217.1	Correlation	1995DEN
pyridine iodide  C–I at 2 site	63.1	264.0	Correlation	1995DEN
3	65.2	272.8		
4	64.9	271.5		
I–C	60.5±8.5	253.1±35.6	Derived	This volume
–CI	49.8±16	208.4±66.9		
$–CI_2$	35.9±14	150.2±60		
$–CH_2$	63.9±2.1	267.4±8.8		

第 7 章　O—X 键能

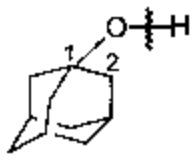
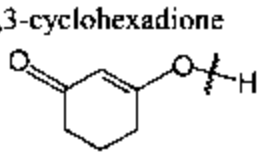
7.1　O—H键能

7.1.1　非酚类分子中的O—H键能

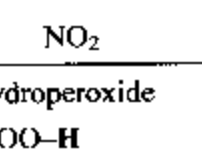
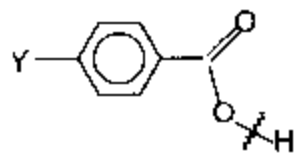
表 7.1.1　非酚类分子中的 O—H BDEs

断裂键 (黑体　离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
water HO–**H** $\Delta_f H^\circ$(R) - 8.91±0.07 (37.28±0.29) O–H	(1) 119.30±0.05 (2) 118.88±0.01 (3) **118.81±0.07** (4) 118.82±0.16 (3) 102.75±0.07	499.15±0.21 497.38±0.06 **497.10±0.29** 497.14±0.67 429.91±0.29	(1) Recommend. (2) Photolysis (3) Recommend. (4) Shock tube	(1) 1994BER/ELL (2) 2000HAR/HWA (3) 2002RUS/WAG (4) 2002HER/HAN
hypofluorous acid FO–**H**	101.6	425.1	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
hypochlorous acid ClO **H**	94.1	393.7	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
hydrobromous acid BrO–**H**	96.8	405.0	Derived from $\Delta_f H^\circ$ in ref.	2001IUPC
hydroiodomous acid IO–**H**	96.4	403.3	Derived from $\Delta_f H^\circ$ in ref.	2001IUPC
methanol CH_3O–**H** $\Delta_f H^\circ$(R) = 4.5±0.7 (18.8±2.9) CD_3O- **H**	(1) 104.4±1 (2) 104.2±0.9 (3) 104.9±0.7 (4) **104.6±0.7** (5) 105.2±0.7 (6) 104.2±2.2	436.8±4.2 436.0±3.8 439±3 **437.7±2.8** 440.2±3 436±9	(1) Kinetics (2) Recommend. (3) CID (4) GPA, revised (5) GPA (6) PES, derived	(1) 1974BAT/CHR (2) 1994BER/ELL (3) 1999DET/ERV (4) 2002ERV/DET (5) 2003REE/HAR (6) 2000RAM/DAV
trifluoromethanol CF_3O–**H** $\Delta_f H^\circ$(R) = –151.8±1.7 (–635.1±7.1)	(1) 109 (2) 120±3 (3) 124.7±3.6 (4) 117.5 (5) **118.8**	456.1 502.1±12.6 521.7±15.1 491.6 **497.1**	(1) Pyrolysis (2) FT-IR (3) FA MS (4) PIMS (5) Recommend.	(1) 1982BAT/WAL (2) 1993WAL/HUR (3) 1996HUE/DUN (4) 1997ASH/APP (5) 2000REI/PRA
ethyn-1-ol HC≡CO–**H**	105.9±2.1	443.1	PES	1983OAK/JON
ethanol C_2H_5O–**H** $\Delta_f H^\circ$(R) = –3.6±0.9 (–15.1±3.3)	(1) 104.2±1 (2) 104.6±0.8 (3) 105.2±1.2 (4) **104.7±0.8** (5) 105.4±1.4	436.0±4.2 437.6±3.3 440±5 **438.1±3.3** 441.0±5.9	(1) Pyrolysis (2) Recommend. (3) CID (4) GPA, revised (5) GPA	(1) 1974BAT/CHR (2) 1994BER/ELL (3) 1999DET/ERV (4) 2002ERV/DET (5) 2003REE/HAR

续表

断裂键 (黑体 = 离解原 f) Δ_fH°(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
C_2H_5O–**D** C_2D_5O–**H**	(6) ≤105.9±0.5 (7) 104.2±2.4	≤443.1±2.1 436±10	(6) Photodissociat. (7) PES, derived	(6) 1999XU/AMA (7) 2000RAM/DAV
vinyl alcohol CH_2=CHO–**H** Δ_fH°(R) = 4.4±0.3 (18.4±1.3)	85	355.6	FT-ICR	2001BOU/CHA
2,2,2-trifluoroethan-1-ol CF_3CH_2O **H**	107.0±2.5	447.7±10.5	GPA	2003REE/HAR
1-propanol nC_3H_7O–**H** Δ_fH°(R) = - 7.2±2 (–30.1±8.4)	(1) 105.9±2 (2) 103.4±1 (3) ≤103.5±0.5	443.1±8.4 432.6±4.2 ≤433±2	(1) Review (2) Pyrolysis (3) Photodissocit.	(1) 1973BEN/ONE (2) 1974BAT/CHR (3) 2003ZHO/YUA
2-propanol iC_3H_7O–**H** Δ_fH°(R) = –11.6±0.8 (-48.5±3.3)	(1) 104.7±1 (2) 103.9 (3) 105.9±1.0 (4) **105.7±0.7** (5) ≤104.0±0.5	438.1±4.2 434.7 443±4 **442.3±2.8** ≤435±2	(1) Pyrolysis (2) AOP (3) CID (4) GPA, revised (5) Photodissociat.	(1) 1974BAT/CHR (2) 1996BOR/LIU (3) 1999DET/ERV (4) 2002ERV/DET (5) 2003ZHO/YUA
1-butanol nC_4H_9O–**H** Δ_fH°(R) = –15 (–62.8)	101.9±1	426.3±4.2	Pyrolysis	1974BAT/CHR
2-butanol sC_4H_9O–**H** Δ_fH°(R) = –16.6 (69.5)	105.5±1	441 4±4.2	Pyrolysis	1974BAT/CHR
tert-butyl alcohol tC_4H_9O–**H** Δ_fH°(R) = –20.5±0.9 (–85.8±3.8)	(1) 105.1±1 (2) 105.5 (3) 105.5 (4) **106.3±0.7** (5) 106.8±1.0	439.7±4.2 441.4 441.4 **444.9±2.8** 446.9±4.2	(1) Pyrolysis (2) AOP (3) PAC (4) GPA, revised (5) GPA	(1) 1974BAT/CHR (2) 1996BOR/LIU (3) 2000REI/PRA (4) 2002ERV/DET (5) 2003REE/HAR
neopentyl alcohol $tBuCH_2O$–**H**	102.3±1	428.0±4.2	Pyrolysis	1974BAT/CHR
benzyl alcohol $C_6H_5CH_2O$–**H** Δ_fH°(R) = 25.6±3 (107.1±12.6)	101.7	425.5	AOP	1996BOR/LIU
1-adamantanol 	103.1	431.5	Derived	2002MIR/LEB
1,3-cyclohexadione 	92	384.9	AOP	1994BOR/SAT

续表

断裂键 (**黑体** · 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ethane-1,1-diol $CH_3C(OH)O$–**H**	106.8±1.5	446.9±6.3	Electrochemical	2002MER/LIN
propane-2,2-diol $(CH_3)_2C(OH)O$–**H**	107.7±1.5	450.6±6.3	Electrochemical	2002MER/LIN
tropolone 	88	368.2	AOP	1994BOR/SAT
formic acid HC(O)O–**H** $\Delta_f H^\circ$(R) = –30±3 (–125.5±12.6)	112±3	468.6±12.6	Recommended	2003BLA/ELL
acetic acid $CH_3C(O)O$–**H** $\Delta_f H^\circ$(R) = –43±3 (–179.9±12.6)	(1) 106.4 (2) 105.8±2 (3) 112 (4) **112±3**	445.2 442.7 468.6 **468.6±12.6**	(1) Electrochem. (2) Review (3) AOP (4) Review	(1) 1963EBE (2) 1973BEN/ONE (3) 2000XIA/ZHU (4) 2003BLA/ELL
propanoic acid $C_2H_5C(O)O$–**H**	(1) 106.4±2 (2) 113	445.2 472.8	(1) Review (2) AOP	(1) 1973BEN/ONE (2) 2000XIA/ZHU
butanoic acid $nC_3H_7C(O)O$–**H**	105.9±2	443.1	Review	1973BEN/ONE
iso-butanoic acid $iC_3H_7C(O)O$–**H**	113	472.8	AOP	2000XIA/ZHU
benzoic acid $C_6H_5C(O)O$–**H** $\Delta_f H^\circ$(R) = –12±4 (–50.2±16.7)	(1) 105 (2) 111 (3) **111±4**	439.3 464.4 **464.4±16.7**	(1) AOP (2) AOP (3) Recommend.	(1) 1994BOR/SAT (2) 2000XIA/ZHU (3) 2003BLA/ELL
benzoic acid, substituted 				
Y = Br	112	468.6	AOP	2000XIA/ZHU
Me	110	460.2		
MeO	109	456.1		
NO_2	119	497.9		
hydroperoxide HOO–**H** $\Delta_f H^\circ$(R) = 3.2±0.5 (13.4±2.1)	(1) 87.2±1.0 (2) 88.2±1.0 (3) 88.4±1.2 (4) 87.9±0.8 (5) **87.8±0.5**	364.8±6.4 369.0±4.2 269.9±5.0 367.8±3.3 **367.4±2.1**	(1) Laser magnetic resonance (2) Review (3) GIB MS (4) GPA (5) PES	(1) 1980HOW (2) 1983SHU/BEN (3) 1990FIS/RM(b) (4) 1998LIT/RUS (5) 2002RAM/BLA

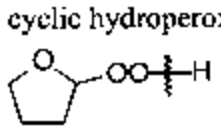
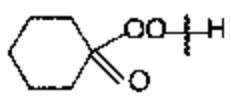
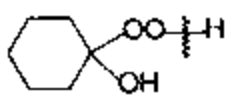
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
hydroperoxy radical **H**-OO	(1) **48.2±0.8** (2) 48.3±1.2	**201.7±3.3** 202.1±5.0	(1) Derived from $\Delta_f H^\circ$ in ref. (2) GIB MS	(1) 2001IUPC (2) 1990FIS/ARM(b)
methyl hydroperoxide CH_3OO–**H** $\Delta_f H^\circ$(R) = 5.1±1.2 (20.1±5.0) CD_3OO–**H**	(1) **88.5±0.5** (2) 87.2 (3) 87.9±1.1 (3) 87.8±1.0	**370.3±2.1** 365 367.8±4.6 367.4±4.2	(1) VLPP (2) Electrochem. (3) GPA	(1) 1984KON/BEN(b) (2) 1996JON (3) 2001BLA/RAM
rifluoromethyl hydroperoxide CF_3OO–**H**	91.5	383	Electrochemical	1996JON
fluoromethyl hydroperoxide CH_2FOO–**H**	90.6	379	Electrochemical	1996JON
trichloromethyl hydroperoxide CCl_3OO–**H**	92.3	386	Electrochemical	1996JON
dichloromethyl hydroperoxide $CHCl_2OO$–**H**	91.5	383	Electrochemical	1996JON
chloromethyl hydroperoxide CH_2ClOO–**H**	90.6	379	Electrochemical	1996JON
tribromomethyl hydroperoxide CBr_3OO–**H**	91.5	383	Electrochemical	1996JON
bromomethyl hydroperoxide CH_2BrOO–**H**	90.6	379	Electrochemical	1996JON
ethyl hydroperoxide C_2H_5OO–**H** $\Delta_f H^\circ$(R) = –6.8±2.3 (–28.5±9.6)	(1) 86.8 (2) 84.8±2.2	363 354.8	(1) Electrochem. (2) GPA	(1) 1996JON (2) 2001BLA/RAM
2-chloroethyl hydroperoxide $CH_3CHClOO$–**H**	90.1	377	Electrochemical	1996JON
2,2-dichloroethyl hydroperoxide CH_3CCl_2OO–**H**	91.5	383	Electrochemical	1996JON
1,1,1-trifluoro-2-chloroethyl hydroperoxide $CF_3CHClOO$–**H**	91.8	384	Electrochemical	1996JON
1,1,2,2-tetrachloroethyl hydroperoxide $CHCl_2CCl_2OO$–**H**	98.4	411.6	Correlation	2004DEN/DEN
pentachloroethyl hydroperoxide C_2Cl_5OO–**H**	(1) 91.5 (2) 98.7	383 413.1	(1) Electrochem. (2) Correlation	(1) 1996JON (2) 2004DEN/DEN
iso-propyl hydroperoxide iC_3H_7OO–**H** $\Delta_f H^\circ$(R) = 15.6±2.7 (–65.4±11.3)	85.1	356	Electrochemical	1996JON

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** - 推荐值; 括号内数字 - 文献编号) kcal/mol	kJ/mol	方法	文献
allyl hydroperoxide CH_2=$CHCH_2OO$–**H** $\Delta_d H^\circ$(R) = 21.2 (88.7)	(1) 89 (2) 86.8	372.4 363	(1) Photolysis (2) Electrochem.	(1) 1981RUI/BAY (2) 1996JON
tert-butyl hydroperoxide t-C_4H_9OO–**H**	(1) 89.4 (2) 82.2 (3) **88.2** (4) 85±2 (5) 84.2±2.1	374.0 344 **369.0** 355.6±8.4 352.3±8.8	(1) VPPR (2) Electrochem. (3) Review (4) PES (5) GPA	(1) 1983HEN/BEN (2) 1996JON (3) 1997BEN/COH (4) 1998CLI/WEN (5) 2001BLA/RAM
benzyl hydroperoxide $C_6H_5CH_2OO$–**H**	86.8	363	Electrochemical	1996JON
p-NO_2-benzyl hydroperoxide p-NO_2-$C_6H_4CH_2OO$–**H**	87.5	366	Electrochemical	1996JON
diphenylmethyl hydroperoxide $(C_6H_5)_2CHOO$–**H**	88.4	370	Electrochemical	1996JON
phenyl hydroperoxide, substituted Y = H	91.8	384	Electrochemical	1996JON
p-Cl	92.0	385		
p-Me	91.5	383		
p-OH	91.3	382		
p-CN	92.1	385		
p-Ph	93.2	390		
p-CO_2	92.0	385		
methaneperoxycarboxylic acid $CH_3C(O)OO$–**H**	92.3	386	Electrochemical	1996JON
benzeneperoxycarboxylic acid $C_6H_5C(O)OO$–**H**	96.5	403.9	Correlation	2004DEN/DEN
2,2-dichloro-2-hydro-peroxyethane $CCl_2(CN)OO$–**H**	91.8	384	Electrochemical	1996JON
hydroperoxymethan-ol $OHCH_2OO$–**H**	88.0	368	Electrochemical	1996JON
2-hydroperoxypropan-ol $(CH_3)_2C(OH)OO$–**H**	86.5	362	Electrochemical	1996JON
1-hydroperoxyacetone $CH_3C(O)CH_2OO$–**H**	88.0	368	Electrochemical	1996JON

续表

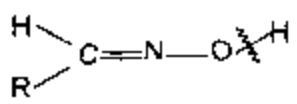
断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
α-CO_2^-–methyl hydro-peroxide (CO_2^-)CH_2OO–**H**	87.5	366	Electrochemical	1996JON
2-hydroperoxyethanenitrile (CN)CH_2OO–**H**	89.9	376	Electrochemical	1996JON
α-CO_2^- -chloromethyl hydro-peroxide (CO_2^-)$CHClOO$–**H**	90.3	378	Electrochemical	1996JON
α-CO_2^- -dichloromethyl hydro-peroxide (CO_2^-)CCl_2OO–**H**	90 3	378	Electrochemical	1996JON
2,2-dichloro-2-hydroperoxy-ethanenitrile (CN)CCl_2OO–**H**	91.8	384	Electrochemical	1996JON
naphth-1-yl hydroperoxide 1-$C_{10}H_7OO$–**H**	93 9	393	Electrochemical	1996JON
naphth-2-yl hydroperoxide 2-$C_{10}H_7OO$–**H**	93.2	390	Electrochemical	1996JON
9-anthracenyl hydroperoxide 9-$C_{14}H_9OO$–**H**	93.9	393	Electrochemical	1996JON
hydroperoxides (R–C_6H_4)CH(OH)OO–**H**	86.0	359.8	Correlation	2004DEN/DEN
ROCH(R)OO–**H**	87.8	367.3		
$R_2CHOC(R)_2OO$–**H**	85.7	358.4		
ROCH(Ph)OO–**H**	89.6	374.8		
$R_3CC(O)OO$–**H**	90.1	376.9		
RC(O)CH(R)COO–**H**	88.4	369.8		
RC(O)OCH(Ph)OO–**H**	90.0	376.4		
cyclic hydroperoxides 	87.9	367.6	Correlation	2004DEN/DEN
	90.1	376.9		
	86.5	362.1		
in enols, R_1R_2C=CR(OH) Mes = mesityl				

续表

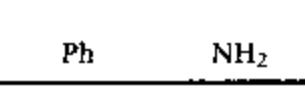
断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)			BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
			kcal/mol	kJ/mol		
R_1	R_2	R				
Mes	Mes	H	82.2	343.9	AOP	1997BOR/ZHA
Mes	Mes	Mes	82.6	345.6		
Mes	Mes	Me_3Si	82.4	344.8		
Mes	Mes	Ph	79.9	334.3		
Mes	Mes	iPr	78.6	328.9		
Mes	Mes	tBu	78.3	327.6		
Mes	Ph	Mes	83.7	350.2		
Mc_5C_6	Mc_5C_6	H	82.3	344.3		
H	H	Me	83.0	347.3		
nitrous acid **H**–ONO $\Delta_f H°$(R) = 7.91 (33.10)			78.3+0.5	327.6±2.1	Review	1976BEN
t,perp-HOONO **H**–OONO			71 5	299.2	Derived from $\Delta_f H°$ in ref.	2002HIP/NAS
nitric acid **H**–ONO_2 $\Delta_f H°$(R) = 17.0 (71.1)			101.2	423.4	Derived from $\Delta_f H°$ in ref.	1998CHA
hyponitrite **H**–ONNOH			45.2	189	Derived from $\Delta_f H°$ in ref.	2004POS/SHA
2,2-*dimethylsilaethanol* **H** -$OSiMe_3$			118.3	495	Derived	1998BEC/WAL

7.1.2 肟和羟胺分子中的O—H键能

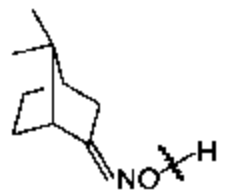
表 7.1.2 肟和羟胺分子中的 O—H BDEs

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
oximes 				

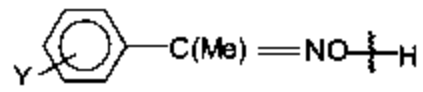
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
R = Me	98.2	410.9	AOP	1992BOR/JI
Et	98.1	410.5		
CH_3CO	89.6	374.9		
PhCO	88.9	372.0		
NH_2	88.8	371.5		
oximes 				
R_1 = Me R_2 = Me	(1) 95.8 (2) 94.1	400.8 393.7	(1) AOP (2) Correlation	(1) 1992BOR/JI (2) 2000DEN/DEN
Et Et	(1) 92.3 (2) 90.6	386.2 379.1		
iPr rPr	(3) 87.7 (2) 86.0	366.9 359.8	(3) AOP	(3) 1995BOR/ZHA(b)
Me tBu	(3) 91.1	381.2		
iPr tBu	(2) 84.3 (4) 84.3 (5) 86.0	352.7 352.7 359.8	 (4) EPR (5) AOP	 (4) 1973MAH/MEN (5) 1996BOR/LIU
tBu tBu	(2) 80.9 (3) 84.2 (4) 80.9 (5) 82.6	338.5 352.3 338.5 345.6		
tBu adamantyl	(3) 81.7 (4) 80.0	341.8 334.7		
tBu c-C_5H_9	(3) 90.7	379.5		
Ph Ph	(1) 89.0	372.4		
$PhCH_2$ $PhCH_2$	(1) 89.1	372.8		
Me Et_2NCH_2	(1) 91.4	382.4		
Me NH_2	(1) 86.7	362.8		
Ph NH_2	(1) 86.9	363.6		

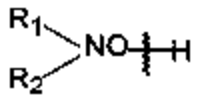
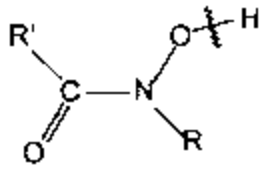
续表

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
cyclohexanone, oximes c-$C_5H_{10}C$=NO–**H**	(1) 90.3 (2) 88.6	377.8 370.7	(1) AOP (2) Correlation	(1) 1995BOR/ZHA(b) (2) 2000DEN/DEN
cycloundecanane, oximes c-$C_{11}H_{22}C$=NO–**H**	90.3	377.8	AOP	1992BOR/JI
oximes, substituted				
(Z)-PhCH=NO–**H**	90.2	377.4	AOP	1995BOR/ZHA(b)
(E)-PhCH=NO–**H**	86.9	363.6		
(Z)-p-MeC_6H_4CH=NO–**H**	89.0	372.4		
(E)-p-MeC_6H_4CH=NO–**H**	86.5	361.9		
(Z)-p-$MeOC_6H_4CH$=NO–**H**	89.9	376.1		
(E)-p-$MeOC_6H_4CH$=NO–**H**	87.5	366.1		
(Z)-m-$NO_2C_6H_4CH$=NO–**H**	88.6	370.7		
(E)-m-$NO_2C_6H_4CH$=NO–**H**	86.9	363.6		
(Z)-p-$NO_2C_6H_4CH$=NO–**H**	88.0	368.2		
(Z)-PhCHCHCH–NO–**H**	88.6	370.7		
(Z)-$CH_3C(Ph)$= NO–**H**	91.1	381.2		
(E)-$CH_3C(Ph)$= NO–**H**	89.4	374.0		
(Z)-$Me_2NCH_2C(CH_3)$=NO–**H**	92.0	384.9		
(E)-$Me_2NCH_2C(Ph)$=NO–**H**	88.5	370.3		
(Z)-(c-C_4H_8N)$CH_2C(Ph)$=NO–**H**	88.6	370.7		
(E)-$Me_2NCH_2C(Ph)$=NO–**H**	87.6	366.5		
(E)-(c-C_4H_8N)$CH_2C(Ph)$=NO–**H**	89.1	372.8		
(Z)-$Me_2NCH_2CH_2C(Ph)$=NO–**H**	88.7	371.1		
2-(hydroxyimino)-1,7,7-trimethylbicyclo(2.2.1)-heptane 	88.1	368.6	AOP	1995BOR/ZHA(b)
norcamphor, oximes R=NO–**H**	87.6	366.5	AOP	1995BOR/ZHA(b)
fluorene, oximes Fl=NO–**H**	87.5	366.1	AOP	1992BOR/JI

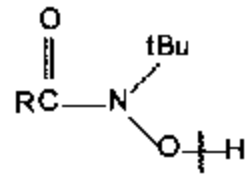
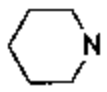
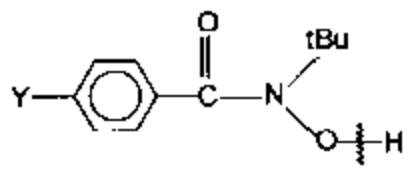
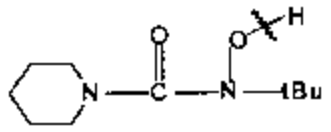
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
(hydroxyimino)-2,7-dibromo-fluorenylmethane 2,7-BrFl=NO–**H**	89.6	374.9	AOP	1992BOR/JI
(hydroxyimino)-2-$PhSO_2$-fluorenylmethane 2-$PhSO_2$Fl=NO–**H**	89.0	372.4	AOP	1992BOR/JI
oximes, substituted  Y = H	88.1	368.6	AOP	1998BOR/ZHA
p-Cl	87.8	367.4		
p-Br	87.6	366.5		
p-MeO	87.8	367.4		
p-Me	88.0	368.2		
p-CF_3	87.9	367.8		
p-CN	87.8	367.4		
m-NO_2	88.6	370.7		
p-NO_2	88.4	369.9		
oximes, substituted  Y = H	88.4	369.9	AOP	1998BOR/ZHA
p-Cl	89.0	372.4		
p-Br	89.0	372.4		
p-Me	89.0	372.4		
p-MeO	88.9	372.0		
p-CF_3	88.9	372.0		
p-CN	88.8	371.5		
p-NO_2	88.8	371.5		

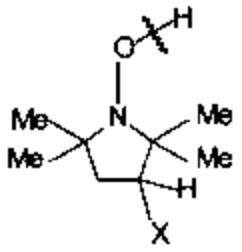
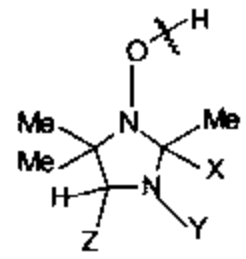
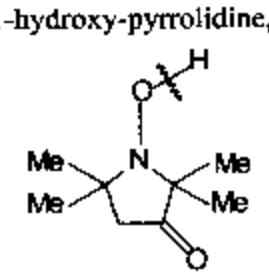
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)		BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
hydroxylamines, substituted 					
R_1 = CF_3	R_2 = CF_3	(1) 85.3	356.9	(1) EPR	(1) 1984DOB/TNG
Et	Et	(2) 69.5	290.8	(2) Kinetics	(2) 1978CAC/LIS
		(3) 75.9	317.6	(3) AOP	(3) 1996BOR/LIU
		(4) 72.8	304.5	(4) Correlation	(4) 2000DEN/DEN
		(5) 69.6±1.9	291.2	(5) GPA	(5) 2003REE/HAR
tBu	tBu	(3) 68.2	285.3		
		(6) <69.6	<291.2	(6) EPR	(6) 1973MAH/MEN
hydroxamic acid, substituted 					
R′ = iPr	R = Ph	(1) 79.3	331.8	(1) EPR	(1) 1990PER/BER
		(2) 81.2	339.7	(2) AOP	(2) 1996BOR/LIU
tBu	Ph	(1) 78.0	326.4		
		(2) 79.9	334.3		
Ph	Ph	(2) 84.1	351.9		
		(3) 80	333.4	(3) EPR	(3) 2002MIN/PUN(a)
Ph	Me	(4) 79.2±0.5	331.4±2.1	(4) EPR	(4) 2003AMO/LUC
Ph	p-BrC_6H_4	(2) 84.0	351.5		
Ph	p-CN-C_6H_4	(2) 84.2	352.3		
tBu	p-O_2N-C_6H_4	(1) 80.2	335.6		
tBu	p-MeO-C_6H_4	(1) 75.9	317.6		
tBu	n-$C_{10}H_{21}$	(1) 75.8	317.1		
tBu	$N(CH_2)_5$	(1) 74.4	311.3		
3,5-(tBu)–C_6H_3	Ph	(1) 80.5	336.8		
3,5-$(NO_3)_2$–C_6H_5	tBu	(4) 80.2±0.5	355.6±2.1		

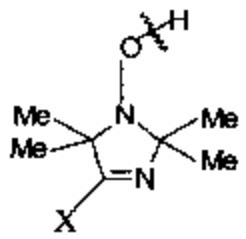
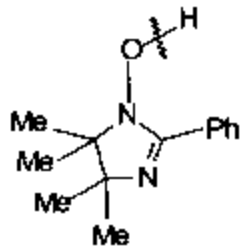
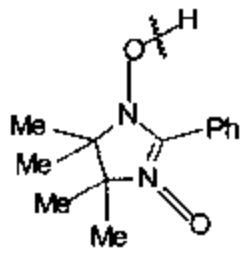
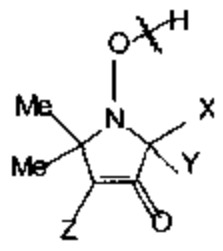
续表

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
hydroxylamines, substituted R(tBu)NO–**H**				
R = $iPrCH_2C(O)$	75.6	316.5	Correlation	2000DEN/DEN
$PhCH_2CH_2C(O)$	76.1	318.6		
$CH_3(CH_2)_9C(O)$	75.8	317.2		
C(O)CHCHPh	76.8	321.3		
4-$NO_2C_6H_4$	80.2	335.6		
4-$MeOC_6H_4C(O)$	73.5	307.5		
N-(tert-butyl)-N-hydroxy-carboxamide, substituted 				
R = PhCH=CH	76.8	321.3	EPR	1983JEN/PER
$PhCH_2CH_2$	76.2	318.8		
$CH_3(CH_2)_9$	75.8	317.1		
$(CH_3)_2CHCH_2$	75.6	316.3		
	74.4	311.3		
N-(tert-butyl)-N-hydroxy-benzamide, substituted 				
Y = H	77.2	323.0	EPR	1983JEN/PER
Ph	76.7	320.9		
NO_2	79.4	332.2		
MeO	75.1	314.2		
hydroxy-N-piperidine, substituted 	74.4	311.1	Correlation	2000DEN/DEN

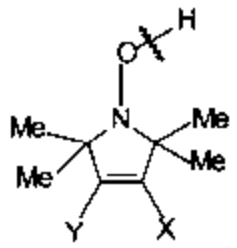
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
phenylamine, substituted $(4\text{-R-}C_6H_4)_2NO\text{–}\mathbf{H}$				
R = MeO	71.8	300.3	Correlation	2000DEN/DEN
t-Bu	70.9	296.5		
1-hydroxy-pyrrolidine, substituted 				
X = $CONH_2$	69.6	291.0	Correlation	2000DEN/DEN
C(O)OH	69.3	290.1		
OH	69.1	289.1		
1-hydroxy-tetrahydro-imidazole 				
X Y Z				
Me OH H	71.9	300.9	Correlation	2000DEN/DEN
Me Me H	69.5	290 8		
Me Me Me	68.6	286.9		
Me Me p-FC_6H_4	69.8	292.0		
Me Me p-MeC_6H_4	69.5	290.7		
Me Me Ph	69.9	292.6		
Me H PhC(O)CH=	71.4	298.7		
1-hydroxy-pyrrolidine, substituted 	71.4	298.7	Correlation	2000DEN/DEN

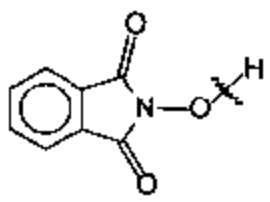
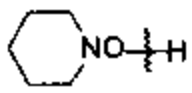
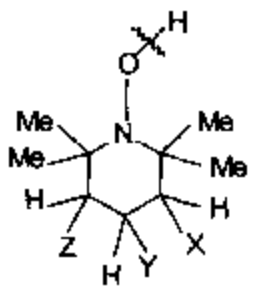
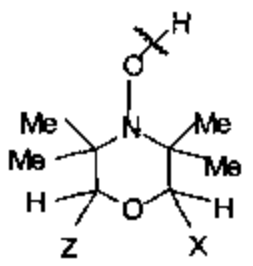
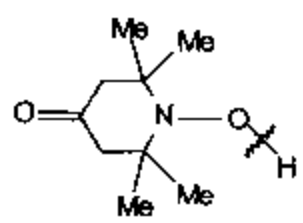
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
hydroimidazole, substituted 				
X = Me	70.6	295.2	Correlation	2000DEN/DEN
iPr	70.5	294.9		
CCl_3	71.0	296.9		
Ph	70.3	294.2		
p-FC_6H_4	70.8	296.1		
p-ClC_6H_4	70.5	294.9		
$C(O)NH_2$	71.0	296.9		
$CH_3C_6H_4$	71.0	296.9		
C(O)Me	71.0	296.9		
CH=N–tBu	70.5	294.8		
CH=NOH	70.8	296.1		
hydroimidazole, substituted 	74.6	312.2	Correlation	2000DEN/DEN
hydroimidazole, substituted 	71.0	297.1	Correlation	2000DEN/DEN
2,5-dihydrioimidazole, substituted 				

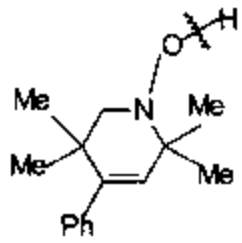
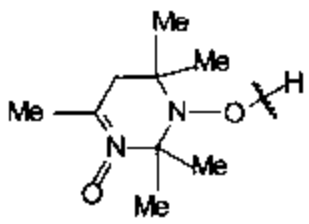
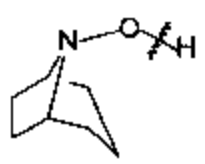
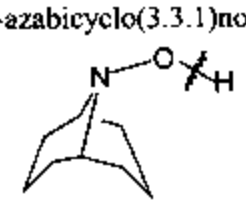
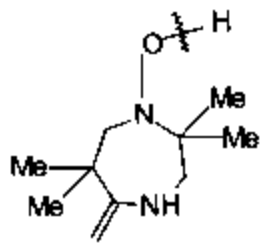
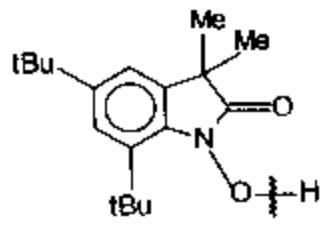
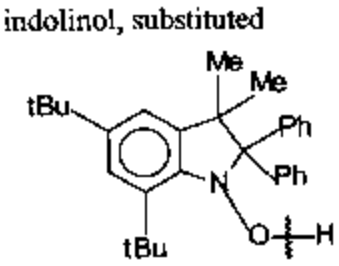
续表

断裂键 (黑体 · 离解原 f) $\Delta_f H^\circ$(R)/kcal (kJ)			BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
			kcal/mol	kJ/mol		
X	Y	Z				
Me	NMeOH	Ph	74.1	310.0	Correlation	2000DEN/DEN
Me	Me	Me	73.1	305.8		
Me	Me	$BrCHCH_3$	73.1	305.8		
Me	Me	p-BrC_6H_4	73.1	305.8		
Me	Me	$CHBr_2$	74.4	311.1		
Me	Me	p-ClC_6H_4	73.2	306.3		
Me	Me	$CHCl_2$	74.0	309.8		
Me	Me	p-FC_6H_4	73.1	305.8		
Me	NHMe	Ph	74.0	309.8		
Me	Me	CH_2Br	73.2	306.3		
Me	Me	p-$MeOC_6H_4$	72.5	303.4		
Me	Me	p-MeC_6H_4	72 6	303.6		
Me	Me	Ph	72.8	304.5		
2,5-dihydropyrrole, substituted 						
X = Cl	Y – H		70.1	293.1	Correlation	2000DEN/DEN
COMe	H		70.3	294.3		
$CONH_2$	H		70.1	293.1		
C(O)OH	H		69.6	291.0		
C(O)OMe	H		70.1	293.1		
Br	Br		70.2	293.7		
C(O)OMe	Br		70.1	293.1		
COMe	Br		70.4	294.5		

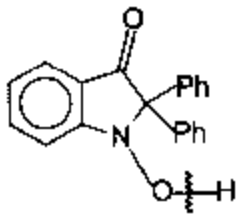
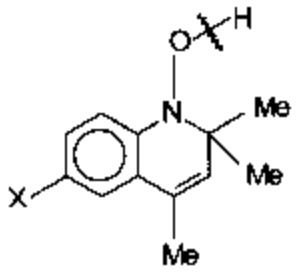
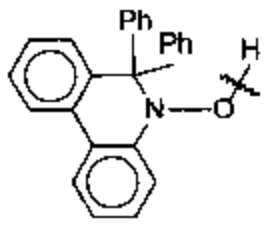
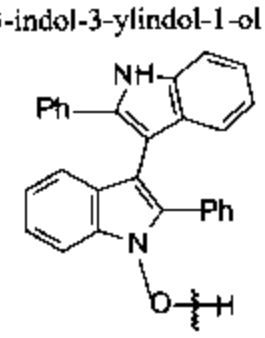
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
N-hydroxyphthalimide (NHPI) 	(1) > 86 (2) 88.1±0.5 (3) 89.6±2.4	>359.8 368.6±2.5 375±10	(1) EPR (2) EPR (3) Polanyi plot	(1) 2002MIN/PUN(b) (2) 2003AMO/LUC (3) 2003KOS/CAI
piperidinol 	77.0	322.2	AOP	1996BOR/LIU(b)
piperdin-1-ol, substituted 				
X Y Z				
H H H	(1) 69.6 (2) 69.7 (3) 71.2	291.2 291.6 297.7	(1) EPR (2) AOP (3) Correlation	(1) 1973MAH/MEN (2) 1996BOR/LIU (3) 2000DEN/DEN
H PhC(O)O H	(3) 71.2	297.7		
H OH H	(3) 72.2	302.2		
1-hydroxy-piperidine, substituted 				
X = Cl Z = H	73.6	307.9	Correlation	2000DEN/DEN
Br H	72.5	303.4		
1-hydroxy-piperidn-4-one, substituted 	71.8	300.4	EPR	1973MAH/MEN

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1-hydroxy-1,2,5,6-tetra-hydropyridine, substituted 	70.7	295.9	Correlation	2000DEN/DEN
1-hydroxy-1,2,5,6-tetra-hydropyrimidine, substituted 	73.8	308.8	Correlation	2000DEN/DEN
7-aza-bicyclo(2.2.1)heptan-7-ol 	(1) 77.0 (2) 78.0	322.2 326.4	(1) EPR (2) AOP	(1) 1973MAH/MEN (2) 1996BOR/LIU
9-azabicyclo(3.3.1)nonane-9-ol 	76.2	318.8	EPR	1973MAH/MEN
hydroxydiazacycloheptane, substituted 	72.7	304.3	Correlation	2000DEN/DEN
1-hydroxyindolin-2-one, substituted 	78.5±0.5	328.4±2.1	EPR	2003AMO/LUC
indolinol, substituted 	69.7±0.4	291.6±1.7	EPR	2003AMO/LUC

续表

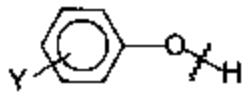
断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1-hydroxyindolin-3-one, substituted 	70.6±0.3	295.4±1.3	EPR	2003AMO/LUC
1,2-dihydroquinoline, substituted 				
X = $C(CF_3)_2OH$	70.5	294.9	Correlation	2000DEN/DEN
CPh_3	69.2	289.5		
5,6-dihydrophenanthridine, methanol, substituted 	71.4±0.3	298.7±1.3	EPR	2003AMO/LUC
3-indol-3-ylindol-1-ol 	72.8±0.1	304.6±0.4	EPR	2003AMO/LUC

7.1.3 酚类分子中的O—H键能

表 7.1.3 酚类分子中的 O—H BDEs

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
phenol PhO–H $\Delta_f H^\circ$(R) = 12.9±1.5 (54±6)	(1) 88.3±1.5 (2) **90.4±1**, in sol. (3) **88.0±1.5**, in gas (4) 88.3±0.8 (5) 88.7±0.5, in gas	369.4±6.3 **378.2±4.2**, **368.2±6.3**, 369.4±3.3 371.1±2.1	(1) SPST (2) AOP (3) Recommend. (4) EPR (5) Recommend.	(1) 1990WAL/TSA (2) 1996BOR/LIU (3) 1996TSA (4) 2003VAL/BRI (5) 2003GUE/COU

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
pentafluorophenol C_6F_5O–**H**	85.5	357.7	Correlation	2000DEN/DEN
phenols, substituted 				
Y = p-F	(1) 91.2 (3) 87.4±0.5 (5) 84.5 (14) 87.2	381.6 365.7±2.1 353.5 365.0	(1) AOP (2) AOP (3) Pulse radiolysis (4) EPR	(1) 1990ARN/AMA (2) 1991BOR/CHE(b) (3) 1990LIN/SHE (4) 1996LUC/PED
m-F	(14) 89.0	372.7	(5) Electrochem	(5) 1992PAR
o-F	(14) 86.3	361.0	(6) EPR	(6) 1973MAH/MEN
p-Cl	(1) 93.4 (2) 90.3 (3) 87.6±0.5 (8) 91.1 (12) 90.9	390.8 378±2 366.5±2.1 381 380.3	(7) PAC (8) AOP (9) AOP	(7) 2001SIL/MAT (8) 1997ZHU/ZHA (9) 1994ZHA/BOR
m-Cl	(2) 91.8 (14) 88.4 (15) 84.2±1	384.1 369.9 352.4±4.2	(10) Electrochem. (11) EPR	(10) 1991PAR/HAN (11) 1994LUC/PED
o-Cl	(2) 90.0 (14) 86.0 (15) 84.7±1 (16) 85.8	376.6 359.9 354.5±4.2 359	(12) AOP (13) Electrochem. (14) Correlation	(12) 1996BOR/LIU (13) 1975MAH/DAR (14) 2000DEN/DEN
p-Br	(2) 90.7 (3) 88.1±0.5 (5) 85.2 (8) 91.3 (14) 89.0	379.5 368.6±2.1 356.5 382 372.3	(15) PAC (16) Derived from $\Delta_f H^\circ$ in ref.	(15) 1998YAN/JIA (16) 2003BUR/KHA
o-Br	(14) 86.5	361.8		
p-I	(3) 87.9±0.3 (5) 85.1	367.8±1.3 356.1		
p-Me	(1) 87.2 (2) 88.7 (3) 86.1±0.5 (4) 88.2±0.6 (8) 89.4	364.8 371.1 360.2±2.1 369.0±2.5 374		

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
m-Me	(2) 89.4	374.0		
	(14) 87.6	366.7		
o-Me	(2) 88.2	369.0		
	(12) 90.0	376.6		
	(14) 86.1	359.9		
p-CN	(1) 93.1	389.5		
	(2) 94.2	394.1		
	(3) 92.9±0.7	388.7±2.9		
	(5) 90.1	377.0		
	(8) 94.9	397		
m-CN	(2) 93.9	392.9		
	(14) 89.3	373.6		
o-CN	(14) 88.0	368.1		
p-NO_2	(1) 93.8	392.5		
	(2) 94.7	396.2		
	(3) 94.2±1.4	394.1±5.9		
	(5) 91.3	382.0		
	(8) 95.4	399		
m-NO_2	(2) 94.3	394 6		
	(14) 87.7	366.9		
o-NO_2	(14) 86.9	363.4		
p-MeO	(1) 86.3	361.1		
	(3) 82.6±0.5	345.6±2.1		
	(4) 82.8±0.2	346.4±0.8		
	(8) 85.1	356		
	(13) 84.0	351.5		
m-MeO	(2) 90.2	377.4		
	(12) 90.8	379.9		
	(14) 88.4	369.8		
o-MeO	(2) 86.0	359.8		
	(14) 84.2	352.1		
p-O	(2) 73.0	305.4		
	(3) 72.4	302.9		

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
p-OH	(2) 81.5	341.0		
	(3) 80.2	335.6		
	(8) 82.2	344		
	(13) 84.6	354.0		
	(14) 84.1	352.0		
m-OH	(2) 90.9	380.3		
	(13) 90.9	380.3		
	(14) 88.2	369.1		
o-OH	(14) 81.2	339.6		
p-NH_2	(2) 77.3	323.4		
	(3) 75.5	315.9		
	(8) 77.9	326		
	(14) 80.8	338.1		
m-NH_2	(2) 88.0	368.2		
	(8) 88.0	368		
	(14) 87.8	367.2		
o-NH_2	(14) 85.3	356.7		
p-CF_3	(2) 95.3	398.7		
	(8) 95.8	401		
	(14) 91.4	382.4		
m-CF_3	(2) 93.8	392.5		
	(14) 92.2	385.7		
p-tBu	(2) 88.7	371.1		
	(4) 85.3±0.5	356.9±2.1		
	(8) 89.4	374		
	(13) 86.5	361 9		
	(14) 86.1	360.1		
o-tBu	(14) 84.6	354.0		
p-Ph	(2) 87.6	366.5		
	(8) 88.2	369		
	(13) 85.0	355.6		
	(14) 88.1	368.7		
o-Ph	(14) 86.5	361.9		
o-C_2H_3	(14) 85.8	358.9		

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
p-CH_2OH	(14) 85.7	358.7		
p-C(O)OH	(14) 88.8	371.7		
p-$MeCO_2$	(1) 88.9	372.0		
m-$EtCO_2$	(13) 89.9 (14) 90.7	376.1 379.4		
p-Me_2N	(2) 80.3 (3) 74.1 (8) 79.8 (14) 78.6	336.0 310.0 334 328.9		
m-Me_2N	(2) 87.9 (14) 86.2	367.8 360.6		
p-$MeSO_2$	(2) 95.0 (8) 95.6	397.5 400		
m-$MeSO_2$	(2) 92.3 (14) 90.7	386.2 379.5		
p-MeCO	(2) 92.8 (3) 90.3±0.5 (5) 87.5 (8) 93.5 (14) 88.8	388.3 377.8±2.1 366.1 391 371.6		
m-MeCO	(2) 91.8 (14) 90.0	384.1 376.5		
o-MeCO	(14) 86.8	363.0		
p-PhCO	(2) 92.5 (8) 93.2 (14) 90.8	387.0 390 379.9		
p-COO^-	(3) 89.9±0.5 (5) 87.1	376.1 364.4		
o-$(CH_2)_3CHO$	(14) 86.9	363.6		
p-BuO	(14) 83.1	347.8		
phenols, di-substituted 3,5-Cl_2	(2) 93.9	392.9	(2) AOP	(2) 1991BOR/CHE(b)

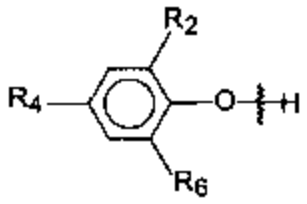
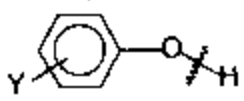
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
	(14) 92.3	386.2		
			(4) EPR	(4) 1996LUC/PED
2,5-Cl_2	(15) 85.0±1	355.7±4.2		
			(7) PAC	(7) 2001SIL/MAT
3,5-Me_2	(2) 89.1	372.8		
	(8) 88.2	369	(8) AOP	(8) 1997ZHU/ZHA
	(12) 89.7	375.3		
	(14) 87.2	364.7	(12) AOP	(12) 1996BOR/LIU
	(16) 86.6±0.4	362.5±1.5		
			(13) Electrochem.	(13) 1975MAH/DAR
2,3-Me_2	(14) 85.0	355.5		
			(14) Correlation	(14) 2000DEN/DEN
2,4-Me_2	(14) 86.2	360.5		
			(15) PAC	(15) 1998YAN/JIA
2,6-Me_2	(2) 85.1	356.1		
	(4) 84.5±0.4	353.5±1.7	(16) EPR	(16) 2003LUC/MUG(b)
	(13) 85.1	356.1		
	(14) 84.8	354.6	(17) EPR	(17) 2003VAL/BRI
	(17) 82.7±0.2	346.1±0.8		
3,4-Me_2	(14) 84.8	354.6		
2-Me-4-tBu	(14) 86.0	359.9		
2-tBu-4-Me	(14) 86.2	360.5		
2,6-tBu_2	(2) 82.1	343.5		
(also see Table 7.1.4)	(4) 82.8±0.2	346.4±0.8		
	(8) 82.7	346		
	(13) 85.1	356.1		
	(14) 82.8	346.4		
2,4-tBu_2	(14) 85.9	359.5		
3,5-tBu_2	(4) 86.6±0.3	362.3		
	(7) 90.3±0.5	377.8		
	(13) 86.9	363.6		
	(14) 86.6	362.4		
2,6-$(MeO)_2$	(4) 83.2±0.2	347.9		
3,5-$(MeO)_2$	(4) 86.7±0.3	362.8		
2-OH-4-tBu	(14) 81.8	342.4		

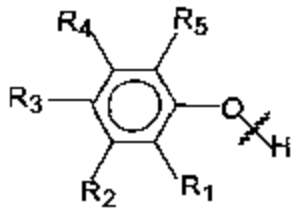
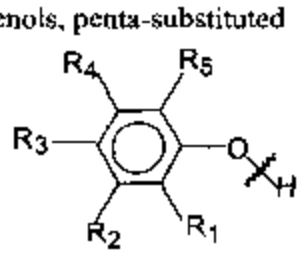
续表

断裂键 (黑体 = 离解原子) $\Delta_f H°(R)$/kcal (kJ)	BDEs (黑体 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
2-Me-4-OH	(14) 83.6	349.8		
2-tBu-4-MeO	(14) 82.1	343.4		
phenols, tri-substituted				
3,4,5-Cl_3	(2) 93.1	389.5	(2) AOP	(2) 1991BOR/CHE(b)
	(14) 91.4	382.4		
			(4) EPR	(4) 1996LUC/PED
2,4,6-Cl_3	(15) 83.7±1	350.3±4.2		
	(20) 85.8	359	(6) EPR	(6) 1973MAH/MEN
2,4,5-Me_3	(14) 85.3	356.8	(8) AOP	(8) 1997ZHU/ZHA
2,4,6-Me_3 (see next cell)	(see next cell)	(see next cell)	(9) AOP	(9) 1994ZHA/BOR
			(11) EPR	(11) 1994LUC/PED
2,4,6-tBu_3	(6) 81.2	339.7		
(also see Table 7.1.4)	(8) 82.2	344	(14) Correlation	(14) 2000DEN/DEN
	(9) 82.6	345.6		
	(11) 81.2±0.1	339.7±0.4	(15) PAC	(15) 1998YAN/JIA
	(18) 81.3	340.2		
			(16) EPR	(16) 2002LUC/MUG
2,4-tBu_2-6-Me	(14) 85.1	355.9		
			(17) EPR	(17) 1988COR/COL
2,6-Me_2-4-Cl	(14) 84.0	351.4		
			(18) EPR	(18) 2000PED/COR
3,5-Me_2-4-$CH_2C(O)OH$	(14) 83.7	350.3		
			(20) Derived from $\Delta_f H°$ in ref.	(20) 2003BUR/KHA
2,6-Me_2-4-CN	(14) 84.6	354.0		
2.6-Me_2-4-NH_2CH_2	(14) 83.2	348.1	(21) EPR	(21) 2003VAL/BRI
2-OH-3,5-tBu_2	(14) 81.3	340.3		
2-OH-3,6-tBu_2	(14) 81.1	339.5		
2,3-MeO-4-OH	(14) 82.2	343.8		
2,3-Me_2-4-MeO	(14) 79 2	331.4		
2-$S(CH_2)_2CN$-4-Me-6-MePhCH	(14) 83.1	347.5		
2-Me-4-NH_2CH_2-6-tBu	(14) 83.8	350.6		
2,6-tBu_2-4-Me	(21) 81.0±0.1	339.0±0.5		

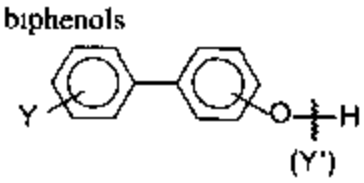
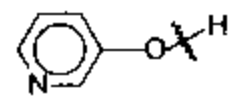
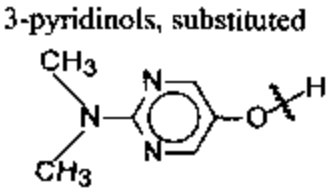
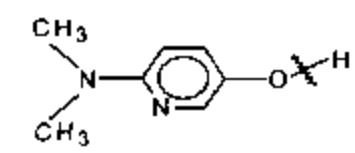
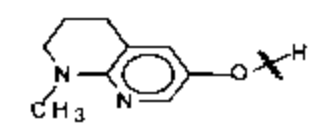
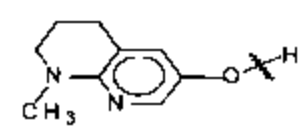
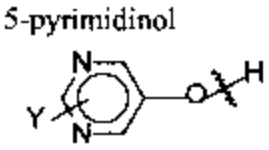
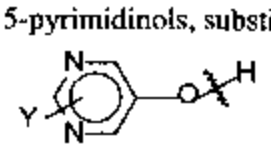
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
3,6-tBu_2-4-Me	(7) 80.5±0.9 (11) 80.7±0.3	336.8 337.6		
2-tBu-4,6-Me_2	(14) 85.1	355.8		
1,3-tBu_2-5-OH	(4) 79.3±0.3 (16) 80.7±0.3	331.8 337.6		
2,5-t-pentyl-4-OH	(16) 80.8±0.2	338.1±0.8		
4-C_3H_7-2,5-di-OH (propyl gallate)	(16) 82.6±0.3	345.6±1.3		
4-C_8H_{17}-2,5-di-OH (octyl gallate)	(16) 82.5±0.3	345.2±1.3		
phenols, substituted 				
R_2 R_4 R_6	in sol. in gas	in sol. in gas		
H H H	(1) 89.2 87.3	373.2 365.3	(1) PAC	(1) 1995WAY/LUS
tBu tBu tBu (also see Table 7.1.4)	(2) 83.2 81.2	348.1 339.7	(2) Calorimetry	(2) 1969MAH/FER
tBu Me tBu	(3) 81.6 79.6 (4) 82.7 80.7 (5) 79.7	341.4 333.0 346.0 337.6 333.5	(3) PAC (4) EPR (5) EPR	(3) 1996WAY/LUS (4) 1994LUC/PED (5) 2000PED/COR
Me Me Me	(1) 83.8 81.8 (6) 82.7	350.6 342.3 346.0	(6) ERP	(6) 2002AMO/FER
Me MeO Me	(3) 79.2 77.2 (4) 79.6 77.6	331.4 323.0 333.0 324.7		
tBu t-Bu H	(3) 84.1 82.1	351.9 343.5		
phenols, substituted 				
	in sol. in gas	in sol. in gas	PAC	(1) 1999HEE/KOR
Y = H	(1) 89.2 86.2	373.2 360.7		

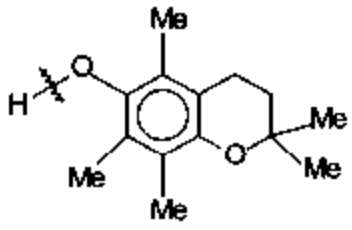
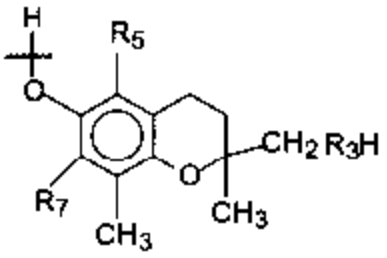
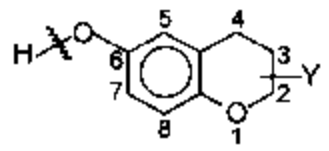
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断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值， 括号内数字 = 文献编号) kcal/mol		kJ/mol		方法	文献
2-MeO	(1) 88.6	86.6	370.7	362.3		
2,6-$(MeO)_2$	(1) 81.9	79.7	342.7	333.5		
2,4-$(MeO)_2$	(1) 83.5	81.5	349.4	341.0		
2,4,6-$(MeO)_3$	(1) 78.9	76.9	330.1	321.7		
4-MeO	(2) 83.8	81.4	350.6	340.6		(2) 1996WAY/LUS
phenols, tetra-substituted 						
$R_1 = R_4 = R_5 = Me$ $R_2 = H$, $R_3 = MeO$	(1) 79.2±0.2		331.4±0.8		(1) EPR	(1) 1996LUC/PED
$R_1 = R_2 = R_4 = R_5 = Me$ $R_3 = H$	(4) 83.1		347.8		(3) EPR	(3) 2002LUC/MUG
$R_1 = R_2 = R_3 = R_5 = Me$ $R_4 = H$	(4) 83.9		351.2		(4) Correlation	(4) 2000DEN/DEN
$R_2 = R_5 = H$, $R_3 = OH$ $R_1 = R_4 = CMe_2Et$	(3) 80.8±0.2		338.1±0.8			
$R_1 = R_5 = OH$, $R_2 = R_4 = H$ $R_3 = C(O)OC_7H_7$	(3) 82.6±0.3		345.6±1.3			
$R_1 = R_5 = OH$, $R_2 = R_4 = H$ $R_3 = C(O)OC_8H_{17}$	(3) 82.5±0.3		345.2±1.3			
$R_1 = R_2 = R_4 = Me$ $R_3 = OH$, $R_5 = H$	(4) 82.4		344.7			
phenols, penta-substituted 						
$R_1 = R_2 = R_4 = R_5 = Me$ $R_3 = MeO$	(1) 81.9±0.2 (2) 78.0±0.1		342.7 326.4		EPR	(1) 1996LUC/PED (2) 1991COR/COL
$R_1 = R_2 = R_3 = R_4 = R_5 = Me$	(3) 81.4 (4) 81.8		340.5 342.3		(3) Correlation (4) EPR	(3) 2000DEN/DEN (4) 2002AMO/FER

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
biphenols 				
Y = 2-OH Y' = 2-OH	(1) 88.9	372	(1) Electrochem.	(1) 2002JON/LIN
2-O⁻ 2-OH	(1) 92.0	385		
4-OH 4-OH	(1) 83.4 (2) 85.2 (3) 85.5	349 356.5 357.7	(2) Electrochem. (3) Pulse radiolysis	(2) 1975MAH/DAR (3) 2001DAS
4-O 4-OH	(1) 78.9	330		
3-pyridinol 	95	397.5	AOP	1993BOR/SIN
3-pyridinols, substituted 	78.2±0.3	327.2±1.3	EPR	2003WIJ/PRA
	77.0±0.5	322.2±2.1		
	76.3±0.6	319.2±2.5		
	75.4±0.7	315.5±2.9		
5-pyrimidinol  Y= H	(1) 91.1 (2) 90.3	381.2 377.8	Estimated by exp.	(1) 2001PRA/DIL (2) 2003VAL/BRI
5-pyrimidinols, substituted 				
Y = 2-CH_3, 6-CH_3, 4-CH_3	(1) 85.20±0.50	356.48±2.09	EPR	(1) 2001PRA/DIL
2-tBu, 6-tBu, 4-CH_3	(1) 84.10±0.25	351.87±1.05		
2-CH_3, 6-CH_3, 4-$N(CH_3)_2$	(1) 78.16±0.25	327.02±1.05		

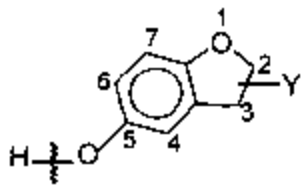
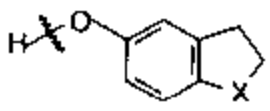
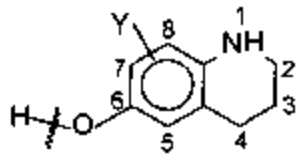
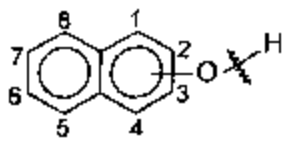
续表

断裂键 （黑体 = 离解原子） $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs （黑体 = 推荐值； 括号内数字 = 文献编号） kcal/mol	kJ/mol	方法	文献
2-CH_3, 6-CH_3, 4-CH_3O	(2) 82.48±0.50	345.10±2.09		(2) 2003VAL/BRI
2-tBu, 6-tBu, 4-$N(CH_3)_2$	(2) 76.64±0.10	320.66±0.42		
chroman-6-ol, substituted 	78.3±0.2	327.6±0.8	EPR	1996LUC/PED
α-tocopherol 				
R = $CH_2CH_2CH(CH_3)CH_2$ $R_5 = R_7 = CH_3$ (vitamin E)	(1) 78.9 (2) 78.9 (3) 80.9±1, in sol. (4) **79.3**, in sol. (4) **77.3**, in gas (5) 78.23±0.25	330.1 330.1 338.5±4.2 **331.8** **323.4** 327.31±1.05	(1) EPR (2) EPR (3) AOP (4) PAC (5) EPR	(1) 1992JAC/HOS (2) 1994LUC/PED (3) 1996BOR/LIU (4) 1996WAY/LUS (5) 2003VAL/BRI
δ-tocopherol $R_5 = R_7 = H$	(4) 82.2, in sol. (4) 80.2, in gas (6) 81.9	343.9 335.6 342.8	 (6) Correlation	 (6) 2000DEN/DEN
β-tocopherol $R_5 = CH_3$, $R_7 = H$	(6) 80.2	335.6		
γ-tocopherol $R_5 = H$, $R_7 = CH_3$	(6) 80.1	335.1		
chroman, substituted 				
Y = 5,7,8-trimethyl	79.1	331.0	Correlation	2000DEN/DEN
2,4,5,7-tetramethyl	78.0	326.4		
2,5,7,8-tetramethyl-2 -COOH	78.6	328.9		
2,5,7,8-tetramethyl-2- $CH_2CH_2C(O)COOH$	78.7	329.1		
2,5,7,8-tetramethyl-2- CH_2COOH	79.7	329.3		

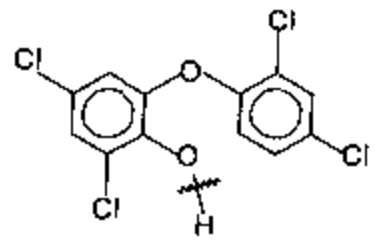
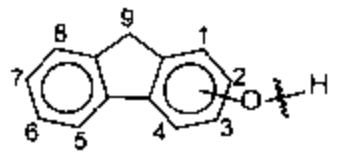
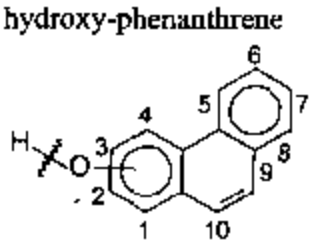
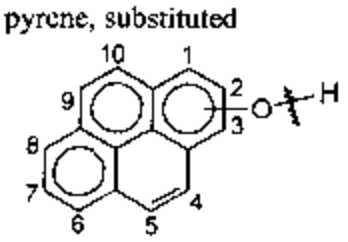
续表

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
2,5,7,8-tetramethyl-2-CH_3O	80.0	334.7		
2,5,7,8-tetramethyl-2-$CH_2CH_2C(O)OCH_3$	78.8	329.7		
2,2,5,7,8-pentamethyl	78.5	328.4		
2,5,7,8-tetramethyl-2-CH_2OH	79.1	331.0		
2H-chromene, substituted 2,2,5,7,8-pentamethyl 	79.2	331.5	Correlation	2000DEN/DEN
ubiquinol-2 R = $(CH_2CHC(CH_3)CH_2)_2H$	82.3	344.3	Correlation	2000DEN/DEN
ubiquinol-6 R = $(CH_2CHC(CH_3)CH_2)_6H$	82.3	344.3	Correlation	2000DEN/DEN
ubiquinol-10 R = $(CH_2CHC(CH_3)CH_2)_{10}H$	in sol. in gas 80.5 78.5	in sol in gas 336.8 328.4	PAC	1999HEE/KOR
5,7-dimethy-tocol, DMT RO–H	79.7	333.5	Correlation	2000DEN/DEN

续表

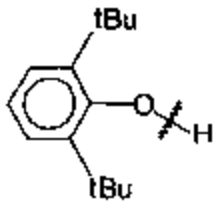
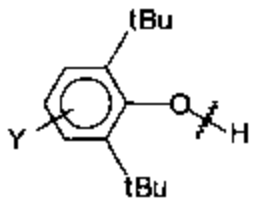
断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
dihydrobenzofuran, substituted 				
Y = 2,2,6,7-tetramethyl	78.8	329.7	Correlation	2000DEN/DEN
2,4,6,7-tetramethyl	78.0	326.4		
2,4,6,7-tetramethyl-2-C(O)OH	79.8	334.0		
2,2,4,6,7-pentamethyl	77.9	326.0		
2,3-dihydrobenzo(b)furan-5-ol and its 1-thio, 1-seleno, and 1-telluro analogues 				
X = O	81.3	340	Electrochemical	2001MAL/JON
S	80.5	337		
Se	80.3	336		
Te	80.5	337		
tetrahydroquinoline, substituted 				
Y = 5,7,8-trimethyl-N-acetyl	83.7	350.3	Correlation	2000DEN/DEN
5,7,8-trimethyl-N-ethyl	79.6	332.9		
hydroxynaphthalene, substituted 				
H-O bond at 1 site $\Delta_f H^\circ$(R) = 39.5 (165.3)	(1) **84.5** (2) 84.0 (3) 82.1	**353.5** 351.5 343.4	(1) Electrochem. (2) AOP (3) Correlation	(1) 1975MAH/DAR (2) 1991BOR/CHE(b) (3) 2000DEN/DEN
2 site $\Delta_f H^\circ$(R) = 41.6 (174.1)	(1) **86.5** (2) 88.0 (3) 84.6	**361.9** 368.2 353.8		

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ(R)$/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
1 site with 5-OH	(1) 83.6	*349.8*		
2 site with 6-Br	(2) 88.5	370.3		
2,4-dichlorophenoxy-1',5'-dichloro-phenyl-6,2'-ether  $\Delta_f H^\circ$(R) = −30.6±6 (128±25)	81.3	340	Derived from $\Delta_f H^\circ$ in ref.	2003BUR/KHA
hydroxyfluorene 				
H–O bond at 1 site	(1) 82.0	343.1	(1) Electrochem.	(1) 1975MAH/DAR
3 site	(2) 80.9	338.3	(2) Correlation	(2) 2000DEN/DEN
hydroxy-phenanthrene 				
H–O bond at 1 site	84.8	354.7	Correlation	2000DEN/DEN
2 site	87.7	367.0		
3 site	86.6	362.5		
4 site	85.1	356.2		
pyrene, substituted 				
H–O bond at 3 site	(1) 80.2	335.6	(1) Electrochem.	(1) 1975MAH/DAR
3 site with 8-OH	(1) 79.0 (2) 75.5	330.5 315.9	(2) Correlation	(2) 2000DEN/DEN
3 site with *10-OH*	(1) 79.2 (2) 75.9	331.4 317.7		

7.1.4 有位阻的酚类分子中的O—H键能

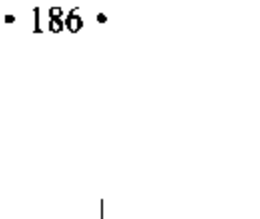
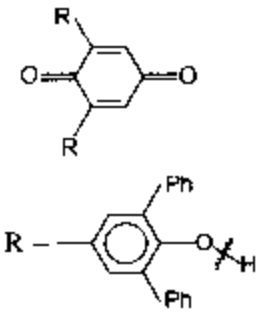
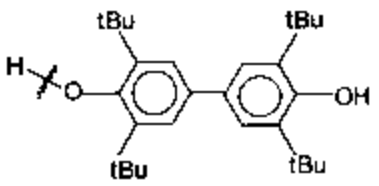
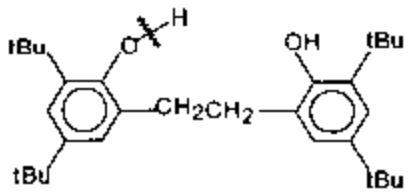
表 7.1.4 有位阻的酚类分子中的 O—H BDEs

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 - 文献编号)		方法	文献
	kcal/mol	kJ/mol		
phenols, substituted  	(2) 82.1 (4) 82.8±0.2 (8) 82.7 (13) 85.1 (14) 82.8	343.5 346.4±0.8 346 356.1 346.4	(2) AOP (4) EPR (8) AOP (13) Electrochem. (14) Correlation	(2) 1991BOR/CHE(b) (4) 1996LUC/PED (8) 1997ZHU/ZHA (13) 1975MAH/DAR (14) 2000DEN/DEN
phenols, substituted  				
Y = p-Cl	(14) 82.3 (15) 82.4	344.5 344.8	(2) AOP (4) EPR	(2) 1991BOR/CHE(b) (4) 1996LUC/PED
p-NC	(14) 84.2	352.4	(6) EPR	(6) 1973MAN/MEN
p-HS	(14) 81.3	340.0	(7) EPR	(7) 2001SIL/MAT
p-Me	(4) 81.0 (7) 80.5±0.9 (8) 80.1 (17) 79.9±0.2 (18) 79.9±0.1	338.9 336.9±3.6 335 334.3±0.8 334.4±0.5	(8) AOP (9) AOP (10) Electrochem.	(8) 1997ZHU/ZHA (9) 1994ZHA/BOR (10) 1991PAR/HAN
p-Et	(8) 80.1	335	(11) EPR	(11) 1994LUC/PED
p-NO	(14) 82.7	346.0	(14) Correlation	(14) 2000DEN/DEN
p-NO_2	(8) 86.3 (10) 86.7 (14) 85.6 (15) 84.9	361 362.8 358.0 355.2	(15) EPR (16) EPR	(15) 2002BRI/LUC (16) 1994LUC/PED
p-NH_2	(14) 80.0	334.6	(17) EPR	(17) 1988COR/COL
p-NH_2CH_2	(14) 77.2	322.9	(18) EPR	(18) 2000PED/COR
p-CN	(15) 84.2	352.4	(19) EPR	(19) 2003LUC/MUG
p-OH	(19) 78.6	328.9		

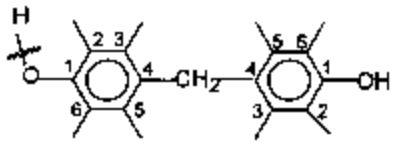
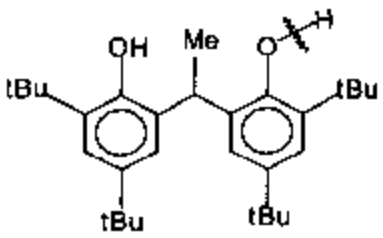
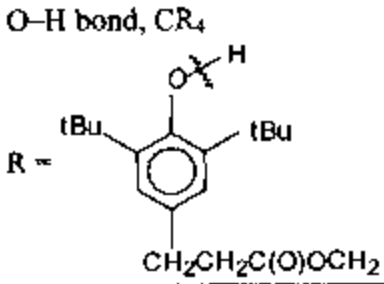
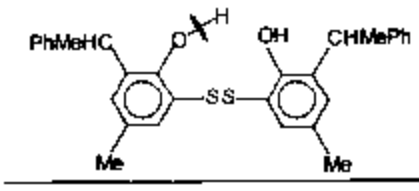
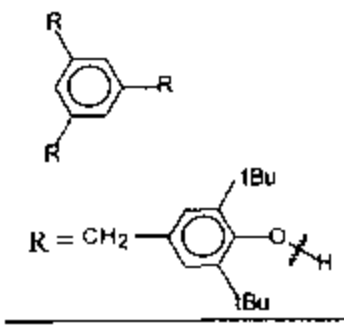
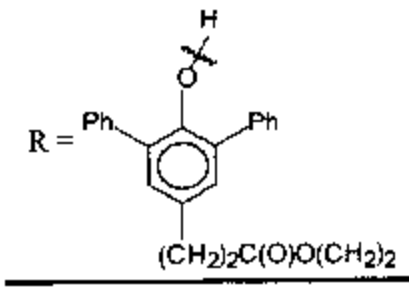
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
p-MeO	(4) 78.3	327.6		
	(8) 79.6	333		
	(9) 79.7	333.5		
	(11) 77.6±0.4	324.7±1.3		
	(14) 78.2	327.1		
p-MeC(O)NH	(14) 78.1	326.7		
p-HO(O)CCH_2	(14) 80.5	336.9		
p-MeC(O)CH_2	(14) 81.9	342.8		
p-$CNCH_2$	(14) 74.4	311.1		
p-MeC(O)	(14) 83.1	347.8		
p-HC(O)	(14) 83.1	347.8		
	(15) 84.2	352.3		
p-HO(O)C	(14) 83.4	348.8		
	(15) 84.3	352.7		
p-MeOC(O)	(8) 82.7	346		
	(9) 84.3	352.7		
	(15) 84.1	351.9		
p-tBuOC(O)	(14) 83.1	347.8		
p-tBu	(6) 81.2	339.7		
	(8) 82.2	344		
	(9) 82.6	345.6		
	(11) 81.2±0.1	339.7±0.4		
	(18) 81.3	334.0		
p-tBuO	(14) 79.2	331.3		
p-BuS	(14) 81.5	341.0		
p-RS	(16) 81.0	338.9		
p-Ph	(14) 80.7	337.7		
	(15) 81.2	339.7		
p-PhO	(14) 80.6	337.2		
p-PhS	(14) 82.8	346.4		
p-$PhCH_2$	(14) 81.2	339.7		
p-PhCH=CH	(15) 78.9	330.1		

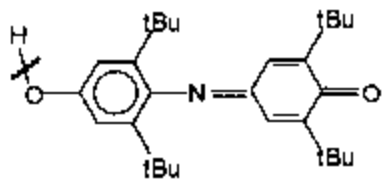
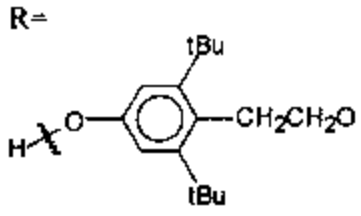
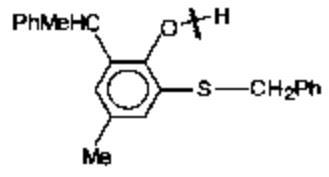
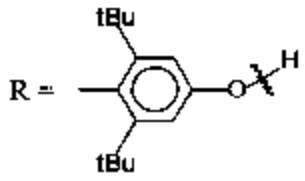
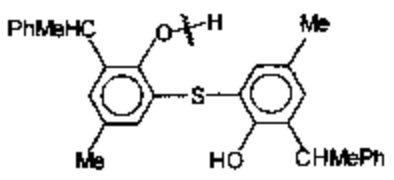
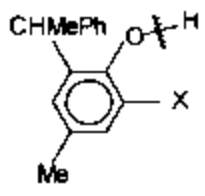
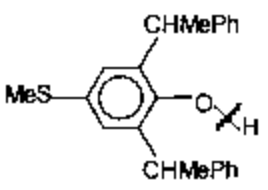
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
p-Ph_2CH	(14) 81.8	342.3		
p-$(CH_2)_2Ph$	(14) 81.3	340.0		
p-$(CH_2)_2$tBu	(14) 81.2	339.8		
p-$C_{18}H_{37}OC(O)CH_2CH_2$ (octadecyloxyoxo-2′-ethyl)	(14) 81.2	339.8		
p-$C_{18}H_{37}O$ (octadecyloxy)	(14) 78.5	328.6		
p-$C_{24}H_{49}O$ (tetracozyloxy)	(14) 78.7	329.2		
phenols, substituted  				
Y − Ph	(8) 84.8 (9) 85.3	354.8 356.9	(8) AOP (9) AOP	(8) 1997ZHU/ZHA (9) 1994ZHA/BOR
$HO(O)CCH_2$	(14) 77.9	325.9	(14) Correlation	(14) 2000DEN/DEN
phenols, substituted O H bond  	81.3	340.0	Correlation	2000DEN/DEN
phenols, substituted  	81.9	342.8	Correlation	2000DEN/DEN
ethane, substituted O–H bond  	81.5	341.0	Correlation	2000DEN/DEN

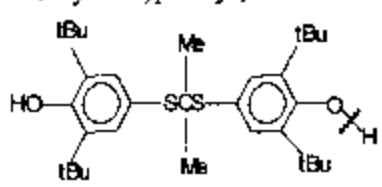
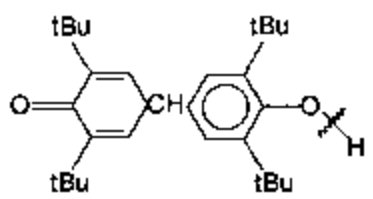
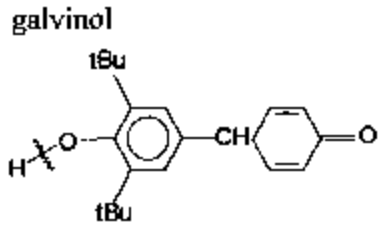
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methane, substituted O-H bond  2,6-tBu_2	(1) 81.3 (2) 81.1±0.1	340.0 339.3±0.4	(1) Correlation (2) EPR	(1) 2000DEN/DEN (2) 2003AMO/LUC
3,5-tBu_2	(1) 81.4	340.5		
ethane, substituted O–H bond 	81.2±0.2	339.7±0.8	EPR	2003AMO/LUC
methane, substituted O–H bond, CR_4 	81.5	340.9	Correlation	2000DEN/DEN
disulfide, substituted O–H bond 	80.0	334.8	Correlation	2000DEN/DEN
benzene, substuted O–H bond 	82.4	344.9	Correlation	2000DEN/DEN
ether, substituted O–H bond, R–O–R 	81.0	339.0	Correlation	2000DEN/DEN

续表

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
indophenol, substituted 	78.2	327.1	Correlation	2000DEN/DEN
silane, substituted O–H bond, SiR_4 R= 	81.5	341.0	Correlation	2000DEN/DEN
sulfide, substituted 	81.3	340.1	Correlation	2000DEN/DEN
sulfide, substituted O–H bond, RCH_2SCH_2R R = 	81.2	339.8	Correlation	2000DEN/DEN
sulfide, substituted 	80.1	335.2	Correlation	2000DEN/DEN
sulfide, substituted  X = $S(CH_2)_4CN$	82.6	345.5	Correlation	2000DEN/DEN
SCH_2CH_3	81.4	340.7		
sulfide, substituted 	81.4	340.4	Correlation	2000DEN/DEN

续表

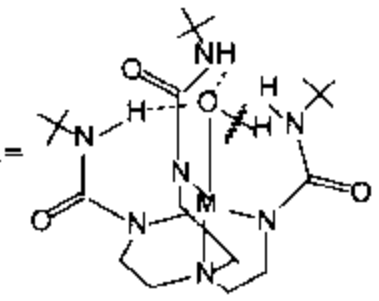
断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
4-((4-hydroxyphenylthio)-methylthio)phenyl, substituted 	81.0±0.4	338.9±1.3	EPR	1994LUC/PED
4-((4-hydrophenyl)-methylene)cyclohexa-2,5-dien-1-one, substituted 	78.8±0.3	329.7±12.6	EPR	1994LUC/PED
galvinol 	78.7	329.1	Correlation	2000DEN/DEN

7.1.5 其他分子中的O—H键能

表 7.1.5 其他分子中的 O—H BDEs

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
permanganic anion $[\mathbf{H}–OMn^{VI}O_3]^-$	(1) 83 (2) **80±3**	347.3 **334.7±12.6**	Electrochemical	(1) 1995COO/MAY (2) 1997GAR/KUE
$\mathbf{H}–OCr(O)Cl_2$	~83	~347	Electrochemical	1995COO/MAY
manganese-oxo cubane complex, $Mn_4O_3(O–\mathbf{H})(O_2PPh_2)_6$	>94.4	>395	Electrochemical	2003CAR/BOU
antion $[Mn(H_2O)_5(HO–\mathbf{H})]^{2-}$	90	376.6	Electrochemical	2003GUP/BOR
$\{L_2Mn^{II}(\mu\text{-}O–\mathbf{H})_2Mn^{II}L2\}(PF_6)_3$	75	313.8	Electrochemical	1997WAN/MAY
$[L_2Mn^{III}(\mu\text{-}O)(\mu\text{-}O–\mathbf{H})Mn^{IV}L_2](PF_6)_3$ L = 1,10-phenanthroline	79	330.5		
$[Mn^{II}Mn^{IV}(\mu\text{-}O)(\mu\text{-}O\text{-}\mathbf{H})(L)_2]$ L = salpn = N,N′-bis(salicylidene)-1,3-propanediamine	76	318.0	Electrochemical	1996BAL/PEC

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^0$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal mol^{-1}	kJ mol^{-1}		
= 3,5-di(Cl)salpn	77	322.2		
= 3,5-di(NO_2)salpn	79	330.5		
= 2,2-bipyridyl	84	351.5		
$Mn^{III}_2L_2$(HO–**H**) L = 2-hydroy-1,3-bis(3,5-X_2-salicylidenamino)propane X = 3,5-H	85	355.6	Electrochemical	1997CAU/PEC
3,5-Cl	89	372 4		
3,5-t-Bu	82	343.1		
$[Mn^{III}Mn^{IV}$L2(HO–**H**)]$^+$ L = 2-hydroy-1,3-bis(3,5-X_2-salicylidenamino)propane X = 3,5-H	89	372.4	Electrochemical	1997CAU/PEC
3,5-Cl	94	393.3		
3,5-t-Bu	86	359.8		
O–H bond in M–O complex, K salts 1= 				
$K_2[Mn^{II}H_31$(O–**H**)]	77	322.2	Electrochemical	2003GUP/BOR
$K[Mn^{III}H_31$(O-**H**)]	110	460.2		
$K_2[Fe^{II}H_3$**1**(O-**H**)]	66	276.1		
$K[Fe^{III}H_3$**1**(O–**H**)]	115	481.2		
cation $[Fe^{II}(H_2O)_5$(HO–**H**)]$^{2+}$	77	322.2	Electrochemical	2002GOL/JON
$[Fe^{II}$(PY5)(MeO-**H**)]$(CF_3SO_3^-)_2$ PY5 = 2,6-bis((2-pyridyl)methyo-methane)pyridine	84	351.5	Electrochemical	1997JON/STA

7.1.6 自由基中的O—H键能

表 7.1.6 自由基中的 O—H BDEs

断裂键 (**黑体** - 离解原子)	BDEs (**黑体** 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
hydroxyl radical **H–O**$^{\bullet}$	102.75±0.07	429.91±0.29	Recommended	2002RUS/WAG
hydroperoxy radical **H–OO**$^{\bullet}$	(1) **48.2±0.8** (2) 48.3±1.2	**201.7±3.3** 202.1±5.0	(1) Derived from $\Delta_f H^\circ$ in ref. (2) GIB MS	(1) 2001IUPC (2) 1990FIS/ARM(b)
H–OC$^{\bullet}$**H**$_2$	30.2±0.2	126.4±0.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
H–OC$^{\bullet}$**H–CH**$_3$	24.6±1	102.9±4		
H–O–C$^{\bullet}$**Cl–CH**$_3$	19.6±3	82.0±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
H–O–C$^{\bullet}$**H–CH**$_2$**CH**$_3$	26.4±1.5	110.5±6.3		
H–OC$^{\bullet}$**(CH**$_3$**)**$_2$	26.5±1.5	110.9±6.3		
H–OC$^{\bullet}$**(C**$_6$**H**$_5$**)**$_2$	27.6±1.7	115.5±7.1		
H–O(O)C$^{\bullet}$	4.6±0.7	19.2±2.9	Derived	This volume

7.2 O—O键能

表 7.2 O—O BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
oxygen **O–O**	119.11±0.04	498.36±0.17	Spectroscopy	1979HUB/HER
oxygen anion **O–O**$^-$	94.6±0.1	395.9±0.6	UV PES	2003ERV/ANU
ozone **O–O**$_2$	25.5	106.6	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
hydroperoxy radical **O–OH**	65.2±0.8	272.8±3.3	Derived from $\Delta_f H^\circ$ in ref.	1998LIT/RUS
hydroperoxide **HO–OH**	(1) 51±1 (2) 50.35±0.10	213.4±4.2 210.66±0.42	(1) Review (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1982MCM/GOL (2) 1998CHA
fluoride hydroperoxide **HO–OF**	45.6±2	199.7±8.4	Derived from $\Delta_f H^\circ$ in ref.	1998COL/GRE

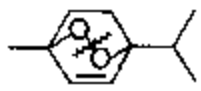
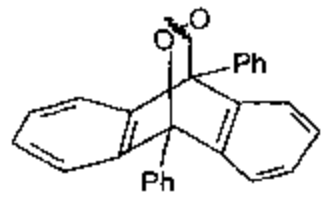
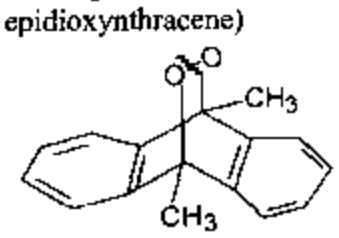
续表

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 ~ 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
bromine hydroperoxide **HO**–OBr	33.1±2	138.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	1998COL/GRE
difluoroperoxide **FO**–OF	47.7	199.6	Derived from $\Delta_f H^\circ$ in ref.	1994FRE/KAB
dichloroperoxide **ClO** OCl	(1) 17.3±0.7 (2) **18.1±0.7**	72.5±3 **75.7±3**	UV photolysis	(1) 1988COX/HAY (2) 1994NIC/FRI
dichlorine trioxide **ClO** OClO	(1) 14.8±2.9 (2) **11.1±1.2**	62±12 **46.4±5**	UV photolysis	(1) 1989HAY/COX (2) 1993BUR/MAU
diiodoperoxide **IO**–OI	17.9±4	74.9±17	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
trant-perp-HOONO **HO**–ONO	(1) 19.8±0.2, at 0 K (2) 18.3, at 0 K (3) ≤16.8	83±1 76.6 ≤70.3	(1) Kinetics (2) Derived (3) Spectroscopy	(1) 2002HIP/NAS (2) 2002DIX/FEL (3) 2003POL/LON
peroxynitric acid **HO**–ONO_2	39±2	163.2±8.4	Derived	1978BAL/GOL
methyl hydroperoxide **HO**–OCH_3	(1) **44.7±1** (2) 46.9±1.5	**187.0±4.2** 196.2±6.3	Derived from $\Delta_f H^\circ$ in ref.	(1) 1998NIST (2) 2001DOR/NOV
trifluoromethyl hydroperoxide **HO**–OCF_3	48.1±5	201.3±20.9	Derived from $\Delta_f H^\circ$ in ref.	1997JPL
ethyl hydroperoxide **HO**–OC_2H_5	42.3±1.5	177.0±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
isopropyl hydroperoxide **HO**–Oi-C_3H_7	44.4±1.5	185.8±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
tert-butyl hydroperoxide **HO**–OtC_4H_9	(1) 44.8±0.5 (2) 44.5±1	187.4±2.1 186.2±4.2	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1992SAH/RIG (2) 1998NIST
1-hydroperoxy-2,2-dimethylpropane **HO**–$OCH_2C(CH_3)_3$	46.3±1.9	193.7±7.9	Pyrolysis	1974BAT/CHR
alkyl hydroperoxide **HO**–OR	44 - 46	184 - 192	Review	2000REI/PRA
methaneperoxycarboxylic acid **HO**–$OC(O)CH_3$	40.6±0.5	169.9±2.1	Pyrolysis	1992SAH/RIG
ethaneperoxycarboxylic acid **HO**–$OC(O)C_2H_5$	40.6±0.5	169.9±2.1	Pyrolysis	1992SAH/RIG
dimethyl peroxide **CH_3O**–OCH_3	(1) 37.6±2 (2) **39.0±1.5** (3) 42.8±2	157.3±8.4 **163.2±6.3** 179.1±8.4	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref. (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1974BAT/CHR (2) 1998NIST (3) 2001DOR/NOV

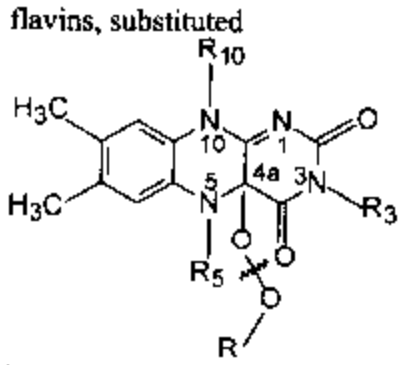
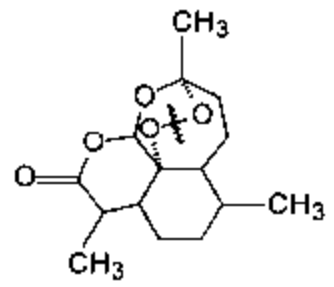
续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ditrifluoromethyl peroxide CF_3O–OCF_3	(1) 40.6±5 (2) 46.2±1 (3) **47.5±0.5**	170±21 193.3±4.2 **198.7±2.1**	(1) Derived (2) Pyrolysis (3) VLPP	(1) 1972LEV/KEN (2) 1976DES/FOR (3) 2000REI/PRA
diethyl peroxide C_2H_5O–OC_2H_5	(1) 37.9±1 (2) 38.9±1.3	158.6±4.2 162.8	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1974BAT/CHR (2) 1998NIST
dipropyl peroxide nC_3H_7O–OnC_3H_7	37.1±1	155.2±4.2	Pyrolysis	1974BAT/CHR
diiso-propyl peroxide iC_3H_7O–OiC_3H_7	37.7	157.7	Pyrolysis	1974BAT/CHR
disec-butyl peroxide sC_4H_9O–OsC_4H_9	36.4±1	152.3±4.2	Pyrolysis	1983BAT
ditert-butyl peroxide **tBuO**–OtBu	(1) 38.0±1 (2) 38.2±0.5 (3) **38.9±0.5** (4) 37.5±2.4 (5) 41.0±1.4	159.0±4.2 159.8±2.1 **162.8±2.1** 156.7±9.9 171.5±5.9	(1) Pyrolysis (2) Pyrolysis (3) VLPP (4) PAC (5) Derived from $\Delta_f H^\circ$ in ref.	(1) 1983BAT (2) 1992SAH/RIG (3) 2000REI/PRA (4) 2001SAN/MUR (5) 1998NIST
dineopentyl peroxide $tBuCH_2O$–OCH_2tBu	36.4±1	152.3	Pyrolysis	1977TRE/WRI
di-1,1-dimethylpropyl peroxide $EtC(Me)_2O$–$OC(Me)_2Et$	39.3±1	164.4±4.2	VLPP	1973PER/GOL
ditert-nonafluorobutyl peroxide $(CF_3)_3CO$–$OC(CF_3)_3$	35.5±1.1	148.5±4.6	Pyrolysis	1977IRE/GOR
hexaphenyl peroxide Ph_3CO–$OCPh_3$	31.4	131.4	Electrochemical	2004DON/WOR
di(sulfur pentafluoro) peroxide SF_5O–OSF_5	37.2	155.6	Pyrolysis	1978CZA/SCH
di(sulfur pentafluoro) trioxide SF_5O–$OOSF_5$	30.3	126.8	Pyrolysis	1981CZA/SCH
tert-butyl 1,1-dimethyl-1-silaethyl peroxide $(CH_3)_3CO$–$OSi(CH_3)_3$	47	196.6	Pyrolysis	1978MAR/COM
2,2-diethyl-2-germabutyl tert-butyl peroxide **tBuO**–$OGeEt_3$	46	192.5	Pyrolysis	1965SKI
2,2-diethyl-2-stannabutyl tert-butyl peroxide **tBuO**–$OSnEt_3$	46	192.5	Pyrolysis	1961HER
HOOO radical **HO**–OO	1.7±2	7.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	This volume
trifluoromethoxy-trifluoro-methyl peroxide CF_3OO -OCF_3	30.3±2	126.8±8.4	Pyrolysis	1981CZA/SCH

续表

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
chlorofluorotrioxide FClOO–**O**	58.4	244.3	Review	1970ONE/BEN
chlorotrioxide ClO–**OO**	7.7<	32.2<	Derived from $\Delta_f H^\circ$ in ref.	1997JPL
zeroane HC(O)O–**OH**	47.6±2	199.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	2003FEL/DIX
bifluoroformyloxy **FC(O)O**–OC(O)F	23	96.2	Pyrolysis	2003MAX/BUR
peroxyacetyl nitrate **$CH_3C(O)O$**–ONO_2	31.4±2	131.4±8.4	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
diacetyl peroxide **$CH_3C(O)O$**–$OC(O)CH_3$	(1) 30.4±2 (2) 36 (3) **33.5±5**	127.2±8.4 150.6 **140.2±21**	(1) Photodetach. (2) Derived (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1975REE/BRA (2) 1998COL/GRE (3) 2001DOR/NOV
bis(trifluoroacetyl) peroxide **$CF_3C(O)O$**–$OC(O)CF_3$	30	125.5	Kinetics	2001KOP/WIL
bis(trifluoromethyl) peroxy-dicarbonate **$CF_3OC(O)O$**–$OC(O)OCF_3$	28.5	119.2	Pyrolysis	2003MAX/BUR
propanoyloxy propanoate **$C_2H_5C(O)O$**–$OC(O)C_2H_5$	(1) 30.4±2 (2) 36	127.2±8.4 150.6	(1) Photodetach. (2) Derived	(1) 1975REE/BRA (2) 1998COL/GRE
butanoyloxy butanoate **$nC_3H_7C(O)O$**–$OC(O)nC_3H_7$	(1) 30.4±2 (2) 36	127.2±8.4 150.6	(1) Photodetach. (2) Derived	(1) 1975REE/BRA (2) 1998COL/GRE
peroxodiphosphate $[$**O_3PO**–$OPO_3]^{4-}$	18.4±4.3	77±18	PAC	2003MES/BIL
Peroxodisulfate $[$**O_3SO**–$OSO_3]^{2}$	28.7±2.6	120±11	PAC	2000BRU/CHU
ascaeidole 	28.5	119.2	Electrochemical	2004DON/WOR
DPA-O_2 (endoperoxide, 9,10-diphenyl-9,10-epidioxynthracene) 	16.3	68.2	Electrochemical	2004DON/WOR
DMA-O_2 (endoperoxide, 9,10-dimethyl-9,10-epidioxynthracene) 	23.2	97.1	Electrochemical	2004DON/WOR

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
flavins, substituted 	< 26	< 108.8	Electrochemical	1991MER/LIN
artemisinin 	23 ~ 24	96.2 ~ 100.4	Electrochemical	1998DON/WOR

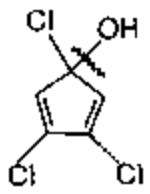
7.3 O—C键能

7.3.1 醇中的O—C键能

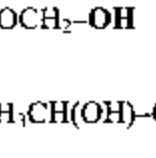
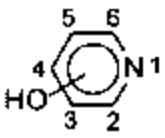
表 7.3.1 醇中的 O—C BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
trifluoromethanol **HO**–CF_3	≤115.2±0.3	≤482.0±1.3	PIMS	1997ASH/APP
methanol **HO**–CH_3	(1) 92.2±0.2 (2) 92.8 (3) **92.00±0.17**	385.8±0.8 388.3 **384.93±0.71**	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived (3) Recommend.	(1) 1986PED/NAY (2) 2001KOS/MIR(a) (3) 2002RUS/WAG
ethynol **HO**–C≡CH	134.6	563.2	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
ethenol **HO**–C_2H_3	111.1	464.8	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
ethanol **HO**–C_2H_5	93.5±0.7	391.2±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2,2,2-trifluoroethanol **HO**–CH_2CF_3	97.6±2	408.4±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
allyl alcohol **HO**–$CH_2CH{=}CH_2$	79.5±1	332.6±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (黑体　离解原子 或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
2-propen-1-ol **HO**–CH=CHCH$_3$	102.5±1.5	428.9±6.3	Derived from $\Delta_f H^\circ$ in ref.	1994PED
1-propanol **HO**–nC$_3$H$_7$	93.7±0.7	392.0±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-propanol **HO**–iC$_3$H$_7$	95.1±1	397.9±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-butanol **HO**–nC$_4$H$_9$	93.2±1	389.9±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-butanol **HO**–sC$_4$H$_9$	94.7±1	396.1±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyl-1-propanol **HO**–iC$_4$H$_9$	94.2±1	394.1±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-methyl-2-propanol **HO**–tC$_4$H$_9$	95.2±1	398.3±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-pentanol **HO**–nC$_5$H$_{11}$	92.3±1.5	386.2±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
2-pentanol **HO**–CH(CH$_3$)(nC$_3$H$_7$)	95.2±1	398.3±4.2	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
3-pentanol **HO**–CH(C$_2$H$_5$)$_2$	95.4±1	399.2±4.2	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
2-methyl-2-butanol **HO**–C(CH$_3$)$_2$(C$_2$H$_5$)	94.6±1.5	395.8±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
1-hexanol **HO**–C$_6$H$_{13}$	92.4±2	386.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
2-hexanol **HO**–C$_6$H$_{13}$	95.6±1.5	400.0±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
phenol **HO**–C$_6$H$_5$	110.8±1.0	463.6±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pentafluorophenol **HO**–C$_6$F$_5$	107	447.7	Derived	1975CHO/GOL
benzyl alcohol **HO**–CH$_2$C$_6$H$_5$	(1) 81.2 (2) **81.3±1.8**	339.7 **340.2±7.5**	(1) VLPP (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1979ROS/GOL (2) 1986PED/NAY
α,α-dimethylbenzyl alcohol **HO**–C(CH$_3$)$_2$C$_6$H$_5$	81.1±1.5	339.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1999VER
cyclopentanol c-C$_5$H$_9$–**OH**	92.2±1.5	385.8±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-hydroxy-1,3,4-trichloro cyclopentadiene 	69.8	292	Derived from $\Delta_f H^\circ$ in ref.	2003BUR/KHA

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
cyclohexanol c-C_6H_{11}–**OH**	95.3±1.5	398.7±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
adamantanol  				
1-OH	(1) 92.0	384.9	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1988LIA/BAR
	(2) 91.6	383.3	(2) Derived	(2) 2002MIR/LEB
	(3) **94.6**	**395.8**	(3) Derived from $\Delta_f H^\circ$ in ref.	(3) 2002MIR/LEB
2-OH	(1) 98.0	410.0		
1-naphthol 1-$C_{10}H_7$–**OH**	112.0±1.5	468.6±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-naphthol 2-$C_{10}H_7$–**OH**	111.8±1.5	467.8±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
dimethylaminomethanol $(CH_3)_2(NH_2)C$–**OH**	74.2±1.5	310.4±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
pyridinol, **HO**-pyridinyl  				
2-OH	95.4±1	399.2±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
3-OH	112.8±2	472.0±8.4		
4-OH	112.2±2	469.4±8.4		
polyols				
$HOCH_2$–**OH**	(1) 98.3	411.3	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1969BEN/CRU
$CH_3CH(OH)$–**OH**	(1) 98.7	413.0		
$HOCH_2CH_2$–**OH**	(2) 81.0	338.9	(2) Derived	(2) 2001KOS/MIR(a)
$(HOCH_2)_2CH$–**OH**	(2) 80.2	335.6		
$HOCH_2CH(OH)CH_2$–**OH**	(2) 79.6	333.0		
$(HOCH_2)_3CCH_2$–**OH**	(2) 80.2	335.6		

7.3.2 醚中的O—C键能

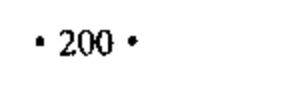
表 7.3.2 醚中的 O—C BDEs

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值; 括号内数字 文献编号)		方法	文献
	kcal/mol	kJ/mol		
dimethyl ether **CH_3**–OCH_3	83.6±1.0	349.8±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl methyl ether **CH_3**–OC_2H_5	83.2±1.0	348.1±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl methyl ether CH_3O–**C_2H_5**	84.4±1.3	353.1±5.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
divinyl ether **C_2H_3**–OC_2H_3	78.1±2.5	326.8±10.5	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
ethyl vinyl ether **C_2H_3**–OC_2H_5	101.7±1.5	425.5±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl vinyl ether **C_2H_5** OC_2H_3	65.2±2.5	272.8±10.5	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
2-chloroethyl vinyl ether **CH_2ClCH_2**–OC_2H_3	66±2.5	276.1±10.5	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
diethyl ether **C_2H_5**–OC_2H_5	85.0±1.5	355.6±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-chloroethyl ethyl ether **CH_2ClCH_2**–OC_2H_5	90.6±2	379.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
methyl 2-methyl-vinyl ether **CH_3**–$OC(CH_3)$=CH_2	66.3	277.4	VLPP	1978ZAB/BEN
methyl propyl ether **CH_3**–OnC_3H_7	84.8±1.5	354.8±6.3	Derived from $\Delta_f H^\circ$ in ref.	1994PED
methyl propyl ether **CH_3O–nC_3H_7**	85.2±1.5	356.5±6.3	Derived from $\Delta_f H^\circ$ in ref.	1994PED
iso-propyl methyl ether **CH_3**–OiC_3H_7	83.7±1.5	350.2±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
iso-propyl methyl ether **CH_3O–iC_3H_7**	85.7±1.0	358.6±4.2	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
ethyl propyl ether **C_2H_5**–OC_3H_7	84.8±2.0	354.8±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl propyl ether **C_2H_5O–C_3H_7**	84.9±1.2	355.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
propyl vinyl ether **C_2H_3**–OC_3H_7	103.0±2.2	431.0±9.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
propyl vinyl ether C_3H_7–OC_2H_3	65.5±2.5	274.1±10.5	Derived from $\Delta_f H^\circ$ in ref.	1994PED
butyl methyl ether **C_4H_9**–OCH_3	82.2±1.5	343.9±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC

续表

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值; 括号内数字 文献编号)		方法	文献
	kcal/mol	kJ/mol		
butyl methyl ether **C_4H_9O–CH_3**	84.4±1.5	353.1±6.3	Derived from Δ_fH° in ref.	2002CRC
tert-butyl methyl ether **tC_4H_9**–OCH_3	83.9±1.5	351.0±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
tert-butyl methyl ether **tC_4H_9O–CH_3**	82.2±1.5	343.9±6.3	Derived from Δ_fH° in ref.	2002CRC
ethyl propyl ether **C_2H_5**–OC_3H_7	86.3±2.2	361.1±9.2	Derived from Δ_fH° in ref	1986PED/NAY
ethyl propyl ether **C_2H_5O–C_3H_7**	85.3±1.5	356.9±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
butyl vinyl ether C_4H_9O–**C_2H_3**	100.2±2	419.2±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
butyl vinyl ether **C_4H_9**–OC_2H_3	65.3±2.5	273.2±10.5	Derived from Δ_fH° in ref	2002CRC
tert-butyl ethyl ether **tC_4H_9**–OC_2H_5	83.0±1.5	347.3±6.3	Derived from Δ_fH° in ref.	2002CRC
tert-butyl ethyl ether tC_4H_9O–**C_2H_5**	82.9±1.5	346.9±6.3	Derived from Δ_fH° in ref.	2002CRC
dipropyl ether **C_3H_7**–OC_3H_7	86.5±2.2	361.9±9.2	Derived from Δ_fH° in ref.	1986PED/NAY
diiso-propyl ether **iC_3H_7**–OiC_3H_7	85.3±2.0	356.9±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
2-ethyl-2-methylpropane **(C_2H_5)C(CH_3)$_2$**–OCH_3	84.8±2.0	354.8±8.4	Derived from Δ_fH° in ref.	1994PED
tert-butyl isopropyl ether t**C_4H_9**–OiC_3H_7	85.6±2.0	358.2±8.4	Derived from Δ_fH° in ref.	1994PED
tert-butyl isopropyl ether tC_4H_9O–**iC_3H_7**	86.1±2.0	360.2±8.4	Derived from Δ_fH° in ref.	1994PED
dibutyl ether **nC_4H_9**–OnC_4H_9	83.3±2.0	348.5±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
disec-butyl ether **sC_4H_9**–OsC_4H_9	85.9±2.0	359.4±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
ditert-butyl ether **tC_4H_9**–OtC_4H_9	77.6±2.0	324.7±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
butyl tert-butyl ether **nC_4H_9** -OtC_4H_9	84.1±2.0	351.9±8.4	Derived from Δ_fH° in ref.	1994PED
butyl tert-butyl ether nC_4H_9O–**tC_4H_9**	83.2±2.0	348.1±8.4	Derived from Δ_fH° in ref.	1994PED
sec-butyl tert-butyl ether **tC_4H_9**–OsC_4H_9	85.8±2.0	359.0±8.4	Derived from Δ_fH° in ref.	1994PED
sec-butyl tert-butyl ether tC_4H_9O–**sC_4H_9**	86.5±2.0	361.9±8.4	Derived from Δ_fH° in ref.	1994PED

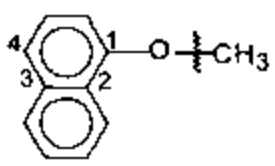
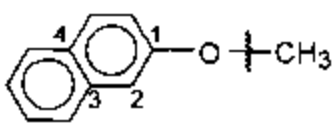
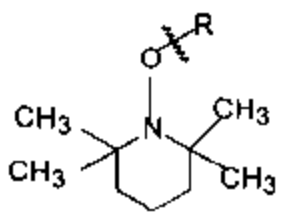
续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
iso-butyl tert-butyl ether **iC_4H_9-OtC_4H_9**	84.4±2.0	353.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1994PED
pentyl tert-butyl ether **nC_5H_{11}–OtC_4H_9**	83.5±2.0	349.4±8.4	Derived from $\Delta_f H^\circ$ in ref.	1994PED
methoxybenzene or anisole **C_6H_5–OCH_3**	99.6±1.4	416.7±5.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methoxybenzene or anisole **CH_3–OC_6H_5**	(1) 64.8 (2) 65.2 (3) 65.3 (4) **64.2±1.7**	271.1 272.8 273.2 **268.6±7.1**	(1) VLPP (2) Tubular flow reactor (3) VLPP (4) Derived from $\Delta_f H^\circ$ in ref.	(1) 1989SUR/KAF (2) 1993ARE/LOU (3) 2001PRA/HEE (4) 1986PED/NAY
methyl pentafluorophenyl ether **CH_3–OC_6F_5**	60.8	254.4	VLPP	1989SUR/KAF
anisoles, substituted 				
Y = m-F	(1) 64.4	269.4	VLPP	(1) 1989SUR/KAF(b)
o-F	(1) 61.6	257.7		(2) 1989SUR/KAF
p-F	(1) 62.4	261.1		(3) 2001PRA/HEE
m-Cl	(2) 63.7	266.5		
o-Cl	(2) 61.3	256.5		
p-Cl	(2) 62.4	261.1		
o-Br	(2) 61.8	258.6		
m-NH_2	(1) 63.1	264.0		
o-NH_2	(1) 56.1	234.7		
p-NH_2	(1) 60.5	253.1		
m-OH	(2) 63.8	266.9		
o-OH	(2) 56.3 (3) 58.1	235.6 243.1		
p-OH	(2) 61.0 (3) 62.6	255.2 261.9		

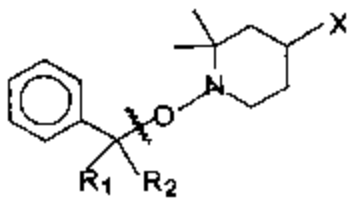
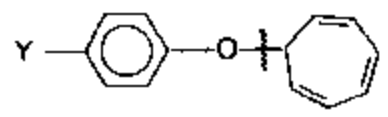
续表

断裂键 (黑体 · 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
m-Me	(1) 63.0	263.6		
o-Me	(1) 60.9	254.8		
p-Me	(1) 61.6	257.7		
m-MeO	(2) 62.4	261.1		
o-MeO	(2) 59.3 (3) 61.2	248.1 256.1		
p-MeO	(2) 59.3 (3) 62.2	248.1 260.2		
o-CH_2OH	(1) 61.0	255.2		
m-$COCH_3$	(1) 63.7	266.5		
o-$COCH_3$	(1) 62.0	259.4		
p-$COCH_3$	(1) 64.1	268.2		
o-$CH{=}CH_2$	(1) 61.0	255.2		
m-CN	(1) 64.6	270.3		
o-CN	(1) 63.4	265.3		
p-CN	(1) 63.8	266.9		
m-NO_2	(1) 63.0	263.6		
o-NO_2	(1) 62.1	259.8		
p-NO_2	(1) 64.6	270.3		
p-CF_3	(3) 67.5	282.4		
2-CHO-4-OH	(3) 62.3	260.7		
1,2-dimethoxybenzene **CH_3-OR**	60.5	253.1	VLPP	1989SUR/KAF
1,4-dimethoxybenzene **CH_3-OR**	60.7	254.0	VLPP	1989SUR/KAF
ethyl phenyl ether **C_2H_5-OC_6H_5**	(1) 64.1 (2) 65.6±2.5	268.2 274.5	(1) VLPP (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1977COL/ZAB (2) 1986PED/NAY

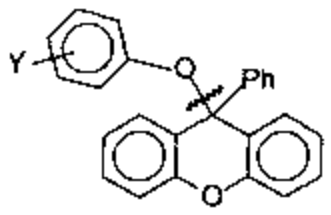
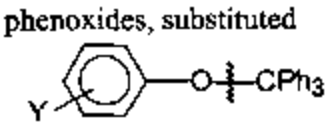
续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
ethyl phenyl ether $\mathbf{C_2H_5O}$–C_6H_5	99.6±1.3	416.7±5.4	Derived from Δ_fH° in ref.	1998NIST
phenyl vinyl ether $\mathbf{C_2H_3}$- OC_6H_5	(1) 70.0 (2) **79.1±2.5** (3) 76.0	292.9 **331.0±10.5** 318.0	(1) Pyrolysis (2) Derived from Δ_fH° in ref. (3) Pyrolysis	(1) 1993HEN (2) 1986PED/NAY (3) 1997SCH/DOR
phenyl vinyl ether C_2H_3O–$\mathbf{C_6H_5}$	(1) **76.6±5** (2) 75.9	**320.5±20.9** 317.6	(1) Derived from Δ_fH° in ref. (2) Pyrolysis	(1) 1986PED/NAY (2) 1997SCH/DOR
(1-methoxyethyl)benzene $\mathbf{C_6H_5CH(CH_3)}$ –OCH_3	72.8±2	304.6±8.4	Derived from Δ_fH° in ref.	2001VER/HEI
(1-ethoxyethyl)benzene $\mathbf{C_6H_5CH(CH_3)}$ –OC_2H_5	72.6±2	303.7±8.4	Derived from Δ_fH° in ref.	2001VER/HEI
*(1-ptopoxyethyl)benzene $\mathbf{C_6H_5CH(CH_3)}$ –OC_3H_7	73.9±2	309.2±8.4	Derived from Δ_fH° in ref.	2001VER/HEI
(1-ios-propoxyethyl)benzene $\mathbf{C_6H_5CH(CH_3)}$ –$OCH(CH_3)_2$	71.3±2	298.3±8.4	Derived from Δ_fH° in ref.	2002VER/HEI
(1-butoxyethyl)benzene $\mathbf{C_6H_5CH(CH_3)}$ –OC_4H_9	71.4±2	298.7±8.4	Derived from Δ_fH° in ref.	2001VER/HEI
(1-sec-butoxyethyl)benzene $\mathbf{C_6H_5CH(CH_3)}$ –OsC_4H_9	71.9±2	300.8±8.4	Derived from Δ_fH° in ref.	2001VER/HEI
diphenyl ether $\mathbf{C_6H_5}$–OC_6H_5	(1) 75.0 (2) **79.4±2** (3) 78.8	313.8 **332.2±8.4** 329.4	(1) Pyrolysis (2) Derived from Δ_fH° in ref. (3) Pyrolysis	(1) 1993ARE (2) 1986PED/NAY (3) 1997SCH/DOR
allyl phenyl ether $\mathbf{CH_2{=}CHCH_2}$–OC_6H_5	49.8±2	208.4±8.4	VLPP	1977COL/ZAB
phenyl benzyl ether $\mathbf{C_6H_5CH_2}$–OC_6H_5	52.1	218.0	Pyrolysis	1993ARE
2,3-benzoanisole 	57.5	240.6	VLPP	1989SUR/KAF
3,4-benzoanisole 	61.0	255.2	VLPP	1989SUR/KAF
piperidinol, substituted 				

续表

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值, 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
R = CH_3	(1) 47±1	196.6	(1) VLPP	1999CIR/KOR
c-C_6H_{11}	(2) 40±1	167.4	(2) PAC	
C_6H_7(1,4-cyclohexadienyl)	(2) 18±1	75.3	(2) PAC	
C_4H_7O(α-tetrahydrofuryl)	(2) 48±1	200.8	(2) PAC	
$(C_2H_5)_2NCHCH_3$	(2) 38±1	159.0	(2) PAC	
$C_6H_5CH_2$	(3) 32	133.9	(3) Re-analyzed	
$C_6H_5CHCH_3$	(3) 30 ～ 34	126 ～ 142		
$C_6H_5C(CH_3)_2$	(3) 26	108.8		
(phenylmethoxy) piperidine, substituted 				
R_1 R_2 X				
H H H	30.6	128.0	Thermolysis	1998SKE/BEL
Me H H	28.4	118.8		
Me Me H	24.6	102.9		
H H OH	31.4	131.4		
tropylium phenoxides, substituted 				
Y = H	(1) 25.5±0.5 (2) 26.8	106.7±6.3 112	AOP	(1) 1993ARN/FLO(b) (2) 1996HAN/HUA
F	(1) 25.8±0.4 (2) 25.8	107.9±1.7 108		
Cl	(1) 28.7±0.6 (2) 28.7	120.1±2.5 120		
Br	(1) 28.2±0.6	118.0±2.5		
Me	(2) 22.0	92		

续表

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
NO_2	(1) 30.9±0.8 (2) 30.8	129.3±3.3 129		
CN	(1) 29.4±0.4 (2) 29.4	123.0±1.7 123		
MeO	(1) 21.4±0.5 (2) 21	89.5±2.1 88		
MeC(O)	(2) 29.4	123		
phenylxanthylium phenoxides, substituted 				
Y = H	25.3	106	AOP	1996HAN/HUA
p-CN	27.2	114		
p-Mc	22.0	92		
p-MeO	20.8	87		
p-MeC(O)	28.0	117		
thiphenylmethylium phenoxides, substituted 				
Y = H	37.0	155	AOP	1996HAN/HUA
p-F	34.7	145		
p-Cl	39.7	166		
p-Br	34.4	144		
p-Me	32.5	136		
p-tBu	34.4	144		
p-MeO	31.8	133		
p-McC(O)	39.0	163		
p-CN	39.7	166		
p-NO_2	39.9	167		

7.3.3 酸、酯、酐中的O—C键能

表 7.3.3 酸、酯、酐中的 O—C BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methyl formate **CH_3**–OC(O)H	(1) 86.8 (2) **91.7±3**	363.2 **383.7±12.6**	(1) Electron capture detect (2) Derived from Δ_fH° in ref.	(1) 1989CHE/ALB (2) 1998NIST
formic acid **HC(O)**–OH	109.4±0.5	457.7±2.1	Derived from Δ_fH° in ref.	1994LIA/LIE
acetic acid **CH_3C(O)**–OH	109.8±1	459.4±4.2	Derived from Δ_fH° in ref.	1994LIA/LIE
propenoic acid **C_2H_3C(O)** –OH	107.2±2.5	448.5±10.5	Derived from Δ_fH° in ref.	1998NIST
propanoic acid **C_2H_5C(O)**–OH	110.0±2	460.2±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
benzoic acid **C_6H_5C(O)**–OH	107.0±2.5	447 7±10.5	Derived from Δ_fH° in ref.	1998NIST
glycolic acid **HO**–CH_2C(O)OH	88.0±2.5	368.2±10.5	Derived from Δ_fH° in ref.	2001DOR/NOV
methyl acetate CH_3C(O)O–**CH_3**	90.9±3	380.3±12.6	Derived from Δ_fH° in ref.	2002CRC
methyl formate **HC(O)**–OCH_3	101.3±1	423.8±4.2	Derived from Δ_fH° in ref.	1994PED
methyl acetate **CH_3C(O)**–OCH_3	100.9±1.5	422.2±6.3	Derived from Δ_fH° in ref.	2002CRC
ethyl chloroformate **ClC(O)**–OC_2H_5	101.8±2	425.9±8.4	Derived from Δ_fH° in ref.	20023CRC
methyl acrylate **CH_2=CHC(O)**–OCH_3	98.8±2	413.4±8.4	Derived from Δ_fH° in ref.	1988LIA/BAR
methyl benzoate **CH_3**–OC(O)C_6H_5	(1) 86.5±2.5 (2) **89.1±4**	361.9±10.5 **372.8±16.7**	Derived from Δ_fH° in ref.	(1) 1986PEN/NAY (2) 2002ROU/TEM
ethyl acetate **C_2H_5**–OC(O)CH_3	91.5±3	382.8±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
iso-propyl acetate **iC_3H_7**–OC(O)CH_3	93.1±3	389.5±12.6	Derived from Δ_fH° in ref.	1994PED
butyl acetate **C_4H_9**–OC(O)CH_3	91.6±3	383.3±12.6	Derived from Δ_fH° in ref.	2002CRC
vinyl acetate **CH_3C(O)**–OC_2H_3	75.8±1.5	317.1±6.3	Derived from Δ_fH° in ref.	2002CRC
vinyl acetate **CH_3C(O)**–OC_2H_3	80.3±3	336.0±12.6	Derived from Δ_fH° in ref.	1994PED
formic acid phenyl ester **HC(O)**–OC_6H_5	74.4±3	311.3±12.6	Derived from Δ_fH° in ref.	1994PED

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
acetic acid phenyl ester **$CH_3C(O)$**–OC_6H_5	77.3±3	323.4±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
methyl benzoate **$C_6H_5C(O)$**–OCH_3	(1) 100.7±3 (2) **98.3±3**	421.3±12.6 **411.3±12.6**	Derived from Δ_fH° in ref.	(1) 1986PED/NAY (2) 2002ROU/TEM
phenyl benzoate **$C_6H_5C(O)$**–OC_6H_5	74.8±3	313.0±12.6	Derived from Δ_fH° in ref.	1986PED/NAY
dimethoxymethane **CH_3OCH_2**–OCH_3	87.8±2	367.4±8.4	Derived from Δ_fH° in ref.	2002CRC
acetic anhydride **$CH_3C(O)$**–$OC(O)CH_3$	(1) 83.5 (2) **91.4±3**	349.4 **382.4±12.6**	(1) Electron capture detect (2) Derived from Δ_fH° in ref.	(1) 1989CHE/ALB (2) 1986PED/NAY
benzoic anhydride **$C_6H_5C(O)$**–$OC(O)C_6H_5$	92.0±4	384.9±16.7	Derived from Δ_fH° in ref.	1986PED/NAY

7.3.4 过氧化合物中的O—C键能

表 7.3.4 过氧化合物中的 O—C BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methyl hydroperoxide **CH_3**–OOH	71.8±3	300.4±12.6	Derived from Δ_fH° in ref.	2001DOR/NOV
ethyl hydroperoxide **C_2H_5**–OOH	79.4±5	332.2±20.9	Derived from Δ_fH° in ref.	1986PED/NAY
tert-butyl hydroperoxide **tC_4H_9**–OOH	73.9±1	309.2±4.2	Derived from Δ_fH° in ref.	1986PED/NAY
hexyl-1 hydroperoxide **n-C_6H_{13}**-OOH	70.1	293.3	Derived from Δ_fH° in ref.	1969BDE/CRU
hexyl-2 hydroperoxide **(n-Bu)(Me)C**–OOH	71.6	299.6	Derived from Δ_fH° in ref.	1969BDE/CRU
hexyl-3 hydroperoxide **(i-Pr)(Et)C**–OOH	69.4	290.4	Derived from Δ_fH° in ref.	1969BDE/CRU
heptyl-2 hydroperoxide **(n-C_5H_{11})(Me)C**–OOH	72.3	302.5	Derived from Δ_fH° in ref.	1969BDE/CRU
cyclohexyl hydroperoxide **cyclo-C_6H_{11}**–OOH	73.8	308.8	Derived from Δ_fH° in ref.	1969BDE/CRU
dimethyl peroxide **CH_3**–$OOCH_3$	(1) 67.3±1.5 (2) 69.9±2	281.6±6.3 292.5±8.4	Derived from Δ_fH° in ref.	(1) 1986PED/NAY (2) 2001DOR/NOV

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
bis(trifluoromethyl) peroxide **CF_3–OOCF_3**	86.4±2	361.5±8.4	Pyrolysis	1983BAT/WAL
diethyl peroxide **C_2H_5–OOC_2H_5**	67.7±2.5	283.2±10.5	Derived from $\Delta_f H^\circ$ in ref.	1969BDE/CRU
tert-butylperoxide **tC_4H_9–OOtC_4H_9**	70.7±2	295.8±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methyl peroxy CH_3–**OO**	(1) >30.3 (2) 32.2±1.5 (3) 32.4±0.7 (4) **32.7±0.9**	>126.8 134.7±6.5 135.6±2.9 **137.0±3.8**	(1) VLPR (2) Equilibrium (3) Derived (4) Re-analyzed	(1) 1984KON/BEN (2) 1982KHA/NIA (3) 1992LIG/COX (4) 1998KNY/SLA(b)
trifluoromethyl peroxy CF_3–**OO**	35.3	147.7	Derived from $\Delta_f H^\circ$ in ref.	1992LIG/COX
chlorodifluoromethyl peroxy $CClF_2$–**OO**	30.5	127.6	Derived from $\Delta_f H^\circ$ in ref.	1992LIG/COX
dichlorofluoromethyl peroxy CCl_2F–**OO**	29.8	124.7	Derived from $\Delta_f H^\circ$ in ref.	1992LIG/COX
chloromethylperoxy CH_2Cl–**OO**	(1) 28.9 (2) 29.3±2.5	120.9 122.4±10.5	(1) Derived (2) Re-analyzed	(1) 1992LIG/COX (2) 1998KNY/SLA(b)
dichloromethylperoxy $CHCl_2$–**OO**	(1) 25.3 (2) 25.9±2.0	105.9 108.2±8.2	(1) Derived (2) Re-analyzed	(1) 1992LIG/COX (2) 1998KNY/SLA(b)
trichloromethylperoxy CCl_3–**OO**	(1) 19.7±0.9 (2) 22±1.5	82.4±3.8 92.0±6.4	(1) Derived (2) Re-analyzed	(1) 1992LIG/COX (2) 1998KNY/SLA(b)
ethylperoxy C_2H_5–**OO**	(1) 34.1±0.5 (2) 35.2±1.5 (3) 31.3±1.1 (4) **35.5±2.0**	142.7±2.1 147.2±6.3 131.0±4.6 **148.4±8.4**	(1) PIMS (2) Derived (3) Review (4) Re-analyzed	(1) 1990WAG/SLA (2) 1992LIG/COX (3) 1997BEN/COH (4) 1998KNY/SLA(b)
vinylperoxy C_2H_3–**OO**	47.3±1.0	197.9±4.0	Derived from $\Delta_f H^\circ$ in ref.	2002SEB/BOC
2-chloroethylperoxy CH_3CHCl–**OO**	31.4±0.4	131.2±1.8	Re-analyzed	1998KNY/SLA(b)
2,2-dichloroethylperoxy CH_3CCl_2–**OO**	26.8±0.5	112.2±2.2	Re-analyzed	1998KNY/SLA(b)
iso-propylperoxy iPr–**OO**	(1) 39.7 (2) 37.7±1.8 (3) 32.2±1.3 (4) **37.1±2.3**	166.1 157.9±7.5 134.7±5.4 **155.4±9.6**	(1) PIMS (2) Derived (3) Review (4) Re-analyzed	(1) 1985SLA/RAT (2) 1992LIG/COX (3) 1997BEN/COH (4) 1998KNY/SLA(b)
allylperoxy CH_2=$CHCH_2$–**OO**	(1) 18.2 (2) 18.4	76.1 77.0	(1) Flash Photolysis (2) PIMS detect.	(1) 1982MOR/PIL (2) 1998KNY/SLA
2-chloro-2-methylethyl-peroxy $(CH_3)_2CCl$–**OO**	32.5±0.9	136.0±3.8	Re-analyzed	1998KNY/SLA(b)

续表

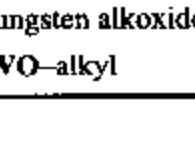
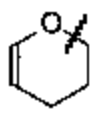
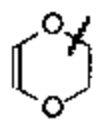
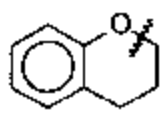
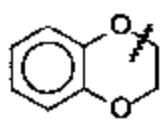
断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
tert-butylperoxy tBu–**OO**	(1) 30.2±1.1 (2) 36.7±1.9 (3) 36.7±1.9 (4) **36.5±1.8**	126.4±4.6 153.6±7.9 153.6±7.9 **152.8±7.4**	(1) VLPR (2) PIMS (3) Derived (4) Re-analyzed	(1) 1983HEN/BEN (2) 1986SLA/RAT (3) 1992LIG/COX (4) 1998KNY/SLA(b)
butenyl-2-peroxy $CH_3CHCHCH_2$–**OO**	15.2±2.0	63.6±8 4	Derived from $\Delta_f H^\circ$ in ref.	1998KNY/SLA
pentadienylperoxy C_5H_7–**OO**	13.4±1.2	56±5	Pulsed-laser photolysis	2001ZIL/INO
neopentyl peroxy neo-C_5H_{11}–**OO**	36.3	151.9	Derived from $\Delta_f H^\circ$ in ref.	2004SUN/BOZ
cyclohetylperoxy c-C_6H_{11}–**OO**	24	100.4	PAC	2000KRA/CIR
cyclohexenylperoxy c-C_6H_9–**OO**	19.2±1.0	80.4±4.2	Pulsed-laser photolysis	1998ZIL/INO
cyclohexadienylperoxy c-C_6H_7–**OO**	12	50 2	PAC	2000KRA/CIR
benzylperoxy $C_6H_5CH_2$–**OO**	(1) 22±1.5 (2) 21±1	92.0±6 87.9±4.2	(1) Photolysis (2) Laser induced fluorescence	(1) 1993FEN/NOZ (2) 1993ELM/MIN
α-OH-methylperoxy $HOCH_2$–**OO**	(1) 16.3±0.3 (2) 34.6	68.2±1.3 144.8	(1) Review (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1997BEN/COH (2) 1992LIG/COX
hydroxycyclohexadienyl-OO $C_6H_6(OH)$ –**OO**	10.4±0.5	43.6±2	UV absorption	2004GRE/KRA
α-NH_2-methylperoxy NH_2CH_2–**OO**	36.5±1.8	152.8±7.4	Re-analyzed	1998KNY/SLA(b)
pyrrolidin-2-yl-peroxy c-C_4H_8N–**OO**	10	41.8	PAC	2000KRA/CIR
(ethylmethylamino)methyl-peroxy $(C_2H_5)N(CH_3)CH_2$–**OO**	25	104.6	PAC	2000KRA/CIR
acetyl peroxy $CH_3C(O)$ –**OO**	34.5±2	144.4±8.4	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
tetrahydrofuran-2-yl-peroxy C_4H_7O–**OO**	32	133.9	PAC	2000KRA/CIR
dioxan-2-yl-peroxy $C_4H_7O_2$–**OO**	34	142.3	PAC	2000KRA/CIR
zeroane HC(O)–**OOH**	69.3	290.0	Derived from $\Delta_f H^\circ$ in ref.	2003FEL/DIX
acetyl peroxide **$CH_3C(O)$**–$OOC(O)CH_3$	75.3	315.1	Derived from $\Delta_f H^\circ$ in ref.	1969BDE/CRU

7.3.5 其他分子中的O—C键能

表 7.3.5 其他分子中的 O—C BDEs

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
carbon monoxide C–**O**	257.26±0.16	1076.38±0.67	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
carbon dioxide **O**=CO	127.2±0.1	532.2±0.4	Spectroscopy	1970DAR
carbon oxysulfide **O**=CS	(1) 158.7±0.9, at 0 K (2) **145.4**	664.0±3.8 **608.4**	(1) GIB MS (2) Derived from $\Delta_f H^\circ$ in ref.	1990PRJ/ARM 2002CRC
formaldehyde **O**=CH_2	180.6	755.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
methanisocynate **O**=$CNCH_3$	133±4	556.5±16.7	Review	1978BEN
trifluoromethyl hypochlorite **ClO**–CF_3	≤88.4±0.3	≤369.9±1.3	PIMS	1997ASH/APP
methyl nitrite **Me**–ONO	58.6	245.2	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
ethyl nitrite **Et**–ONO	62 2	260.2	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
propyl nitrine **n-C_3H_7**–ONO	59.6±1.5	250.2±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
iso-propyl nitrine **i-C_3H_7**–ONO	60.8±1.5	254.4±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
butyl nitrine **n-C_4H_9**–ONO	61.3±1.5	256.5±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
iso-butyl nitrine **i-C_4H_9**–ONO	60.7±1.5	254.0±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
sec-butyl nitrine **s-C_4H_9**–ONO	60.6±1.5	253.6±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
tert-butyl nitrine **t-C_4H_9**–ONO	60.4±1.5	252.7±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
2-methylbytanyl nitrine **(C_2H_5)(CH_3)$_2$C**–ONO	60.7±2	254.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
methyl nitrate **Me**–ONO_2	(1) 81.3 (2) 81.0	340.2 338.9	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived	(1) 1998NIST (2) 2001MIR/KOS
ethyl nitrate **Et**–ONO_2	(1) 82.4 (2) 79.5	344.8 332.6	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived	(1) 1998NIST (2) 2001MIR/KOS
propyl nitrate **n-C_3H_7**–ONO_2	79.6	333.0	Derived	2001/MIR/KOS

续表

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
iso-propyl nitrate **i-C_3H_7–ONO_2**	80.2	335.6	Derived	2001MIR/KOS
nitrates **R**–ONO_2 R = $CH_2CH_2ONO_2$	73.5	307.4	Derived	2001MIR/KOS
$CH_2CH(ONO_2)CH_2ONO_2$	77.2	323.0		
$CH_2C(CH_2ONO_2)_3$	**74.2**	310.5		
$CH(CH_2ONO_2)_2$	69.6	291.2		
1-adamantyl nitrate 	(1) 79.7 (2) **81.5**	333.3 **341.0**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	2002MIR/LEB
1-methoxy-1,1-dimethyl-1-silaethane **Me**–$OSiMe_3$	96.3	403	Derived	1998BEC/WAL
1-ethoxy-1,1-dimethyl-1-silaethane **Et**–$OSiMe_3$	98.5	412	Derived	1998BEC/WAL
2H-3,4-dihydropyran 	61.2	256	Derived	1997DOR/PUG
2,3-dihydro-1,4-dioxin 	60.5	253	Derived	1997DOR/PUG
chromane 	60.9	255	Derived	1997DOR/PUG
2,3-dihydro-1,4-benzodioxin 	60.2	252	Tubular flow reactor	1994SCH/ARE
methoxyacetonitrile **CH_3O–CH_2CN**	94.0	393.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
ethoxyacetonitrile **C_2H_5O–CH_2CN**	94.0	393.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
tungsten alkoxide **WO**–alkyl	<33±10	<138±42	Est. by exp.	1997CRE/MAY

7.3.6 自由基中的O—C键能

表 7.3.6 自由基中的 O—C BDEs

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值，括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
HO–C•H$_2$	106.3±1	444.8±4 2	Derived	This volume
HO–CHClC•H$_2$	31.4±3	131.4±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
–CCl$_2$C•H$_2$	33.2±3	138.9±12.6		
–CH$_2$C•H(CH$_3$)	32.6±3	136.4±12.6		
–CH$_2$C•H$_2$	30.1±2.5	125.9±10.5		
–CH(CH$_3$)C•H$_2$	28.8±3	120.5±12.6		
–C(CH$_3$)$_2$C•H$_2$	39.8±3	166.5±12.6		
CH$_3$–O•	90.1±0.8	377.0+3 3	Derived from $\Delta_f H^\circ$ in ref.	2002ERV/DET
CH$_2$=CHCH$_2$–O•	79.7±1	333.5±4.2		
C$_6$H$_5$CH$_2$–O•	82.4±3	344.3±12.6	Derived	This volume
HC(O) O•	99.8±3	417.6±12.6		
CH$_3$–OC•H$_2$	9.1±2	38 1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
CH$_3$–OC•HCH$_3$	8.1±2	33.9±8.4		
CH$_3$CH$_2$–OC•H$_2$	13.2±3	55.2±12.6		
CH$_3$CH$_2$–OC•HCH$_3$	7±3	29.3±12.6		
C$_6$H$_5$C(O)–OC•H$_2$	18.5±3	77.4±12.6		
trans-HO–C•(O)	29.0±1	121.3±4.2	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
cis-HO–C•(O)	35.0	146.4		
CH$_3$–OC•(O)	–18.5±2	–77.4±8.2	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
CH$_3$O–C•(O)	18.6±2	77.8±8.2		
HO–C(O)C•H$_2$	47.5±4	198.7±16.7		
CH$_3$O–C(O)C•H$_2$	40.2±3	168.2±12.6		
CH$_3$CH$_2$O–C(O)C•H$_2$	44.9±3	187.9±12.6		
C$_6$H$_5$O–C(O)C•H$_2$	–1.3±3	–5.4±12.6		

续表

断裂键 (**黑体** – 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
HOO–$CH_2C^{\bullet}H_2$	4.7±1.5	19.7±6.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
–$CH_2C^{\bullet}HCH_3$	5.6±2	23.4±8.4		
–$CH(CH_3)C^{\bullet}H_2$	7.5±2.5	31.4±10.5		
–$CH_2C^{\bullet}(CH_3)_2$	6.2±2.5	25.9±10.5		
–$C(CH_3)_2C^{\bullet}H_2$	5.4±2.5	22.6±10.5		
–$C(O)C^{\bullet}H_2$	15.4±2.5	64.4±10.5		

7.4 O—N键能

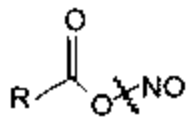
表 7.4 O—N BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
O-**N**	150.71±0.03	630.57±0.13	Spectrometry	2002CRC
dinitrogen oxide O–$\mathbf{N_2}$	40.0	167.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
nitrogen dioxide O–**NO**	72.9	305.0	Review	1965BEN
nitrate O–$\mathbf{NO_2}$	(1) 47.3±0.8, at 0 K (2) 50.5	197.9±3.3 211.3	(1) Photodissoc. (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1993DAV/KIM (2) 1998CHA
nitric oxide NO–**NO**	9.7±0.5	40.6±2.1	Review	1976BEN
dinitrogen pentoxide O_2N–$\mathbf{ONO_2}$	24.6	102.9	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
nitrous acid HO–$\mathbf{NO_x}$ x= 0 1	 49.4 49.3	 206.7 206.3	 Review	 1982MCM/GOL
fluoronitrooxy FO–**NO**	31.7±4	132.5±17	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
chloronitrooxy cis-ClO–**NO** trans-ClO–**NO**	 30.5±2 27.9±2	 127.6±8.4 116.6±8.4	 Derived from $\Delta_f H^\circ$ in ref.	 2003NASA/JPL

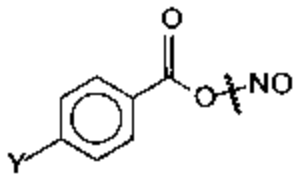
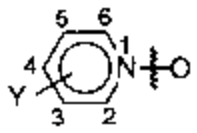
续表

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** – 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
bromonitrooxy cis-BrO–**NO** trans-BrO–**NO**	33.0±2 29.1±2	138.1±8.4 121.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
tanns-perp-HOONO HOO–**NO**	27.3±1	114 2±4	Derived	2002HIP/NAS
methyl nitrite CH_3O–**NO**	(1) 41.8±1 (2) 41.7±0.8	174.9±4.2 174.5±3.3	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref	(1) 1977BAT/MIL (2) 1998NIST
ethyl nitrite C_2H_5O–**NO**	(1) 42.0±1 3 (2) 43.9±1	175.7±5.4 183.7	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref	(1) 1977BAT/MIL (2) 1998NIST
propyl nitrite nC_3H_7O–**NO**	(1) 40.1±1.8 (2) 42.8±1.5	167.8±7.5 179.1±6.3	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref	(1) 1974BAT/CHR (2) 1998NIST
1-propyl nitrite iC_3H_7O- **NO**	(1) 41.0±1.3 (2) 41.9±1	171.5±7.5 175.3±4.2	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref	(1) 1974BAT/CHR (2) 1998NIST
butyl nitrite nC_4H_9O–**NO**	42.5±1.5	177.8±6.5	Pyrolysis	1974BAT/CHR
iso-butyl nitrite iC_4H_9O–**NO**	42.0±1.5	175.7±6.5	Pyrolysis	1974BAT/CHR
sec-butyl nitrite sC_4H_9O–**NO**	41.5±0.8	173.6±3.3	Pyrolysis	1974BAT/CHR
tert-butyl nitrite tC_4H_9O–**NO**	(1) 40.9±0.8 (2) 42.1±1.4	171.1±3.3 176.1±5.9	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref	(1) 1974BAT/CHR (2) 1998NIST
tert-amyl nitrite tAmO–**NO**	40.9±1	171.1±0.4	Kinetics	1979ISL
alkyl nitrite RO–**NO**	40.8±1	170.7±4.2	Review	1981BAT/ROB
phenyl nitrite C_6H_5O–**NO**	20.8	87.0	Kinetics	1998BER/CAR
nitric acid HO–NO_2	48.8	204.2	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
fluoronitrooxy FO–NO_2	31.5±3	131.8±12.6	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
chloronitrooxy ClO–NO_2	26.7±0.5	111.8±2.1	Derived from $\Delta_f H^\circ$ in ref.	1990AND/FAH
bromonitrooxy BrO–NO_2	26.4±2	110.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	1996ORL/TYN
alkyl nitrate RO–NO_2	40.7±0.5	170.3±2.1	Review	1981BAT/ROB

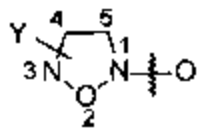
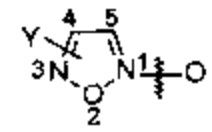
续表

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methyl nitrate CH_3O–**NO_2**	41.6±1	174.1±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl nitrate C_2H_5O **NO_2**	41.3±1	172.8±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
propyl nitrate C_3H_7O **NO_2**	42.3±1	177.0±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
iso-propyl nitrate iC_3H_7O–**NO_2**	42.0±1	175.7±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
nitric peracid HOO–**NO_2**	(1) 23±2 (2) 22.8±0.8, at 0K (4) **23.9±0.7**	96.2±8.4 95.3±3.4 **100.0±2.9**	(1) Pyrolysis (2) Derived (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1978BAL/GOL (2) 1995ZAB (3) 1997REG/MOZ
methyl nitroperoxy CH_3OO–**NO_2**	20.7±2	86.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	1983PAT/GOL
trifluoromethyl nitroperoxy CF_3OO–**NO_2**	25	105	Kinetics	1990DES/TRO
chlorodifluoromethyl nitroperoxy CF_2ClOO–**NO_2**	25.5	106.7	Derived from $\Delta_f H^\circ$ in ref.	1991KOP/ZAB
dichlorofluoromethyl nitroperoxy $CFCl_2OO$–**NO_2**	25.5	106.7	Derived from $\Delta_f H^\circ$ in ref.	1991KOP/ZAB
trichloromethyl nitroperoxy CCl_3OO–**NO_2**	22.9	95.8	Derived from $\Delta_f H^\circ$ in ref.	1991KOP/ZAB
ethyl nitroperoxy C_2H_5OO–**NO_2**	16.5±3	69.0±12.6	Derived from $\Delta_f H^\circ$ in ref.	1990DES/TRO
peroxyacetyl nitrate $CH_3C(O)OO$ **NO_2**	(1) 26±2 (2) **28.4±0.7**	108.8±8.4 **118.8±2.9**	(1) Pyrolysis (2) Kinetics	(1) 1977HEN/KEN (2) 1991BRI/CAR
1-methylvinyl nitroperoxy CH_2=$C(CH_3)OO$–**NO_2**	26±2	108.8±8.4	Pyrolysis	1977HEN/KEN
(hydroxyimino)ethane **HO**–N=$CHCH_3$	49.7	207.9	Review	1970ONE/BEN
nitroso formate, substituted  R = CH_3	35.2	147.3	AOP	2000XIA/ZHU
CH_2CH_3	37.9	158.6		
$CH(CH_3)_2$	36.7	153.6		

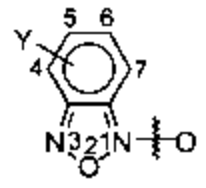
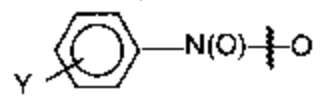
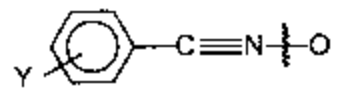
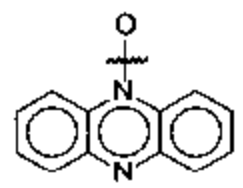
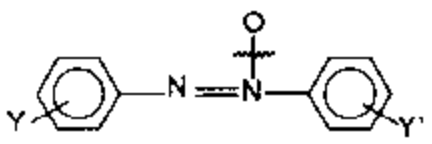
续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** – 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitroso benzoate, substituted 				
Y = H	33.9	141.8	AOP	2000XIA/ZHU
Br	34.3	143.5		
Me	32.8	137.0		
MeO	32.5	136.0		
NO_2	38.6	161.5		
hydroxyamine HO–**NH_2**	63.0±2	263.6±8.4	Derived from $\Delta_f H^\circ$ in ref.	1999AND
methoxyamine CH_3O–**NH_2**	54.6	228.4	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
methylhydroxylamine **HO**- $NHCH_3$	64.9	271.5	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
N-methyoxymethanamine **CH_3O**–$NHCH_3$	57.0	238.5	Derived from $\Delta_f H^\circ$ in ref.	1994NIST
nitromethyl radical **$C^{\bullet}H_2N(O)$** –O	72±6	301±25	Derived	1993CYR/LEA
trialkyl-N-oxides R_3N–**O**				
R = CH_3	61.2±1.2	256±5	Calorimetry	1995ACR/TUC
C_2H_5	16.0±1.2	67±5		
n C_4H_9	–17.7±1.4	–74±6		
pyridine N-oxides, substituted 				
Y = H	(1) 63.3±0.5 (2) 72.1±0.7	264.9±2.0 301.7±2 8	Calorimetry	(1) 1998SIL/MAT (2) 1988LI/PIL
2-Me	(1) 62.1±0.6	259.9±2.4		
3-Me	(1) 63.2±0.6	264.6±2.6		
4-Me	(1) 62.7±0.8 (3) 65.7±1.2	262.4±3.4 274.7±5		(3) 1995LEB/CHI

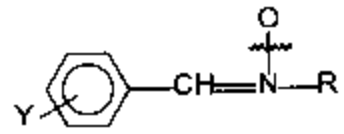
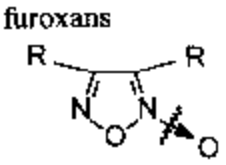
续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
3-CN	(1) 60.8±0.7	254.3±3.1		
4-CN	(1) 63.5±1.1	265.5±4.6		
2-OH	(4) 66.6±0.5	278.8±2.3		(4) 2004SIL/MAT
3-OH	(1) 60.9±1.1	255.0±4.8		
3-HOO	(5) 60.4±0.6	252.8±2.7		(5) 1995ACR/TUC
2-C(O)OH	(1) 65.9±1.2	275.9±5.1		
3-C(O)OH	(4) 60.4±0.6	252.8±2.7		
4-C(O)OH	(1) 62.0±1.2	259.5±5.0		
3-NO_2	(6) 64	267 8		(6) 1969MIR/LEB
4-NO_2	(3) 65.7±1.2 (5) 61.8±1.3	274.6±5 258.5±5.3		
3-Me-4-NO_2	(1) 63.0±1.7	263.4±7.1		
3-$NH_2C(O)$	(7) 71.7±1.2	300.3±5.0		(7) 2001SIL/GON
4-$NH_2C(O)$	(7) 69.0±0.9	288.6±3.7		
2,4,6-$(NO)_3$	(3) 42.3±1.2	176.8±5		
furazan N-oxides, substituted 				
Y = 4,5-Me_2	60.8±1.0	254.2±4.0	Calorimetry	1996ACR/BOT
4,5-$(CH_2ONO_2)_2$	57.1±0.5	238.8±2.1		
4,5-$(CN)_2$	57.4±2.4	240±10		
furazan N-oxides, substituted 				
Y = 4,5-Me_2	60.8±1.0	254.2±4.0	Calorimetry	1996ACR/BOT
4,5-$(CH_2ONO_2)_2$	57.1±0.5	238.8±2.1		
4,5-$(CN)_2$	57.4±2.4	240±10		

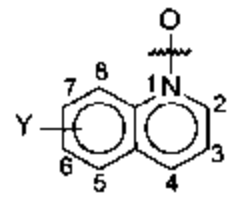
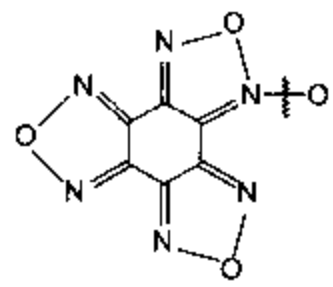
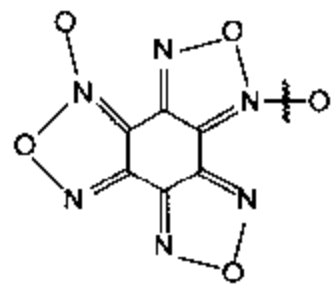
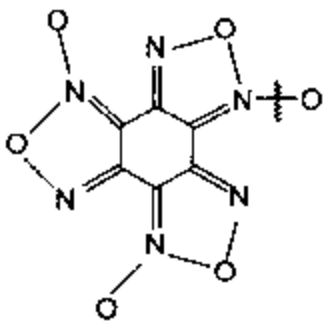
续表

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
benzofurazan N-oxides, substituted 				
Y = H	60.0±0.7	(1) 250.9±3.0	Calorimetry	(1) 1990LEI/PIL
5-Cl	58.3±0.8	(2) 244.1±3.5		(2) 1996ACR/BOT
5-Me	59.7±0.8	(2) 249.8±3.2		
5-MeO	59.3±0.9	(2) 248.0±3.7		
4-NO_2	61.2±1.6	(2) 255.9±6.7		
nitrobenzen, substituted, 				
Y = H	(1) 93.6±1.9	391.5±8.0	Calorimetry	(1) 1993ACR/TUC(a)
2,6-Me_2	(1) 90.9±0.5	380.4±2.3		
2,4,6-Me_3	(1) 91.6±0.7	383.4±2.9		
2,4,6-$(tBt)_3$	(2) 76.9±1.7	321.8±7.0		(2) 1995ACR/BOT
4-$N(Me)_2$	(3) 88.8±0.8	371.4±3.5		(3) 1994ACR/TUC
benzonitrile N-oxide, substituted 				
Y = 2,4,6-Me_3	53.1±1.1	222.2±4.6	Calorimetry	1991ACR/TUC
2,4,6-$(MeO)_3$	55.6±0.9	232.8±3.8		
phenazine N-oxide 	67.1±1.3	280.7±5.6	Calorimetry	1990LEI/PIL
azoxybenzenes, substituted 				

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
E-structure Y, Y' = H	(1) 76.8±0.7 (2) **73.9±0.8**	321.5±2.9 **309.4±3.5**	(1) Calorimetry (2) Calorimetry, revised	(1) 1986KIR/PIL (2) 1993ACR/TUC(b)
OH	(2) 75.8±1.8	317.2±7.6	(3) Calorimetry	(3) 1986KIR/ACR
OCH_2CH_3	(2) 76.6±1.7	320.4±7.0		
iPr	(3) 79.2±0.9	331.5±3.8		
tBu	(3) 76.8±1.0	321.2±4.2		
Z-structure Y, Y' = H	(4) 62.8±0.8	262.8±3.3	(4) Calorimetry	(4) 1989ACR/KIR
di-N-oxides RN(O)=N(O)R R = tBu	(1) 65.8±0.8	275.1±3.3	Derived	(1) 1989ACR/KIR
Ph	(2) 62.8±0.8	262.8±3.3		(2) 1975PEP/LEB
benzylidene N-oxides, substituted  E structure				
R = tBu, Y = H	(1) 67.7±1.6	283.1±6.5	Calorimetry	(1) 1989ACR/KIR
4-NO_2	(1) 68.7±1.2	287.6±5.1		
4-iPr	(1) 68.4±1.9	286.0±7.9		
R = Ph Y = H	(2) 63.3±0.7	264.9±3.0		(2) 1986KIR/ACR
4-MeO	(2) 63.9±1.5	267.5±6.1		
4-iPr	(2) 63.9±1.5	267.3±6.4		
2-OH	(2) 70.5±1.4 (3) 57.1±1.1	294.8±6.0 238.9±4.6		(3) 2002LEB/CHI
furoxans 				
R = CH_3	(1) 60.7	254.0	Calorimetry	(1) 1971MAT/PEP
CH_2ONO_2	(1) 57.1±0.9	238.9±3.8		(2) 1975PEP/MAT

续表

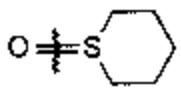
断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
quinoline N-oxides, substituted  Y = 6-OCH_3	64.3±1.2	269.2±5.0	Calorimetry	2003SIL/SAN
benzo furoxans 	58.2±1.9	243.5±7.9	Calorimetry	2002MAT/LEB(b)
	57.8±1.8	241.8±7 5		
	57.4±1.5	240.2±6.3		

7.5 O—S 键能

表 7.5 O—S BDEs

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
sulfur monoxide **O**=S	(1) 124.6	521.3	(1) Derived from $\Delta_f H°$ in ref.	(1) 1998NIST
	(2) 124.7±1	521.7±4.2	(2) Spectroscopy	(2) 2002CRC
	(3) 122.7±2.6	513.4±10.9	(3) Spectroscopy	(3) 2000RED/AHA
oxythio radical **O**–SH	36.2	151.5	Derived from $\Delta_f H°$ in ref.	1993BAL/CAS

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 文献编号) kcal/mol	 kJ/mol	方法	文献
sulfur dioxide **O**=SO	(1) 132±2 (2) 130.1±0.2, at 0K (3) **131.7**	552.3±8.4 544.3±0.9 **551.1**	(1) Spectroscopy (2) Spectroscopy (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1970DAR (2) 1971OKA (3) 1998NIST
sulfur trioxide **O**=SO_2	83.3	348.5	Derived	1978BEN
disulfur oxide **O**=SS	103.8	434.3	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
formylthio **O**=SH_2	71±4	297.1±16.7	Derived	1978BEN
fluoroformyl fluoride **O**=SF_2	118.7	496.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
chloroformyl chloride **O**=SCl_2	105	439.3	Derived	1978BEN
sulfurous acid **O**=$S(OH)_2$	118±6	493.7±25	Derived	1978BEN
sulfur tetrafluorooxide **O**=SF_4	102±6	426.8±25	Derived	1978BEN
dimethyl sulfoxide **O**=$S(CH_3)_2$	86.6	362.3	Derived	1978BEN
diethyl sulfoxide **O**=$S(C_2H_5)_2$	88.7	371.1	Derived	1978BEN
diphenyl sulfoxide **O**=$S(C_6H_5)_2$	89.3	373.6	Derived	1978BEN
(methoxysulfinyl)methoxy **O**=$S(OMe)_2$	116±6	485.3±25	Derived	1978BEN
difluorosulfone **O**=$S(O)F_2$	110±5	460.2±21	Derived	1978BEN
dichlorosulfone **O**=$S(O)Cl_2$	95	397.5	Derived	1978BEN
dimethylsulfone **O**=$S(O)(CH_3)_2$	112	468.6	Derived	1978BEN
diethylsulfone **O**=$S(O)(C_2H_5)_2$	112	468.6	Derived	1978BEN
thian-1-one 	86.0	360.0	Calorimetry	2003ROU/TEM
thiane-1,1-dione 	112.4	470.0	Calorimetry	2003ROU/TEM
diphenylsulfone **O**=$S(O)(C_6H_5)_2$	113	472.8	Derived	1978BEN

续表

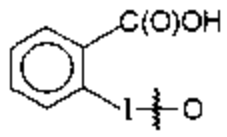
断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值， 括号内数字　文献编号)		方法	文献
	kcal/mol	kJ/mol		
phenylsulfone **O**=S(O)(C_6H_5)	109	456.1	Derived	1978BEN
sulphuric acid **O**=S(O)($OH)_2$	110±3	460.2±12.6	Derived	1978BEN
dimethoxy sulfate **O**=S(O)($OMe)_2$	108	451.9	Derived	1978BEN
diethoxy sulfate **O**=S(O)($OEt)_2$	109	456 1	Derived	1978BEN
phenyl phenylsulfonyl sulfate **O**=S(O)(Ph)($PhSO_2$)	122	510.4	Derived	1978BEN
phenyl phenylthiooxy sulfate **O**=S(O)(Ph)(PhSO)	122±3	510.4±12.6	Derived	1978BEN
phenyl thiophenyl sulfate **O**=S(O)(Ph)(PhS)	115±4	481.2±16.7	Derived	1978BEN
hydroxythiol **HO**–SH	70.1±4	293.3±16.7	Derived from $\Delta_f H^\circ$ in ref.	1993OHA/DEP
methylthio peroxy **OO**-SCH_3	11	46.0	Pulse laser Photolysis	1992TUR/BAR
oxyhydrosulfide radicals **HO**–S	70±4	292.9±16.7	Derived	1978BEN
oxyhydrodisulfide **HO**–S_2	13.2±2	55.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	1997JPL
sulfenic acid **HO**–SOH	74.9±3	313.4±12.6	Derived from $\Delta_f H^\circ$ in ref.	1978BEN
sulfuric acid **HO**–S(OH)O_2	92.0±2	384.9±8.4	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
adduct **HO**–SCS	35 3±1.5	147.7±6.3	Derived from $\Delta_f H^\circ$ in ref	1990MUR/LOV
methanesulfenic acid **HO**–SCH_3	72.6±3	303.8±12.6	Derived from $\Delta_f H^\circ$ in ref.	1996HUN/SHE
methanesulfonic acid **HO**–SO_2CH_3	86.1±3	360.2±12.6	Derived from $\Delta_f H^\circ$ in ref.	2000GUT/GAL
hydrooxy methylsulfonate **HOO**–SO_2CH_3	116.8	488.7	Derived from $\Delta_f H^\circ$ in ref.	1978BEN
methoxy methylsulfonate CH_3**OO**–SO_2CH_3	111.6	466.9	Derived from $\Delta_f H^\circ$ in ref.	1978BEN
methylthiyl peroxy CH_3S–**OO**	~11	~46	Pulsed laser photolysis	1992TUR/BAR

7.6 O—X(卤) 键能

表 7.6 O—X(卤) BDEs

断裂键 (**黑体** · 离解原子)	BDEs (**黑体** - 推荐值: 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
hypofluorous acid F–OH	51.4	215.1	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
difluorine monoxide F–OF	(1) 39.2	164.1	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 2003NASA/JPL
F–O	(1) 52.6 (2) 53.1±4	220 222±17	(2) Spectroscopy	(2) 2002CRC
fluorine dioxide O–FO	–5±6	-21±25	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
fluoro peroxy F–OO	12.9±0.5	54.0±2.1	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
trifluoromethyl hypofluorite F–OCF_3	(1) 43.5±0.5 (2) 40.2±2.5 (3) **48±1**	182.0±2.1 168.2±10.5 **200.8±4.2**	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref. (3) Re-evalated	(1) 1968CZA/CAS (2) 1994SCH/WAL (3) 2002REI/PRA
methyl hypofluorite F–OCH_3	(1) ≤47 4+1 2, at 0 K (2) >46.5	≤198±5 >197	(1) PIMS (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1991RUS/APP (2) 1998NIST
fluoronitrooxy F–ONO_2	33.6	140.6	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
hypochlorous acid Cl–OH	55.8	233.5	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
dichlorine monoxide Cl–OCl	(1) 33.9	142	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 2003NASA/JPL
Cl–O	(2) 64.3 (3) 74.9±2.3	269.1 313.6±9.6	(2) Spectroscopy (3) Spectroscopy	(2) 2002CRC (3) 2001RAJ/FER
chloro peroxy Cl–OO	5.6±1	23.4±4.2	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
dichlorine dioxide Cl–OOCl	21.8	91.2	Derived from $\Delta_f H^\circ$ in ref.	1994NIC/FRI
dichlorine trioxide O–ClOOCl	59.2	247.7	Derived from $\Delta_f H^\circ$ in ref.	1994NIC/FRI
trifluoromethyl hypochlorite Cl–OCF_3	≤52.8±2	≤220.9±8.4	PIMS	1997ASH/RUS

续表

断裂键 (**黑体** = 离解原子)	BDEs (**黑体** = 推荐值， 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methyl hypochlorite **Cl**–OCH_3	47.5	198.7	Derived from $\Delta_f H^\circ$ in ref.	1994NIST
chlorine dioxide **O**–ClO	(1) 59±3 (2) 61.3±0.3	246.9±12.6 256.3±1.3	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1968CZA/CAS (2) 2003NASA/JPL
chloro trioxide **Cl**–O_3	17.1	71.5	Derived from $\Delta_f H^\circ$ in ref.	1994NIC/FRI
chloronitrooxy **Cl**–ONO_2	40.5	169.5	Derived from $\Delta_f H^\circ$ in ref.	1990AND/FAH
bromine dioxide **O**–BrO	49.0±2	204.8±8.4	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
hypobromous acid **Br**–OH	(1) 51±1 (2) 50.1±1	213.4±4.2 209.6±4.2	(1) Review (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1999JUR (2) 2003NASA/JPL
dibromine oxide **Br** OBr **Br**–O	(1) 29.9 (2) 56.2±0.5	125 235.1±2.4	Derived from $\Delta_f H^\circ$ in ref.	(1) 2003NASA/JPL (2) 1998CHA
bromo peroxy **Br**–OO	0.7±10	3.1±42	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
bromo trioxide **Br**–O_3	7.8	32.8	Derived from $\Delta_f H^\circ$ in ref.	1994NIC/FRI
bromonitrooxy **Br** ONO_2	33.6	140.6	Derived from $\Delta_f H^\circ$ in ref.	1996ORL/TYN
hypoiodous acid **I**–OH	51.0	213.4	Derived from $\Delta_f H^\circ$ in ref.	2001IUPC
diiodo oxide **I** OI **I**–O	(1) 31.1 (1) 57.4 (2) 59.5±0.3	130.1 240 249.0±1.3	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Spectroscopy	(1) 2003NASA/JPL (2) 2002CRC
iodo peroxy **I**–OO	2.5±4	10.5±17	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
iodo rioxide **I**–O_3	1.6	6.7	Derived from $\Delta_f H^\circ$ in ref.	1994NIC/FRI
2-iodosobenzoic acid 	63.2±1.9	264.5±8.1	Calorimetry	1999SIL/MAT

7.7 O—P键能

表 7.7 O—P BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Also see Section 10.1				
phosphoryl fluoride **O**=PF_3	(1) 130±5 (2) 129	544±21 540	Review	(1) 1966KER (2) 1973BEN
phosphoryl chloride **O**=PCl_3	(1) 122±5 (2) 124	510.4±21 519	Review	(1) 1966KER (2) 1973BEN
phosphoryl bromide **O**=PBr_3	(1) 119±5 (2) 122	498±21 510	Review	(1) 1966KER (2) 1973BEN
phosphoryl iodide **O**=$P(CH_3)_3$	139	582	Review	1973BEN
ethyl ethylphosphate **O**=$P(OC_2H_5)_3$	148	619	Review	1973BEN
phosphinotris(dimethylamino)- 1-one **O**=$P(N(CH_3)_2)_3$	128	536	Review	1973BEN
triphenylphosphino-1-one **O**=PPh_3	130	544	Review	1973BEN

第 8 章　N—X键能

8.1　N—H键能

8.1.1　非芳胺中的N—H键能

表 8.1.1　非芳胺中的 N—H BDEs

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体**　推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
ammonia **H**–NH_2 $\Delta_f H^\circ$(R) = 44.5±0.3 (186±1)	(1) 108.2±0.3 (2) 107.57±0.06 (3) 108.5±0 3 (4) **107.6±0.1**	452.7±1.3 450.07±0.25 454.0±1 3 **450.2±0.4**	(1) Recommend. (2) Photolysis (3) GPA (4) Review	(1) 1994BER/ELL (2) 1996MOR/ASH (3) 2003REE/HAR (4) 2003BLA/ELL
H–NH	(5) 97.6	408.4	(5) Derived from $\Delta_f H^\circ$ in ref.	(5) 1998NIST
H–N	(6) **78.4±3.7** (7) ≤81.0	**328.0±15.4** ≤338.9	(6) Spectroscopy (7) Spectroscopy	(6) 1968GAY (7) 2002CRC
difluoroamonia **H**–NF_2	75.7±2.5	316.7±10.5	Calorimetry	1969PAN/ZER
(Z)-diazene **H**–NNH $\Delta_f H^\circ$(R) = 59.6 (249.5)	(1) 75±5 (2) **60.8**	314±21 **254.4**	(1) Pyrolysis (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1970LIK/SHI (2) 1998NIST
hydrazoic acid **H**–N_3 $\Delta_f H^\circ$(R) = 112±5 (468.6±20.9)	(1) 92±5 (2) 92.7±3.1 (3) ≤88.7±0.5, at 0 K (4) **93.8±5** (5) 93.7	384.9±20.9 387.9±13.0 ≤371.1±2.1 **392.5±20.9** 392.0	(1) ICR (2) Correlation (3) UV Photolysis (4) Derived from $\Delta_f H^\circ$ in ref. (5) AOP	(1) 1981PEL/JAC (2) 1993JEN (3) 1999ZHA/XU (4) 2002CRC (5) 2002ALN/ZHA
methanimine **H**–N=CH_2	(1) 85±5, at 0 K (2) 87±6	356±21 364±25	(1) PES (2) Derived	(1) 1991COW/TRA (2) 1994SUN/PAN
nitrosyl hydride **H**–NO $\Delta_f H^\circ$(R) = 21.58 (90.29)	(1) 49 (2) 48.1±0.1, at 0 K (3) **47.7**	205 201.2±0.4 **199.5**	(1) Kinetics (2) Spectrometry (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1962HOL (2) 1996DIX (3) 1999AND
isocyanic acid **H**–NCO $\Delta_f H^\circ$(R) = 31.5 (131.8)	(1) 110.1±0.5 (2) ≤109.6±0.4, at 0K (3) 107.7	460.7±2.1 ≤458.6 ±1.7 450.6	(1) Photodissoc. (2) Photolysis (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1995ZHA/DUL (2) 1996BRO/BER (3) 1998NIST

续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
isothiocyanic acid **H**–NCS	(1) 96±6 (2) ≤**94.8±1.1**	402±25 ≤**396.6±4.6**	(1) PES (2) PIMS	(1) 1993BRA/KIM (2) 1994RUS/BER(b)
cyanoamino radical **H**–NCN	83±2	347.3±8.4	PES	1997CLI/WEN
methylamine $CH_3N\mathbf{H}_2$ $\Delta_f H^\circ$(R) = 44.0±2 (184.1±8.4)	(1) 103±2.5 (2) 101.2±3 (3) **101.6±2** (4) 100.0±2.5	431.0±10.5 423.4±12.6 **425.1±8.4** 418.4±10.5	(1) VLPP (2) AE (3) Review (4) Derived	(1) 1972GOL/SOL (2) 1973SHA/FRA (3) 1988COL (4) 1994SUN/PAN
tert-butylamine $tBuN\mathbf{H}_2$ $\Delta_f H^\circ$(R) = 22.8±3 (95.4±12.6)	(1) 100 (2) 93.3±2 (2) 95±2	418.4 390.4±8.4 397.5±8.4	(1) AOP (2) PAC	(1) 1998BOR/LIU (2) 2002LAU/ALL
benzylamine $C_6H_5CH_2N\mathbf{H}_2$ $\Delta_f H^\circ$(R) = 68.9±3 (288.3±12.6)	100	418.4	AOP	1998BOR/LIU
1-naphthanlenamine $RN\mathbf{H}_2$	89.6	374.7	Correlation	2000DEN/DEN
2-naphthanlenamine $RN\mathbf{H}_2$	90.7	379.5	Correlation	2000DEN/DEN
dimethylamine $(CH_3)_2N\mathbf{H}$ $\Delta_f H^\circ$(R) = 37.8±2 (158.2±8.2)	(1) 95±2.5 (2) **94.6±2** (3) 91.5±2.0	397.5±10.5 **395.8±8.4** 382.8±10.5	(1) VLPP (2) Review (3) Derived	(1) 1972GOL/SOL (2) 1988COL (3) 1994SUN/PAN
propylamine phosphonium bromide (n-Pr**N**H–P^+Ph_3) Br	92.7	387.9	AOP	1995CHE/LIU
hydrazine **H**–N**H**NH_2 $\Delta_f H^\circ$(R) = 58.2 (243.5)	(1) 87.5 (2) 80.8±0.3, at 0 K	366.1 338.1±1.3	(1) Pyrolysis (2) PIMS	(1) 1988GRE/COL (2) 1991RUS/BER
hydrazine radical **H**–N_2H_2	(1) 43.8±1.1, at 0 K (2) 44.8	183.3±4.6 187.4	(1) PIMS (2) Derived from $\Delta_f H^\circ$ *in ref.*	(1) 1991RUS/BER (2) 1998NIST
methylhydrazine **H**–NHNH(CH_3)	(1) 88 (2) 66±5	368 276±21	(1) Pyrolysis (2) MS	(1) 1964EBE (2) 1970FON/HUD
methylhydrazine radical HNN(CH_3)–**H**	53±6	222±25	MS	1970FON/HUD
1,1-dimethylhydrazine $(CH_3)_2$NNH–**H**	(1) 88 (2) 85±5	368 356±21	(1) Pyrolysis (2) MS	(1) 1964EBE (2) 1970FON/HUD
amonomethanenitrile **NH**-CN	99	414.2	AOP	1990BOR/HAR(b)
urea $(N\mathbf{H}_2)_2$C=O $\Delta_f H^\circ$(R) = 0.2±3 (0.8±12.6)	111	464.4	AOP	1991BOR/JI(b)

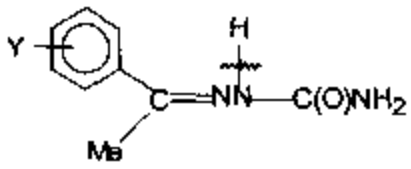
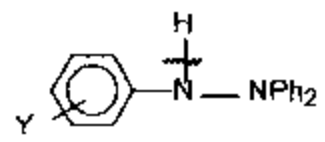
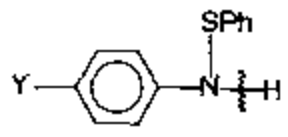
续表

断裂键 （黑体 = 离解原子） Δ_fH°(R)/kcal (kJ)	BDEs （黑体 = 推荐值； 括号内数字 = 文献编号） kcal/mol	kJ/mol	方法	文献
thiourea $(NH_2)_2C{=}S$ Δ_fH°(R) = 46.4±3 (194.1±12.6)	93	389.1	AOP	1991BOR/JI(b)
1-aminoethane-1-thione CH_3CSNH_2	91	380.7	AOP	1991BOR/JI(b)
aminophenylmethane-1-thione $PhCSNH_2$	91	380.7	AOP	1991BOR/JI(b)
bis(phenylamino)methne-1-thione $(PhNH)_2C{=}S$	87	364.0	AOP	1991BOR/JI(b)
aminomethanamidine $(NH_2)_2C{-}NH$ Δ_fH°(R) = 59.9±3 (250.6±12.6)	104	435.1	AOP	1991BOR/JI(b)
diphenylmethanimine $Ph_2C{-}NH$	117	489.5	AOP	1991BOR/JI(b)
benzylphenylthioamine $C_6H_5CH_2NHSPh$	86.9	363.6	AOP	1998BOR/LIU
formamide $HCONH_2$ Δ_fH°(R) = 11.9±3 (49.8±12.6)	108.5	454.0	AOP	1995BOR/ZHA
acetamide CH_3CONH_2 Δ_fH°(R) = -1.6±3 (-6.7±12.6)	107.5	449.8	AOP	1991BOR/JI(b)
2-ethyl-pentanamide Et_3CCONH	109	456.1	AOP	1995BOR/ZHA
tert-butanamide $tBuCONH_2$	109	456.1	AOP	1995BOR/ZHA
benzamide $PhCONH_2$	107	447.7	AOP	1991BOR/JI
methyl aminooate $CH_3OC(O)NH_2$	105	439.3	AOP	1997ZHA/BOR
ethyl aminooate $C_2H_5OC(O)NH_2$	105.3	440.6	AOP	1994ZHA/BOR(e)
N-methylacetamide $CH_3CONHMe$	(1) 103.9 (2) **106.5**	434.7 **445.6**	AOP	(1) 1990BOR/ZHA (2) 1995BOR/ZHA
N-(tert-butyl)-2,2-dimethyl propanamine $tBuCONHtBu$	110.5	462.3	AOP	1995BOR/ZHA

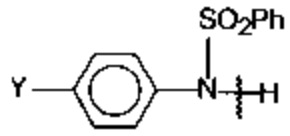
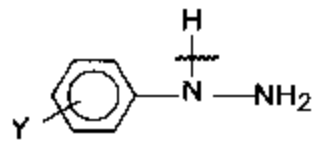
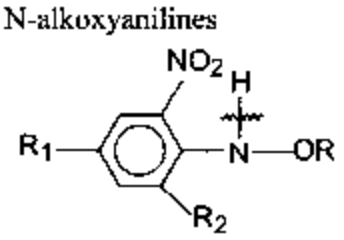
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
acetohydrazide $MeCONHNH_2$	82	343.1	AOP	1997ZHA/BOR
benzenecarbohydrazide $PhCONHNH_2$	80.3	336.0	AOP	1997ZHA/BOR
diacetamide $(CH_3C(O))_2NH$	107.5	449.8	AOP	1992BAU/DAV
diuret $(NH_2C(O))_2NH$	108.5	454.0	AOP	1992BAU/DAV
diacelhydrazine $(NHC(O)CH_3)_2$	91.5	382.8	AOP	1992BAU/DAV
dibenzoylhydrazine $(NHC(O)Ph)_2$	89.5	374.5	AOP	1992BAU/DAV
N-((1E)-buta-1,3-dienyl)-benzamide PhCONHPh	97	405.8	AOP	1991BOR/JI(b)
benzenesulfonamide $PhSO_2NH_2$	105	439.3	AOP	1997ZHA/BOR
hydrazinophenyl sulfone $PhSO_2NHNH_2$	81	338.9	AOP	1997ZHA/BOR
ethanamidine $CH_3C(=NH)NH_2$	102	426.8	AOP	1991BOR/JI(b)
benzenecarboxamidine $PhC(=NH)NH_2$	102	426.8	AOP	1991BOR/JI(b)
diethyl(iminophenylmethyl)-amine $PhC(=NH)NEt_2$	119	497.9	AOP	1991BOR/JI(b)
((1Z)-2-aza-1,2-diphenyl-vinyl)phenylamine PhC(=NPh)NHPh	92	384.9	AOP	1991BOR/JI(b)
(((1Z)-2-aza-1,2-diphenyl-vinyl)amino)dimethylamine $PhC(=NPh)NHNMe_2$	85	355.6	AOP	1991BOR/JI(b)
(imino(phenylamino)methyl)-phenylamine $(PhNH)_2C=NH$	92	384.9	AOP	1991BOR/JI(b)
((1E)-2-aza-1,2-diphenyl-vinyl)amino)amino)-dimethylamine PhC(NHNMe2)=NPh	84.7	354.4	AOP	1992BOR/JI
(tert-buytl)phenylthioamine tBuNHSPh	87.1	364.4	AOP	1998BOR/LIU
phenyl-N-(phenylcarbonyl-amino)carboxamide PhCONHNHCOPh	89.3	373.6	AOP	1997ZHA/BOR

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
N-[(1E)-1-aza-2-phenylprop-1-enyl]aminoamide, substituted 				
Y = H	91.7	383.5	AOP	1994ZHA/HUA
p-Cl	92.4	386.4		
p-Br	92.3	386.0		
p-Me	91.4	382.3		
p-MeO	91.0	380.6		
p-CF_3	92.7	387.7		
p-CN	92.7	387.7		
p-NO_2	92.4	386.4		
diphenyl(phenylamino)amine, substituted 				
Y = H	81.1	339.3	AOP	1997ZHA/BOR
2,4-$(NO_2)_2$	83.1	347.7		
2,4,6-$(NO_2)_3$	80	334.7		
phenylphenylthioamine, substituted 				
Y = H	82.6	345.6	AOP	1998BOR/LIU
Br	83.0	347.3		
MeO	81.6	341.4		
CN	84.2	352.3		

续表

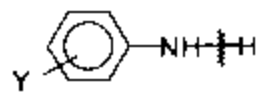
断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
phenyl(phenylsulfonyl)-amine, substituted 				
Y = H	(1) 93.2 (2) 92.6	389 9 387.4	AOP	(1) 1998BOR/LIU (2) 1998CHE/XIA
Cl	(2) 93.8	392.5		
Br	(1) 94.4	395.0		
Me	(2) 91.7	383.7		
MeO	(1) 89.1 (2) 89.0	372.8 372.4		
CN	(1) 96.6	404.2		
MeCO	(2) 95.2	398.3		
NO_2	(2) 97.1	406.3		
di-2-naphthamine $(2\text{-}C_{10}H_7)_2NH$	86.1	360.2	Correlation	2000DEN/DEN
hydrazines, substituted 				
Y = H	72.6	303.8	AOP	1997ZHA/BOR
p-Cl	73.0	305.4		
p-Me	71.9	300.8		
p-Et	76.3	319.2		
p-CF_3	77.9	325.9		
p-CN	77.8	325.5		
N-alkoxyanilines 				

续表

断裂键 (黑体 - 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值, 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
R R_1 R_2				
Me H NO_2	75.4	315.3	AOP	1996STA/ZAR
Me NO_2 H	76.1	318 2		
Me NO_2 NO_2	77.6	324.8		
i-Pr NO_2 NO_2	78.0	326.2		
bis(1,1-dimethyl-1-silaethyl)-amine **H**–N($SiMe_3$)$_2$	110.9	464.0	Derived	1998BEC/WAL
isocyanic acid **H**–NCO	110.5±3.8	462.3±15.9	PIMS	1994RUS/BER(c)
H–NHC$^\bullet$H$_2$	31.8±3	133.1±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
H–N(CH$_3$)C$^\bullet$H$_2$	32.6±3	136.4±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
H–NHC$^\bullet$HCH$_3$	31.4±3	131.4±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST

8.1.2 芳胺中的N—H键能

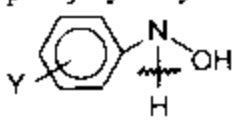
表 8.1.2 芳胺中的 N—H BDEs

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
Aniline or benzenamine PhNH–H $\Delta_f H^\circ$(R) = 58.4±1 (244.3±4.2)	(1) 88.0±2 (2) 92 3 (3) 89.1 (4) **92.2** in sol. (4) **89.7** in gas (5) 92.2	368.2±8.4 386.2 373 **385.8** **375.3** 385 8	(1) VLPP (2) AOP (3) Electrochem. (4) PAC (5) AOP	(1) 1978COL/BEN (2) 1993BOR/ZHA (3) 1994JON/LIN (4) 1997MAC/WAY (5) 1997CHE/WAN
anilines, mono-substituted  Y = 4-F	(3) 88.8 in gas (3) 91.3 in sol. (8) 92.9±2.1	371.5 382.0 388.7±8 8	(1) Electrochem. (2) Electrochem.	(1) 1994JON/LIN (2) 1995JON/LIN

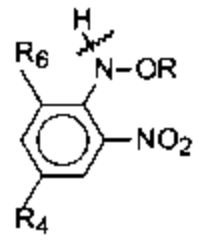
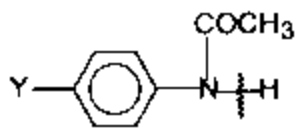
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
2-Cl	(4) 93.1	389.5	(3) PAC	(3) 1997MAC/WAY
3-Cl	(4) 92.6	387.4	(4) AOP	(4) 1993BOR/ZHA
4-Cl	(4) 92.4	386.6	(5) AOP	(5) 1997ZHU/ZHA
	(7) 92.3	386.2		
			(6) Correlation	(6) 2000DEN/DEN
3-Br	(4) 93.2	389.9		
			(7) AOP	(7) 1997CHE/WAN
4-Br	(4) 92.3	386.2		
	(7) 92.2	385.8	(8) GPA	(8) 2003REE/HAR
4-I	(1) 89.1	373		
2-CN	(4) 95.1	397.9		
3-CN	(4) 94.1	393.7		
4-CN	(1) 91.8	384		
	(4) 95.2	398.3		
	(7) 95.1	397.9		
2-CF_3	(2) 92.5	387		
3-CF_3	(2) 93.2	390		
	(4) 95.7	400.4		
	(5) 96.6	404.2		
4-CF_3	(1) 92.0	385		
	(4) 96.5	403.8		
	(7) 96.4	403.4		
2-CH_3	(2) 90.6	379		
4-CH_3	(1) 88.7	371		
	(3) 87.5 in gas	366.1		
	(3) 90.0 in sol.	376.6		
	(4) 92.0	384.9		
	(7) 91.9	384.6		
4-NH_2	(1) 86.0	360		
4-NO_2	(4) 96.7	404.6		
4-tBu	(1) 88.9	372		
	(6) 92.1	385.6		

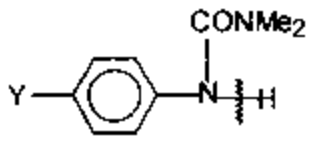
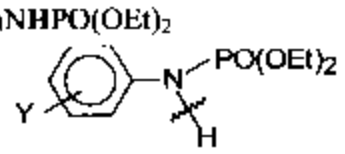
续表

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
4-CH_3CO	(1) 90.6 (4) 94.2 (6) 93.8	379 394.1 392.6		
2-CH_3O	(2) 88.7 (4) 90.4	371.0 378.2		
3-CH_3O	(4) 93.9	392.9		
4-CH_3O	(1) 87.2 (7) 90.3	365 377.9		
3-CF_3SO_2	(4) 95.7	400.4		
anilines, di- and trisubstituted				
2,4-Me_2	(2) 88.0	368	(2) Electrochem.	(2) 1995JON/LIN
3,4-Me_2	(2) 88.7	371	(4) AOP	(4) 1993BOR/ZHA
3,5-Me_2	(2) 90.3	378		
2,4-$(MeO)_2$	(2) 87.7	367		
3,4-$(MeO)_2$	(2) 88.4	370		
3,5-$(MeO)_2$	(2) 91.5	383		
3,5$(CF_3)_2$	(4) 97.2	406.7		
2-NO_2-4-Cl	(4) 97.6	408.4		
3-NO_2-4-Cl	(4) 97.6	408.4		
2,4,6-Cl_3	(4) 95.5	399.6		
phenylhydroxylamine  				
Y = H	69.8	292	AOP	1998CHE/LU
p-Me	67.9	284		
p-Br	72.4	303		
N-methyl-phenylamine PhNHMe $\Delta_f H°$(R) = 57.6±1.5 (241.0±6.3)	(1) **89.3** (2) 87.5±2 (3) 91.9	**373.6** 366.1±8.4 384.5	(1) AOP (2) VLPP (3) Correlation	(1) 1993BOR/ZHA (2) 1978COL/BEN (3) 2000DEN/DEN

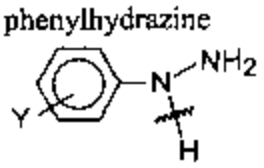
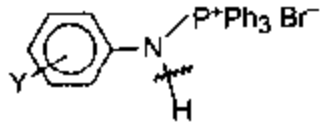
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 - 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
phenyl-1-naphthlamine 1-$C_{10}H_7$N**H**C_6H_5	85.3	357.1	Correlation	2000DEN/DEN
phenyl-2-naphthlamine 2-$C_{10}H_7$N**H**C_6H_5	86.7	362.9	Correlation	2000DEN/DEN
4-methoxy-N-phenyl-benzenamine 4-$CH_3OC_6H_4$N**H**Ph	85.1	355.9	Correlation	2000DEN/DEN
N-(4-phenoxy)phenyl-2-naphthalenamine 2-$C_{10}H_7$N**H**C_6H_4(4'-C_6H_5O)	83.5	349.5	Correlation	2000DEN/DEN
alkyloxy(2-nitrophenyl)amine  				
R R4 R6			AOP	1996STA/ZAR
Me H NO_2	75.4	315.5		
Me NO_2 H	76.1	318.4		
Me NO_2 NO_2	77.6	324.7		
iPr NO_2 NO_2	78.0	326.4		
N-phenylacetamide, substituted  				
Y = H	(1) 98.9 (3) 99.5	413.8 416.3	AOP	(1) 1993BOR/ZHA(b) (2) 1993CHE/ZHA
p-Cl	(2) 98.7	413.0		(3) 1991BOR/JI
p-Br	(2) 99.1	414.6		
p-Me	(2) 97.1	406.3		
p-MeO	(2) 95.3	398.7		
p-MeCO	(2) 100.0	418.4		
p-CF_3	(2) 101.6	425.1		
p-CN	(2) 101.1 (2) 101.5	423.0 424.7		
p-NO_2	(2) 102.0	426.8		

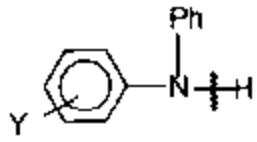
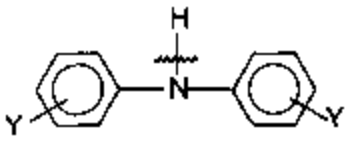
续表

断裂键 (黑体 - 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 - 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
N-phenylacetamide, substituted 				
Y = H	92.7	387.9	AOP	1998CHE/XIA
p-Cl	93.4	390 8		
p-Br	93.5	391.2		
p-I	93.4	390.8		
p-Me	91.8	384.1		
p-MeO	90.4	378.2		
p-MeCO	94.9	397.1		
p-NO_2	96 4	403.3		
diethyl(phenylamino)-phosphino-1-one, substituted PhNHPO(OEt)$_2$ 				
Y = H	(1) 94.7 (2) 94.9	396.2 397	AOP	(1) 1991BOR/ZHA (2) 1998CHE/LU
p-Cl	(3) 95.7	400.4		(3) 1998CHE/XIA
p-Br	(3) 95.7	400.4		
p-Me	(2) 93.5	391		
p-MeCO	(2) 97.3	407		
p-CN	(2) 98.9	414		
p-NO_2	(2) 100.6	421		
phenyl(phenylsulfonyl)amine PhNHSO$_2$Ph	93 2	389.9	AOP	1998BOR/LIU
phenyl-N-benzamide PhNHCOPh	97.3	407.1	AOP	1993CHE/ZHA
(dimethylamino)-N-benzamide PhNHCONMe$_2$	92.7	387.9	AOP	1998CHE/XIA

续表

断裂键 (**黑体** - 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
2,2,2-trifluoro-N-phenyl-acetamide PhNHCOCF$_3$	99.6	416.7	AOP	1993ZHA/BOR(b)
phenylphenylthioamine PhNHSPh	82.6	345.6	AOP	1998BOR/LIU
phenyl(phenylamino)methane-1-thione PhNHSOPh	90.2	377.4	AOP	1998BOR/LIU
phenylhydrazine  				
X = H	(1) 72.9	305.1	AOP	(1) 1997CHE/WAN
p-Cl	(1) 73.2	306.4		(2) 1998CHE/LU
p-Me	(1) 72.2	302.2		
p-CF$_3$	(1) 78.3	327.3		
p-CN	(1) 78.1 (2) 77.9	326.9 326		
p-EtC(O)O	(1) 76.6	320.6		
aminotriphenylphosphonium bromides X–NH$^+$PPh3 Br$^-$				
X = nPr	(1) 92.8 (2) 92.7	388.3 388	AOP	(1) 1995CHE/LIU (2) 1998CHE/LU
nBu	(1) 91.8	384.1		
CH_2Ph	(1) 89.3	373.7		
aniline phosphonium bromide, substituted  				
Y = H	(1) 81.9 (2) **68.4**	342.8 **286**	AOP	(1) 1995CHE/LIU (2) 1998CHE/LU
p-Cl	(1) 81.9	342.8		
p-Me	(1) 83.1 (2) **68.8**	347.8 **288**		

续表

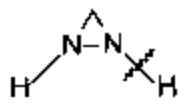
断裂键 (**黑体** = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
p-CN	(2) 64.8	271		
p-CF_3	(2) 64.5	270		
N-(phenylamino)acetamide PhN**H**NHCOMe	78.6	328.9	AOP	1997ZHA/BOR
1,2-diphenylhydrazine PhN**H**N**H**Ph	73.1	305.9	FT-ICR	1991ING/FOK
diphenylamine Ph_2N–**H** $\Delta_f H°$(R) = 87.5±1.5 (366.1±6.3)	(1) 87.3 (2) 85.8±0.7 (3) 89.2, in sol. (3) **87.2**, in gas (4) 87.2 (5) 87.5	365.3 359.0 373.2 **364.8** 364.7 366.1	(1) Kinetics (2) EPR (3) PAC (4) Correlation (5) AOP	(1) 1987VAR/DEN (2) 1999LUC/PED (3) 1997MAC/WAY (4) 2000DEN/DEN (5) 2002ALN/ZHA
diphenylamine, substituted  				
Y = m-Cl	(1) 88.4	369.9	(1) AOP	(1) 1993BOR/ZHA
p-Me	(1) 86.9	363.6		
m-Me	(1) 87.6	366.5		
p-MeO	(1) 85.6 (4) 85.1	358.2 356.1		
p-PhNH	(1) 79.2 (2) 79.9	331.4 334.3	(2) AOP	(2) 1994ZHA/BOR
p-NO_2	(1) 90.4 (3) 91.0 (4) 89.1	378.2 380.7 372.9	(3) AOP (4) Correlation	(3) 1991BOR/ZHA (4) 2000DEN/DEN
diphenylamine, substituted  				
Y = p-Br	(1) 88.1 (2) 87.0	368.6 364.2	(1) AOP (2) Correlation	(1) 1993BOR/ZHA (2) 2000DEN/DEN
p-MeO	(1) 84.2 (2) 83.3 (4) 81.8	352.3 348.6 342.2		
p-Me	(2) 85.4 (3) 86.3, in sol. (3) **86.2**, in gas (4) 83.3	357.5 361.1 **360.7** 348.5	 (3) PAC (4) EPR	 (3) 1997MAC/WAY (4) 2002PRA/DIL

续表

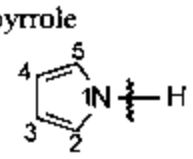
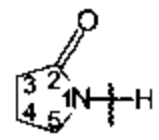
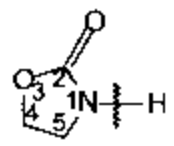
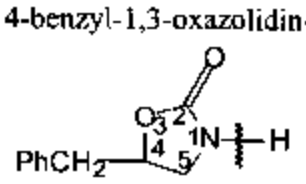
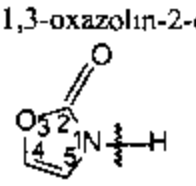
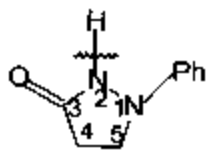
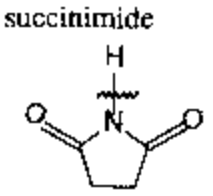
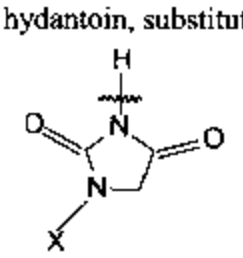
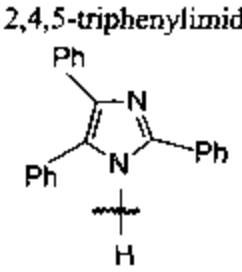
断裂键 (**黑体** - 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
p-tBu	(2) 85.8	358.8		
p-$N(CH_3)_2$	(4) 79 5	332.6		
N-1-(3,7-bis(1.1-dimethyl-ethyl)napthalenyl-benzenamine 1-(3,7-tBu_2-$C_{10}H_5$)N**H**Ph	82.4	344.9	Correlation	2000DEN/DEN
4-(1,1-dimethylethyl)-N-phenyl-benzenamine 4-tBu-C_6H_4N**H**Ph	86.1	360.3	Correlation	2000DEN/DEN
N,N′-di(4-isopropylphenyl-)-p-phenylendiamine 4-tBu-C_6H_4NH-4-C_6H_4N**H**C_6H_4-t-Bu	79.7	333.6	Correlation	2000DEN/DEN
N,N′-di-2naphthyl-p-phenylendiamine 4-(2-$C_{10}H_7$NH)C_6H_4N**H**-2′-$C_{10}H_7$	82 8	346.6	Correlation	2000DEN/DEN
N,N′-dioctyl-p-phenyl-endiamine 4-C_8H_{17}NHC_6H_4NHC_8H_{17}	82.9	346.9	Correlation	2000DEN/DEN
N,N′-diphenyl-p-phenylen-diamine 4-C_6H_5NH-4-C_6H_4NHPh	85 1	355.9	Correlation	2000DEN/DEN
N-phenyl-N′-isopropyl-p-phenylendiamine 4-(C_6H_5NH)C_6H_4NH–iPr	83.5	349.2	Correlation	2000DEN/DEN
9H-carbazole 1,2-C_6H_4N**H**-1′,2′-C_6H_4	88.8	371.6	Correlation	2000DEN/DEN
4-(1,1-dimethylethyl)-N-(4-(1,1-dimethylethyl)phenyl)-1-naphthalenamine 1(N**H**C_6H_4-4tBu)-4′-Bu$C_{10}H_6$	84.2	352.1	Correlation	2000DEN/DEN

8.1.3 环状分子中的N—H键能

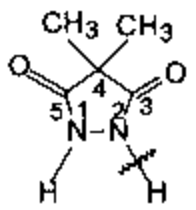
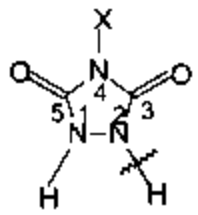
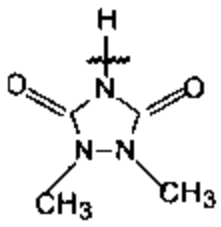
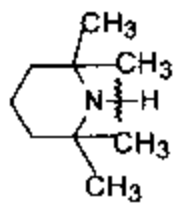
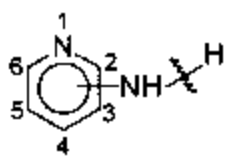
表 8.1.3 环状分子中的 N—H BDEs

断裂键 (**黑体** = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1,2-diaziridine 	88±4	368 2±16.7	GPA	2002KAS/BRO

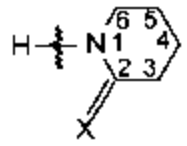
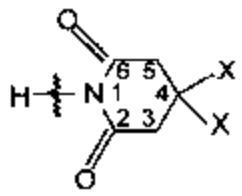
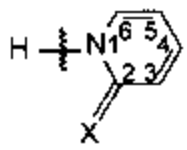
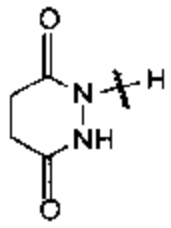
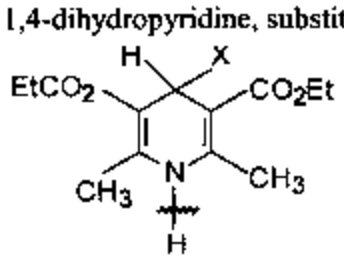
续表

断裂键 (**黑体** = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 文献编号) kcal/mol	kJ/mol	方法	文献
pyrrole  $\Delta_f H°$(R) = 70.8±3 (296.2±12.6)	(1) 99±6 (2) **97** (3) 97±2 (4) 88±2	414.2±25.1 **405.8** 405.8±8.4 368.2±8 4	(1) Photodetach. (2) AOP (3) Derived (4) Photoioniz.	(1) 1975RIC/STE (2) 1991BOR/JI(b) (3) 1994SUN/PAN (4) 1994BLA/NOR
2-pyrrolidone 	107	447.7	AOP	1995BOR/ZHA
1,3-oxazolidin-2-one 	105.8	442.7	AOP	1994ZHA/BOR(e)
4-benzyl-1,3-oxazolidin-2-one 	105.7	442.2	AOP	1994ZHA/BOR(e)
1,3-oxazolin-2-one 	91.0	380.7	AOP	1994ZHA/BOR(e)
1-phenylpyrazolidin-3-one 	73.9	309.2	AOP	1997ZHA/BOR
succinimide 	(1) 91.7 (2) 92.5 (3) 118±3	383.7 387.0 493.7	(1) AOP (2) AOP (3) Electrochem.	(1) 1992ARN/VEN (2) 1992BAU/DAV (3) 1993LIN/JON
hydantoin, substituted  X = H CH_3	92.5 92.5	387.0 387.0	AOP	1992BAU/DAV
2,4,5-triphenylimidazole 	89.5	374.5	AOP	1994ZHA/BOR

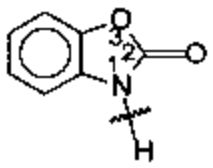
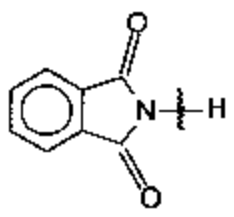
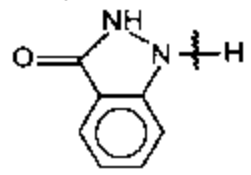
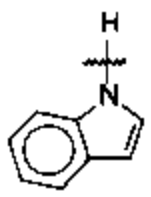
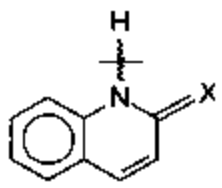
续表

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
4,4-dimethylpyrazolidine-3,5-dione 	82.5	345.2	AOP	1992BAU/DAV
urazole, 4-substituted 				
X = 4-CH_3	78.5	328.4	AOP	1992BAU/DAV
4-Ph	78.5	328.4		
4-(p-$MeOC_6H_4$)	78.5	328.4		
4-(p-MeC_6H_4)	78.5	328.4		
4-(p-ClC_6H_4)	78.5	328.4		
4-(m-ClC_6H_4)	79.5	332.7		
1,2-dimethylurazole 	94.5	395.4	AOP	1992BAU/DAV
2,2,6,6-tetramethylpiperidine 	87.6±4	366.5±17	PAC	2002LAL/ALL
aminopyridine 				
H–N at site 2	87	364.0	AOP	1993BOR/SIN
3	94	393.3		
4	84	351.5		

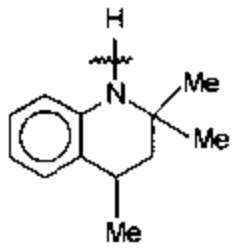
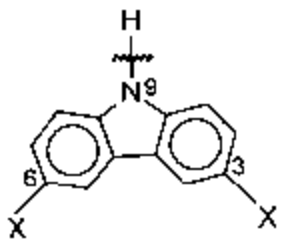
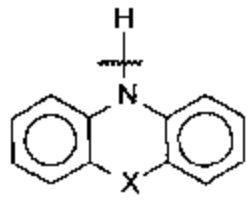
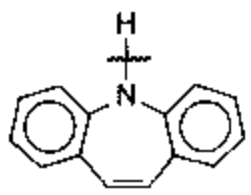
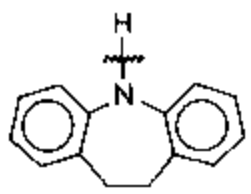
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
2-piperidone, analogues 				
X = O	109.5	458.1	AOP	1995BOR/ZHA
S	91	380.7		
2,6-piperidione 				
X = H	(1) 115±3	481.2	Electrochemical	(1) 1998LIN/MER
CH_3	(2) 104.5	437.2		(2) 1992BAU/DAV
2-pyridone, analogues 				
X = O	98	410.0	AOP	1993BOR/SIN
S	81	338.9		
4-pyridone, analogues 				
X = O	99	414.2	AOP	1993BOR/SIN
S	82	343.1		
1,2,4,5-tetrahydropyridazine-3,6-dione 	87.7	366.9	AOP	1997ZHA/BOR
1,4-dihydropyridine, substituted 				
X = H	86.2	360.7	AOP	2000CHE/LU
i-Pr	89.4	374.0		

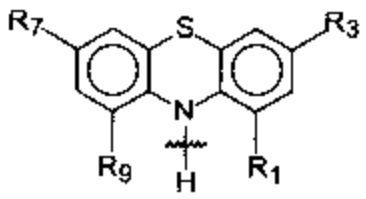
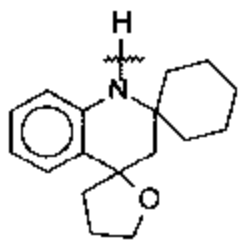
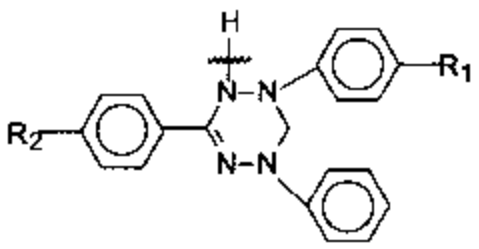
续表

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Ph	90.8	379.9		
4-$MeOC_6H_4$	90.5	378.7		
4-MeC_6H_4	90.6	379.1		
4-ClC_6H_4	91.2	381.6		
4-CNC_6H_4	92.8	388.3		
3-hydrobenzoxazol-2-one 	94.8	396.6	AOP	1994ZHA/BOR(e)
phthalimide 	89.1	372.8	AOP	1992ARN/VEN
1H-2-hydroindazol-3-one 	77.7	325.1	AOP	1997ZHA/BOR
indole 	(1) 90.8 (2) 94.1	380 393.7	(1) Electrochem. (2) AOP	(1) 1994JON/LIN (2) 2000ZHU/HE
2-quinolone, analogues 				
X = O	101	422.6	AOP	1993BOR/SIN
S	83	347.3		
2,3-dihydrophthalazine-1,4-dione 	86.8	363.2	AOP	1997ZHA/BOR

续表

断裂键 (黑体 = 离解原子) $\Delta_f H°$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
2,2,4-trimethyl-1,2,3,4-tetrahydroquinoline 	88.1	368.6	Correlation	2000DEN/DEN
carbazole 				
X = H $\Delta_f H°$(R) = 91.6±2 (383.3±8.4)	(1) 92.7 (2) **93.6** (3) 93.0	387.9 **391.6** 389.1	AOP	(1) 1991BOR/ZHA (2) 1992ARN/VEN (3) 2000ZHU/HE
Br 3,6-dibromocarbazole	(1) 93.6 (2) 94.3 (3) 93.8	391.6 394.6 392.5		
phenothiazine, analogues 				
X = O	(1) 79.7 (2) 77.2±0.3 (3) 80.0	333.5 323.0±1.3 334.7	(1) AOP (2) EPR (3) AOP	(1) 1993BOR/ZHA (2) 1999LUC/PED (3) 2000ZHU/HE
S	(1) 82.3 (2) 79.3±0.3	344.3 331.8±1.3		
Se	(2) 80.4±0.4	336.4±1.7		
iminostilbene, or 5H-dibenzo(b,f)azepine 	(1) 84.6 (2) 85.3 (3) 82.4±0.5 (4) 84.8	354.0 356.9 344.8±2.1 354.8	(1) AOP (2) AOP (3) EPR (4) AOP	(1) 1991BOR/CHE (2) 1994ZHA/BOR (3) 1999LUC/PED (4) 2000ZHU/HE
5H,10H,11H-dibenzo(b,f)azepine 	(1) 87.0 (2) 87.2	(1) 364.0 (2) 364.8	AOP	(1) 1991BOR/ZHA (2) 2000ZHU/HE

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
phenothioazine, substituted 				
$R_1 = R_9 = Me$, $R_3 = R_7 = H$	77.7±0.4	325.1±1.7	EPR	1999LUC/PED
$R_1 = R_9 = H$, $R_3 = R_7 = OMe$	76.2±0.3	318.8±1.3		
$R_1 = R_9 = H$, $R_3 = R_7 = CMe_3$	78.1±0.4	326.8±1.7		
$R_1 = R_9 = H$, $R_3 = R_7 = Cl$	79.8±0.4	333.9±1.7		
$R_1 = R_9 = H$, $R_3 = R_7 = NO_2$	81.0±1.0	338.9±4.2		
2-spirocyclohexyl-4-(spiro-tetrahydrofuran-2)-1,2,3,4-tetrahydroquinoline 	86.2	360.7		
2,6-diaryl-4-phenyl-1,2,3,4-tetrahydro-sym-tetrazines 				
R_1 = H R_2 = H	69.6	291	ESR	1989MIS/POL
H MeO	70.0	293		
H Me	69.8	292		
H Cl	69.1	289		
H NO_2	68.1	285		
MeO H	68.4	286		
Me H	68.8	288		

续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/kcal (kJ)		BDEs (黑体 = 推荐值; 括号内数字 文献编号)		方法	文献
		kcal/mol	kJ/mol		
Cl	H	70.3	294		
NO_2	H	72.9	305		
MeO	NO_2	67.2	281		
NO_2	MeO	73.4	307		

8.2 N—N键能

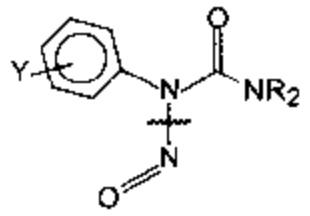
表 8.2 N—N BDEs

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitrogen N≡N	225.94±0.14	945.33±0.59	Spectroscopy	2002CRC
azide radical N–N_2	(1) –0.7±2.3	–2.9±9.6	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1993CON/CYR
	(2) 6.2±1.8, at 0 K	26.1±7.7	(2) CID	(2) 1995MAY/FRY
azide cation N^+–N_2	86.2±1.8, at 0 K	360.8±7.7	CID	1995MAY/FRY
nitrogen dimer cation N_2^+–N_2	(1) 22.8	95.4	(1) HP MS	(1) 1970PAY/KEB
	(2) 24.4	102.1	(2) MS	(2) 1973TEN/CON
	(3) 26.2±1.8	109.6±7.5	(3) AE	(3) 1989NOR/LUO
	(4) 25.1±1.4	105.2±5.8	(4) CID	(4) 1991SCH/ARM
	(5) 25.8±1.5	107.9±6.3	(5) HP MS	(5) 1994HIR/YAM
dinitrogen oxide ON–N	114.9	480.7	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
nitric oxide dimer ON–NO	2.03±0.03	8.49±0.12	Photodissociation	2003POT/DRI
dinitrogen trioxide ON–NO_2	8.8	36.8	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
dinitrogen tetroxide O_2N–NO_2	13.2	55.2	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
diazene HN=NH	(1) ≤123.8±1.1, at 0 K	≤518±5	(1) PIMS	(1) 1991RUS/BER
	(2) 119.7	501	(2) Derived from $\Delta_f H^\circ$ in ref.	(2) 1998CHA
hydrazine H_2N–NH_2	(1) 65.5±0.4	274.1±1.7	(1) PIMS	(1) 1991RUS/BER
	(2) 66.2	277.0	(2) Derived from $\Delta_f H^\circ$ in ref.	(2) 2002CRC

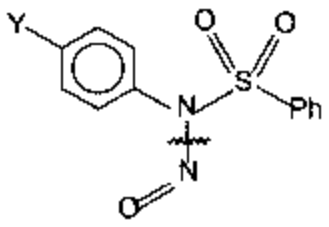
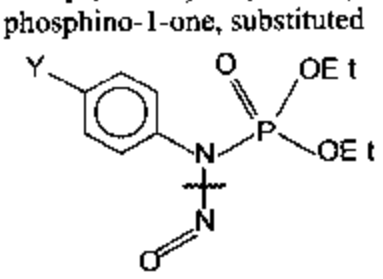
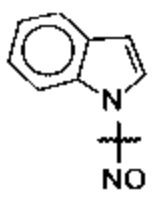
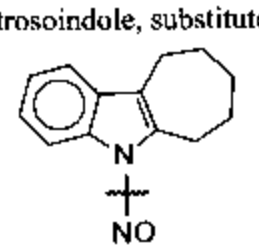
续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
tetrafluorohydrazine $\mathbf{F_2N}$-$\mathbf{NF_2}$	(1) 21±1 (2) **22.2±3**	87.9±4.2 92.9±12.6	(1) Calorimetry (2) Derived from Δ_fH° in ref.	(1) 1969PAN/ZER (2) 1998CHA
methylhydrazine $\mathbf{NH_2}$–NHCH$_3$	(1) 67 (2) **65.9±2**	280 **275.8±8.4**	(1) Pyrolysis (2) Derived from Δ_fH° in ref.	(1) 1964EBE (2) 1986PED/NAY
1,1-dimethylhydrazine $\mathbf{NH_2}$–N(CH$_3$)$_2$	62.1±2	259.8±8.4	Derived from Δ_fH° in ref.	2002CRC
phenylhydrazine $\mathbf{NH_2}$–NHC$_6$H$_5$	54.4±2	227.6±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
1,2-dimethylhydrazine (CH$_3$)$\mathbf{NH}$–$\mathbf{NH}$(CH$_3$)	66.0±3	276.1±12.6	Derived from Δ_fH° in ref.	2002CRC
dimethyl(methylamino)amine (CH$_3$)$_2$N–NH(CH$_3$)	60.8	254.4	Derived from Δ_fH° in ref.	1988LIA/BAR
tetramethylhydrazine (CH$_3$)$_2$N–N(CH$_3$)$_2$	59.6	249.4	Derived from Δ_fH° in ref.	1994NIST
[(dimethylamino)diazenyl]dimethyl-anine (CH$_3$)$_2$N–NNN(CH$_3$)$_2$	16.5	69	Kinetics	1961GOW/JON
1,2-diphenyl hydrazine $\mathbf{PhNH}$–NHPh	38.8±2	162.3±8.4	Derived from Δ_fH° in ref.	1994NIST
nitroamine H$_2$N–$\mathbf{NO_2}$	(1) **58.6** (2) 55.0	**245.2** 230.0	(1) Derived from Δ_fH° m ref. (2) Derived	(1) 1991GUR/VEY (2) 2000KOS/MIR
N-nitromethylamine CH$_3$HN–$\mathbf{NO_2}$	50	209.2	Derived	2000KOS/MIR
N-nitrodimethylamine (CH$_3$)$_2$N–$\mathbf{NO_2}$	(1) 43.8 (2) 39.6	183.3 165.7	(1) Derived from Δ_fH° in ref. (2) Derived	(1) 1986PED/NAY (2) 2000KOS/MIR
1,1-dinitroethane CH$_3$N(NO$_2$)–$\mathbf{NO_2}$	(1) 27.6 (2) 28.3	115.6 118.4	(1) Pyrolysis (2) Calorimetry	(1) 1975MAT/NAS (2) 1987MIR/KOR
1,1-dinitropropane C$_2$H$_5$N(NO$_2$)–$\mathbf{NO_2}$	29.0	121.5	Pyrolysis	1975MAT/NAS
1,1-dinitrobutane C$_3$H$_7$N(NO$_2$)–$\mathbf{NO_2}$	31.0	129.7	Pyrolysis	1975MAT/NAS
1,1-dinitropentane C$_4$H$_9$N(NO$_2$)–$\mathbf{NO_2}$	29.6	123.8	Pyrolysis	1975MAT/NAS
methyl((methylnitroamino)-methyl)nitroamine CH$_3$N(NO$_2$)CH$_2$N(CH$_3$)–$\mathbf{NO_2}$	40.0	167.4	Derived	2000KOS/MIR

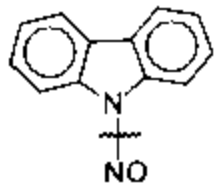
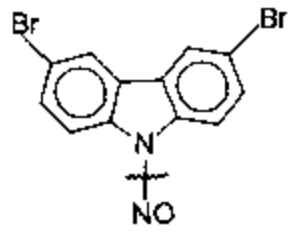
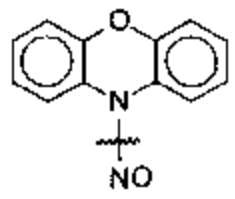
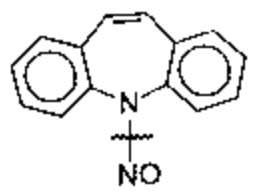
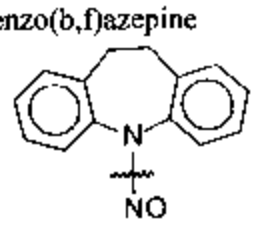
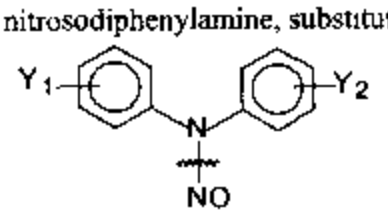
续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** – 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitrozoamines $((NO_2)_3CCH_2)_2N$–**NO_2**	40.0	167.4	Derived	2001MIR/KOS
$(H(NO_2)_2CCH_2)_2N$–**NO_2**	45.5	190.4		
$(NO_2)_3CCH_2N((CH_2)_2C(NO_2)_3)$ –**NO_2**	40.0	167.4		
$((NO_2)_3CCH_2N(NO_2)CH_2CH_2N$– $C(NO_2)_3)$–**NO_2**	40.0	167.4		
$(H(NO_2)_2CCH_2N(NO_2)CH_2CH_2N$– $CH(NO_2)_2)$–**NO_2**	40.0	167.4		
$((NO_2)_3CCH_2)_2N$–**NO_2**	39.0	163.2		
$((NO_2)_3CCH_2N(NO)CH_2CH_2N$– $C(NO_2)_3)$–**NO**	40.0	167.4		
aminomethylnitrosoamino $H_2NN(CH_3)$–**NO**	42.9	179.6	Derived	1998LEB/CHJ
amino-N-nitroso-N-phenyl-amide, substituted 				
R = Me Y = H	29.1	121.8	AOP	1998CHE/XIA
2-Cl	23.1	96.7		
4-Cl	29.2	122.2		
3-Br	30.3	126.8		
4-Br	29 4	123.0		
4-I	28.9	120.9		
2-Me	27.5	115.1		
4-Me	28.7	120.1		
4-MeO	28.3	118.4		
4-MeCO	30.5	127.6		
4-NO_2	33.1	138.5		
R = i-Pr Y = 4-Me	26.6	111.3		
R = $C_6H_5CH_2$ Y = 4-Me	25.4	106.3		

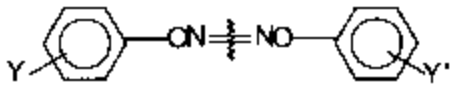
续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** – 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitrosophenyl(phenyl-solfonyl)-amine, substituted 				
Y – H	13.2	55.2	AOP	1998CHE/XIA
Cl	13.1	54.8		
Me	11.4	47.7		
MeO	12.4	51.9		
MeCO	14.5	60.7		
NO_2	18.0	75.3		
diethyl(nitrosophenylamino)-phosphino-1-one, substituted 				
X = H	35.0	146.4	AOP	1998CHE/XIA
Cl	36.2	151.5		
Br	36.2	151.5		
Me	34.5	144.3		
NO_2	40.4	169.0		
nitrosoindole 	28.7	120.1	AOP	2000ZHU/HE
nitrosoindole, substituted 	29.7	124.3	AOP	2000ZHU/HE

续表

断裂键 (黑体 = 离解原子 或原子团)	BDEs (黑体 = 推荐值, 括号内数字 - 文献编号)		方法	文献
	kcal/mol	kJ/mol		
9-nitrosocarbazole 	27.4	114.6	AOP	2000ZHU/HE
3,6-dibromo-9-nitrosocarbazole 	28.3	118.4	AOP	2000ZHU/HE
10-nitrosophenoxazine 	13.6	56.9	AOP	2000ZHU/HE
5-nitroso-benzo(b,f)azepine 	19.2	80.3	AOP	2000ZHU/HE
5-nitroso-10H, 11H-dibenzo(b,f)azepine 	22.9	95.8	AOP	2000ZHU/HE
nitrosodiphenylamine, substituted 				
Y_1 = H Y_2 = H	22.6	94.6	AOP	2000ZHU/HE
m-Cl H	24.1	100.8		
m-Me H	22.3	93.3		
p-Me H	21.4	89.5		
p-NO_2 H	24.3	101.7		
p-MeO H	21.4	89.5		
p-MeO p-MeO	21.0	87.9		

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
hydrogen azide $HN{=}N_2$	15.0	62 8	Derived from $\Delta_f H^\circ$ in ref.	1994FRE/KAB
methyl azide $CH_3N{=}N_2$	41.7	174.4	Pyrolysis	2001ORL
ethyl azide $C_2H_5N{=}N_2$	38.0	159.0	Pyrolysis	2001ORL
phenyl azide $C_6H_5N{=}N_2$	36.8	153.9	Pyrolysis	1986STE/KRU
benzyl azide $C_6H_5CH_2N{=}N_2$	38.2	159.7	Pyrolysis	1986STE/KRU
cyclohexyl azide $c\text{-}C_6H_{11}N{=}N_2$	38.2	159 7	Pyrolysis	1986STE/KRU
4-aza-4-diazobut-4-en-2-one $CH_3C(O)CH_2N{=}N_2$	37.8	158.1	Pyrolysis	1986STE/KRU
1-aza-1-diazopent-1-en-3-one $C_2H_5C(O)CH_2N{=}N_2$	38.0	159.0	Pyrolysis	1986STE/KRU
p-NO_2-benzyl azide 4-$NO_2C_6H_4CH_2N{=}N_2$	38.6	161.5	Pyrolysis	1986STE/KRU
azobenbenzene-N,N-dioxides substituted 				
Y, Y' = H	(1) 21.8±2.0	91.1±8.5	(1) Derived	(1) 1993ACR/TUC
2,4-Me_2	(1) 17.7±2.9	74.1±12.2	(1) Calorimetry	
2,4,6-Me_3	(1) 17.3±2.9	72.2±12.2		
2,3,5,6-Me_4	(2) 14.6±1.2	61.1±5.0	(2) NMR	(2) 1970OKA/INA
2,3,4,5,6-Me_5	(2) 12.0±1.2	50.2±5.0		
4-$N(Me)_2$	(3) 12.2	51	(3) Derived	(3) 1994ACR/TUC

8.3 N—C键能

表 8.3 N—C BDEs

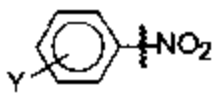
断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
CN radical C≡N	(1) 175.9±4.3 (2) **179.3±0.7**	736.2±18.0 **750.0±2.9**	(1) Spectroscopy (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 2003RED/AHA (2) This volume

续表

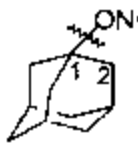
断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
CH_2N radicals CH_2=**N**	144±6, at 0 K	602±25	PES	1991COW/TRA
CNN radicals C–N_2	29.5+0 8	123.4±3.3	Derived from $\Delta_f H^\circ$ in ref.	2000BIS/HOO
diazomethylene CH_2=N_2	<41.8	<174.9	UV Photolysis	1971LAU/OKA
isocyanic acid **HN**=CO	(1) ≤122.1±0.3 (singlet-triplet) (2) 86.6±1.2	≤510.9±1.3 362.3±5.0	(1) Photolysis (2) Derived from $\Delta_f H^\circ$ in ref.	1996BRO/BER
cyanogen azide N_3–CN	109.5±5	458.1±20.9	Derived from $\Delta_f H^\circ$ in ref	1998NIST
1-aza-1-diazoethane N_3–CH_3	(1) 71.7 (2) 80.1±5	300.0 335.1±20.5	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1993PEP/MAT (2) 1988LIA/BAR
azacyclopentyldiazomethen cyclo-C_5H_9–N_3	76.2±3.3	318.8±13.8	Calorimetry	1993PEP/MAT
azacyclohexyldiazomethen cyclo-C_6H_{11}–N_3	81.1±3.7	339.3±15.5	Calorimetry	1993PEP/MAT
azadiazophenylmethane N_3–C_6H_5	(1) 89.0±4.4 (2) 89.8±5	372.4±18.4 375.7±20.9	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1993PEP/MAT (2) 1988LIA/BAR
1-aza-1-diazo-2-phenylethane N_3–$CH_2C_6H_5$	50.5±3.4	211 3±14.2	Calorimetry	1993PEP/MAT
1-aza-1-diazo-2,2,2-triphenylethane N_3–$C(C_6H_5)_3$	46.6	195.0	Review	1974PEP/ERL
3-aza-3-diazoprop-3-en-1-ol N_3–CH_2CH_2OH	56.2±3.9	235.1±16.3	Calorimetry	1993PEP/MAT
ethyl-3-aza-3-diazopro-3-enoate N_3–$CH_2C(O)OC_2H_5$	66.8±3 9	279.5+16 3	Calorimetry	1993PEP/MAT
1-aza-1-diazo-2,2,2-trinitroethane N_3–$C(NO_2)_3$	70.6±3.7	295.4±15.5	Calorimetry	1993PEP/MAT
1-aza-1-diazo-2,2-dinitroprop-1-ene N_3–$C(NO_2)_2Me$	66.4±3.7	277.8±15.5	Calorimetry	1993PEP/MAT
nitrosyl cyanide NC–**NO**	28.8±2.5	120.5±10.5	Electron impact	1975GOW/ION

续表

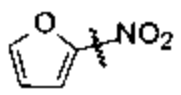
断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitrosomethane CH_3–**NO**	(1) 40±0.8 (2) **41.1**	167.4±3.3 **172.0**	(1) Pyrolysis (2) Visible spectroscopy	(1) 1973BAT/MIL (2) 1990MCC/PFA
nitroso-trifluoromethane CF_3–**NO**	(1) 31±3 (2) 42.8±2 (3) **39.9**	129.7±12.6 179.1±8.4 **167**	(1) Electron impact (2) Pyrolysis (3) Visible spectroscopy	(1) 1973CAR/GOW (2) 1979GLA/MAI (3) 1990MCC/PFA
nitroso-trichloromethane CCl_3–**NO**	(1) 32±3 (2) **29.9**	133.9±12.6 **125**	(1) Electron impact (2) Pulse photolysis	(1) 1973CAR/GOW (2) 1995LEY/MAS
nitrosoethane C_2H_5–**NO**	41.0	171.5	Derived from $\Delta_f H^\circ$ in ref.	1994NIST
3-nitroso-1-propene CH_2CHCH_2–**NO**	26.3	110	Flash photolysis	1995BOY/NOZ
2-nitroso-propane iC_3H_7–**NO**	36.5±3	152.7±12.6	Electron impact	1972CAR/GOW
nitroso-tert-butane tC_4H_9–**NO**	(1) 29±3 (2) 39.5±1.5 (3) **39.9**	121.3±12.6 165.3±6.3 **167**	(1) Electron impact (2) VLPP (3) Laser excitation	(1) 1973CAR/GOW (2) 1974CHO/MEN (3) 1986NOB/QUI
2,2-dimethyl-1-nitrosopropane $tBuCH_2$–**NO**	36	150.6	Electron impact	1972CAR/GOW
nitrosobenzene C_6H_5–**NO**	(1) 51.5±1 (2) **54.2±0.5** (3) 52.4±1.4	215.5 **226.8±2.1** 219.2±5.9	(1) VLPP (2) Pyrolysis (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1975CHO/GOL (2) 1997PAR/DYA (3) 1998NIST
nitroso-pentafluorobenzene C_6F_5–**NO**	(1) 62±5 (2) **50.5±1**	259.4±20.9 **211.3±4.2**	(1) Electron impact (2) VLPP	(1) 1973CAR/GOW (2) 1975CHO/GOL
nitrosotoluene $C_6H_5CH_2$–**NO**	29.4	123	Flash Photolysis	1995BOY/NOZ
nitromethyl radical $C^{\bullet}H_2$–NO_2	71.2±3	298±13	Derived	1993CYR/LEA
nitromethane CH_3–NO_2	(1) 60.8 (2) 63.7 (3) 60.8 (4) 62.3±2.3 (5) **62.3±0.5**	254.4 266.5 254.4 260.7±9.6 **260.7±2.1**	(1) Review (2) Electron capture detect. (3) Derived (4) Electron capture detect. (5) Derived from $\Delta_f H^\circ$ in ref.	(1) 1981BAT/ROB (2) 1989CHE/ALB (3) 2000MIR/VOR(a) (4) 2002CHE/CHE (5) 1998NIST
nitroethylene C_2H_3–NO_2	71.5	299.2	Derived from $\Delta_f H^\circ$ in ref.	1999BUR

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** 推荐值; 括号内数字 文献编号) kcal/mol	 kJ/mol	方法	文献
nitroethane C_2H_5–**NO_2**	(1) 58.6 (2) **60.8**	245.2 **254.4**	(1) Review (2) Derived from Δ_fH° in ref.	(1) 1981BAT/ROB (2) 1986PED/NAY
(E)-nitro-propylene-2 $(CH_3)CH{=}CH$–**NO_2**	69.3	290.0	Derived from Δ_fH° in ref.	1999BUR
nitrocyclopropane cyclo-C_3H_5–**NO_2**	70.6	295.4	Derived from Δ_fH° in ref.	1999BUR
1-nitropropane nC_3H_7–**NO_2**	61.3	256.5	Derived from Δ_fH° in ref.	1986PED/NAY
2-nitropropane iC_3H_7-**NO_2**	(1) 59.0 (2) **62.1**	246.9 **259.8**	(1) Review (2) Derived from Δ_fH° in ref.	(1) 1981BAT/ROB (2) 1986PED/NAY
1-nitrobutane nC_4H_9–**NO_2**	(1) 60.9 (2) 61.2	254.8 256.0	Derived from Δ_fH° in ref.	(1) 1986PED/NAY (2) 2002KOS/MIR
2-nitrobutane sC_4H_9–**NO_2**	62.9	263.2	Derived from Δ_fH° in ref.	1986PED/NAY
2-methyl-2-nitropropane tC_4H_9–**NO_2**	(1) 58.5 (2) **61.8** (3) 58.8	244.8 **258.6** (3) 246.0	(1) Review (2) Derived from Δ_fH° in ref. (3) Derived	(1) 1981BAT/ROB (2) 1986PED/NAY (3) 2001MAT/LEB
nitropentane nC_5H_{11}–**NO_2**	(1) 60.4±1.5 (2) 60.2±1.5	252.7±6.3 251.9±6.3	Derived from Δ_fH° in ref.	(1) 1997VER (2) 1999BUR
nitrocyclohexane c-C_6H_{11}–**NO_2**	64.0±1.5	267.8±6.3	Derived from Δ_fH° in ref.	1997VER
nitrohexane nC_6H_{13}–**NO_2**	60.2	251.9	Derived from Δ_fH° in ref.	1999BUR
nitrobenzene C_6H_5–**NO_2**	(1) 71.3±1 (2) 71.4±2 (3) **70.7±1** (4) 71.8	298.3±4.2 298.7±8.4 **295.8±4.2** 300.4	(1) Review (2) VLPP (3) Derived from Δ_fH° in ref. (4) Derived from Δ_fH° in ref.	(1) 1981BAT/ROB (2) 1985GON/LAR (3) 1986PED/NAY (4) 2002KOS/MIR
nitrobenzene, substituted  Y = 3-NH_2 Δ_fH°(3-NH_2-C_6H_4) = 76.5 (320.1) Y = 4-NH_2 Δ_fH°(4-NH_2-C_6H_4) = 78.3 (327.8)	(1) 70.5 (1) 72.2	295.0 302.0	(1) Pyrolysis	(1) 1975MAT/NAS

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 · 文献编号) kcal/mol	 kJ/mol	方法	文献
3-NO_2 $\Delta_f H^\circ$(3-NO_2-C_6H_4) = 81.4±2.4 (340.6±10.0)	(1) 66.5 (2) 73.2±2.4	278.2 306.3±10.0	(2) VLPP	(2) 1985GON/LAR
4-NO_2 $\Delta_f H^\circ$(4-NO_2-C_6H_4) = 72.3 (302.7)	(1) 67.0	280.3		
2-Me $\Delta_f H^\circ$(2-Me-C_6H_4) = 75.3±2.5 (315.1±10.5)	(2) 70.2±2.5	293.7±10.5		
4-Mc $\Delta_f H^\circ$(3-NO_2-C_6H_4) = 70.9±2.3 (296.6±9.6)	(2) 71.4±2.3	298.7±9.6		
3,5-$(NO_2)_2$ $\Delta_f H^\circ$(3,5-$(NO_2)_2$-C_6H_3) = 73.0 (305.4)	(1) 66.0	276.1		
2-Me-4-NO_2 $\Delta_f H^\circ$(2-Me-4-NO_2-C_6H_3) = 70.6±2 (295.4±8.4)	(2) 70.6±2	295.4±8.4		
phenylnitromethane $C_6H_5CH_2$–**NO_2**	(1) 49.0±2.0 (2) 47.0±2.3	205.0±8.4 196.6	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Electron capture detection	(1) 1986PED/NAY (2) 1999CHE/WEL
1-nitronaphthalene 1-naphtyl–**NO_2**	77.3±1.6	323.4±6.7	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-nitroadamantane 	(1) 58.8 (2) **62.2**	246.0 **260.2**	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref.	2002MIR/LEB
dinitromethane $(NO_2)CH_2$ –**NO_2**	(1) 48.8±2.5 (2) 49.5 (3) 52.2	204.2±10.5 207.1 218.4	(1) Review (2) Derived from $\Delta_f H^\circ$ in ref. (3) Derived	(1) 1981BAT/ROB (2) 1986PED/NAY (3) 2000MIR/VOR(a)
1,1-dinitroethane $(CH_3)CH(NO_2)$–**NO_2**	50 5	211.3	Derived	2000MIR/VOR(b)
1,1-dinitropropane $(C_2H_5)CH(NO_2)$–**NO_2**	49 9	208.8	Derived	2000MIR/VOR(b)
2,2-dinitropropane $(CH_3)_2C(NO_2)$–**NO_2**	49.9	208.8	Derived	2000MIR/VOR(b)

续表

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1,1-dinitrobutane $(C_3H_7)CH(NO_2)$–**NO_2**	50.5	211.3	Derived	2000MIR/VOR(b)
1,1-dinitropentane $(C_3H_7)CH(NO_2)$–**NO_2**	49.3	206.1	Derived	2000MIR/VOR(b)
trinitromethane $(NO_2)_2CH$–**NO_2**	(1) 43 7+2.5 (2) 45.1	182 8±10.5 188.7	(1) Review (2) Derived	(1) 1981BAT/ROB (2) 2000MIR/VOR(a)
1,1,1-trinitroethane $(CH_3)(NO_2)_2C$–**NO_2**	42.7	178.7	Derived	2000MIR/VOR(b)
1,1,1-trinitropropane $(C_2H_5)(NO_2)_2C$–**NO_2**	41.9	175.3	Derived	2000MIR/VOR(b)
1,1,1-trinitrobutane $(C_3H_7)(NO_2)_2C$–**NO_2**	41 5	173.6	Derived	2000MIR/VOR(b)
1,1,1-trinitropentane $(C_4H_9)(NO_2)_2C$–**NO_2**	40.7	170.3	Derived	2000MIR/VOR(b)
tetra-nitromethane $(NO_3)_3C$–**NO_2**	(1) 40.5±1 (2) 42.1	169.5±4.2 176.1	(1) Review (2) Derived	(1) 1981BAT/ROB (2) 2000MIR/VOR(a)
1,1,1,2,2,2-hexanitroethane $(NO_2)_3C(NO_2)_2C$–**NO_2**	35.8	149.8	Derived	2000MIR/VOR(b)
2-nitrofuran 	70.4	294.6	Pyrolysis	1987PRO/NAZ
methylamine CH_3–**NH_2**	(1) 85.1±0.5 (2) 86.0	356.1±2.1 359.8	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived	(1) 1986PED/NAY (2) 2001KOS/MIR
difluoro(trifluoromethyl)-amine **CF_3**–NF_2	67.1	280.7	Derived from $\Delta_f H^\circ$ in ref.	1977PED/RYL
acetaldimine C_2H_3–**NH_2**	102.1	427.2	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/LIE
ethylamine C_2H_5 **NH_2**	84.2±1.5	352.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclopropylamine c-C_3H_5–**NH_2**	92.8±0.6	388.3±2.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-propylamine nC_3H_7–**NH_2**	85.1±0.7	356.1±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
2-propylamine iC_3H_7 **NH_2**	85.5±0.9	357.7±3.8	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
cyclobutylamine c-C_4H_7–**NH_2**	86.0±1.2	359.8±5.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
1-butylamine nC_4H_9–**NH_2**	85.1±0.7	356.1±2.9	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (**黑体**：离解原子或原子团)	BDEs (**黑体** 推荐值，括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
2-butylamine sC_4H_9–**NH_2**	85.8±0.7	359.0±2.9	Derived from Δ_fH° in ref.	1986PED/NAY
iso-butylamine iC_4H_9-**NH_2**	84.8±1.2	254.8±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
2-methyl-2-propylamine tC_4H_9-**NH_2**	85.0±1.5	355.6±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
cyclopentyamine c-C_5H_9-**NH_2**	82.9±1.2	346.9±5.0	Derived from Δ_fH° in ref.	1986PED/NAY
2-pyridylamine pyridin-2-yl-**NH_2**	103.0	431.0	Derived from Δ_fH° in ref.	1988LIA/BAR
3-pyridylamine pyridin-3-yl-**NH_2**	104.0	435.1	Derived from Δ_fH° in ref	1988LIA/BAR
4-pyridylamine pyridin-4-yl-**NH_2**	107.0	447.7	Derived from Δ_fH° in ref.	1988LIA/BAR
aniline or benzenamine C_6H_5–**NH_2**	102.6±1.0	429.3±4.2	Derived from Δ_fH° in ref.	1986PED/NAY
cyclohexylamine c-C_6H_{11}–**NH_2**	87.6±1.5	366.5±6.3	Derived from Δ_fH° in ref.	1986PED/NAY
benzylamine $C_6H_5CH_2$–**NH_2**	(1) 71.1±1 (2) **72.0±1.8** (3) 72.9±1, at 0K	297.5±4.2 **301.2±7.5** 305±4	(1) VLPP (2) Derived from Δ_fH° in ref. (3) Shock tube	(1) 1972GOL/SOL (2) 1986PED/NAY (3) 2002SON/GOL
α-methylbenzylamine $C_6H_5CH(CH)_3$–**NH_2**	71.9±2	300.8±8.4	Derived from Δ_fH° in ref.	1999VER
α,α-dimethylbenzylamine $C_6H_5C(CH_3)_2$-**NH_2**	71.2±2	301.9±8.4	Derived from Δ_fH° in ref.	1999VER
1-naphthylamine 1-naphtyl–**NH_2**	102.8±2	430.1±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
2-naphthylamine 2-naphtyl-**NH_2**	108.3±2	453.1±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
formamide HC(O) –**NH_2**	100.8±2	421.7±8.4	Derived from Δ_fH° in ref.	2002CRC
acetamide $CH_3C(O)$ –**NH_2**	99.1±2	414.6±8.4	Derived from Δ_fH° in ref.	2002CRC
2,2-bis(difluoroamino) propane $(CH_3)_2(NF_2)C$–**NF_2**	(1) ~47 (2) **47.8**	~196.6 **200.0**	(1) Pyrolysis (2) Pyrolysis/ FTIR	(1) 1993FOK/GRE (2) 2002PAR/CHA
methyl hydrazine CH_3-**$NHNH_2$**	70.7±2.5	295.8±10.5	Derived from Δ_fH° in ref.	1986PED/NAY
phenyl hydrazine C_6H_5-**$NHNH_2$**	88.6±2.5	370.7±10.5	Derived from Δ_fH° in ref.	1986PED/NAY

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
N,N,N'N'-methyl-methanediamine $(CH_3)_2N$-$CH_2N(CH_3)_2$	55.6±3	232.6±12.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
dimethylamine CH_3–$NHCH_3$	(1) 82.2±2.5 (2) 81 9	343.9±10.5 342.7	Derived	(1) 1982MCM/GOL (2) 2001KOS/MIR
ethyl methylamine C_2H_5–$NHCH_3$	79.8±1	333.9±4.2	Derived	1982MCM/GOL
phenyl methylamine C_6H_5–$NHCH_3$	100.6±2.5	420.9±10.5	Derived	1982MCM/GOL
benzyl methylamine $C_6H_5CH_2$–$NHCH_3$	68.7±2	287.4±8.4	VLPP	1972GOL/SOL
N-methyl acetamide $CH_3C(O)$ –$NHCH_3$	100.9	422.2	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
trimethylamine CH_3–$N(CH_3)_2$	(1) 75.5±2.5 (2) **78.6±2** (3) 79.3	315 9±10.5 328 9 331.8	(1) Derived (2) Derived from $\Delta_f H^\circ$ in ref. (3) Derived	(1) 1982MCM/GOL (2) 1998NIST (3) 2001KOS/MIR
ethyl dimethylamine C_2H_5- $N(CH_3)_2$	72.3±2	302.5±8.4	Derived	1982MCM/GOL
1,1-dimethylhydrazine CH_3–$N(CH_3)NH_2$	90	377	Pyrolysis	1964EBE
phenyl dimethylamine C_6H_5- $N(CH_3)_2$	93.2±2.5	389.9±10.5	Derived	1982MCM/GOL
benzyl dimethylamine $C_6H_5CH_2$–$N(CH_3)_2$	(1) 62.1±2.5 (2) **66.8**	259 8±10.5 **279.5**	(1) VLPP (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1972GOL/SOL (2) 1999VER
1-methylpyrrile CH_3-pyrrol-1-yl	81.3±2	340.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
N-methylaniline CH_3–NHC_6H_5	(1) **71.4±2** (2) 68.9	**298.7±8.4** 288.3	(1) VLPP (2) Pyrolysis	(1) 1978COL/BEN (2) 1990BEC/DOG
N-ethylaniline C_2H_5 -NHC_6H_5	(1) 73.3±2 (2) **70.9±2**	306 7±8.4 **296.6±8.4**	Derived from $\Delta_f H^\circ$ in ref.	(1) 1986PED/NAY (2) 1997VER(b)
diphenylamide C_6H_5–NHC_6H_5	87.4	365.7	Derived from $\Delta_f H^\circ$ in ref.	1969BEN/CRU
N-benzylaniline $PhCH_2$--NHC_6H_5	57.6	241.0	Derived from $\Delta_f H^\circ$ in ref.	1997VER(b)
N,N'-methylaniline CH_3 $N(CH_3)C_6H_5$	70.8	296.2	VLPP	1978COL/BEN
dimethyl phenylamine $C_6H_5(CH_3)N$–CH_3	70.8±2	296.2±8.4	VLPP	1978COL/BEN
dimethyl benzylamine $(CH_3)_2N$–CH_2Ph	62.1±2	259.8±8.4	VLPP	1972GOL/SOL
azomethane CH_3–N_2CH_3	52.5	219.7	Pyrolysis	1970BEN/ONE

续表

断裂键 (**黑体** - 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
azohexafluoroethane **CF_3**–N_2CF_3	55.2	231.0	Pyrolysis	1970BEN/ONE
azoethane **C_2H_5**–$N_2C_2H_5$	50	209.2	Pyrolysis	1970BEN/ONE
azoisopropane **iC_3H** –$N_2iC_3H_7$	47.3	197.9	Pyrolysis	1970BEN/ONE
azobutane **nC_4H_9**–$N_2nC_4H_9$	50	209.2	Pyrolysis	1970BEN/ONE
azoisobutane **iC_4H_9**–$N_2iC_4H_9$	49	205.0	Pyrolysis	1970BEN/ONE
azo-2-butane **sC_4H_9**–$N_2sC_4H_9$	46.7	195.4	Pyrolysis	1970BEN/ONE
azotertbutane **tC_4H_9**–$N_2tC_4H_9$	43.5	182.0	Pyrolysis	1970BEN/ONE
azobenzene **C_6H_5**–$N_2C_6H_5$	82.3±1.2	344.4±4.8	Photoionization	2001CHE/ZHA
azotoluene **$C_6H_5CH_2$**–$N_2CH_2C_6H_5$	37.6	157.3	Pyrolysis	1970BEN/ONE
p-hydroxyazobenzene **p-OH–$C_6H_4N_2$**–C_6H_5	48.0±1.2	200.7±4.8	Photoionization	2001CHE/ZHA
p-aminoazobenzene **p-NH_2 $C_6H_4N_2$**–C_6H_5	63.0±2.3	263.4±9.6	Photoionization	1999WU/SHE
formamide **HC(O)** –NH_2	99.0	414.2	Derived from Δ_fH° in ref.	1998NIST
acetamide **$CH_3C(O)$** –NH_2	99.1	414.6	Derived from Δ_fH° in ref.	1998NIST
N-methyl-acetamide **$CH_3C(O)$** –$NH(CH_3)$	100.9	422.2	Derived from Δ_fH° in ref.	1998NIST
propanamide **$C_2H_5C(O)$** –NH_2	98.7	413.0	Derived from Δ_fH° in ref.	1998NIST
benzamide **$C_6H_5C(O)$** –NH_2	96.4	403.3	Derived from Δ_fH° in ref.	1998NIST
N,N-dimethyl-propanamide **$C_2H_5C(O)$** –$N(CH_3)_2$	89.9	376.1	Derived from Δ_fH° in ref.	1998NIST
1-(dimethylamino)-2-propanone **$CH_3C(O)CH_2$**–$N(CH_3)_2$	72.7	304.2	Derived from Δ_fH° in ref.	1998NIST
methylnitroamine **CH_3**–$NHNO_2$	71.0	297.1	Derived	2001KOS/MIR
dimethylnitroamine **CH_3**-$N(CH_3)NO_2$	69.8	292.0	Derived	2001KOS/MIR
methyl((methylnitroamino)-methyl)nitroamine $CH_3N(NO_2)CH_2$–**$N(NO_2)CH_3$**	70.1	293.3	Derived	2001KOS/MIR

续表

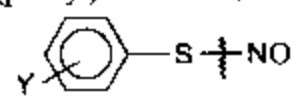
断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitrozoamines $\mathbf{(NO_2)_3CCH_2}$-$N(NO_2)H_2C(NO_2)_3$	53.5	223.8	Derived	2001MIR/KOS
$\mathbf{(NO_2)_2CHCH_2}$–$N(NO_2)$– $CH_2CH(NO_2)_2$	59.0	246.9		
$\mathbf{(NO_2)_3CCH_2}$–$N(NO_2)$– $CH_2CH_2C(NO_2)_3$	64.0	267.8		
$\mathbf{(NO_2)_3CCH_2}$–$N(NO_2)$– $CH_2N(NO_2)CH_2C(NO_2)_3$	52.6	220.1		
$\mathbf{(NO_2)_2CHCH_2}$-$N(NO_2)$– $(CH_2)_2N(NO_2)CH_2CH(NO_2)_2$	57.9	242.3		
$\mathbf{(NO_2)_3CCH_2}$–$N(NO)$- $CH_2C(NO_2)_3$	53.3	223.0		
$\mathbf{(NO_2)_3CCH_2}$ $N(NO)$– $(CH_2)_2N(NO)CH_2C(NO_2)_3$	49.5	207.1		
bis(1,1-dimethyl-silacthyl)-methylamine $\mathbf{CH_3}$–$N(SiMe_3)_2$	87	364	Derived	1998BEC/WAL
methyl isocyanide CH_3–**NC**	101.5±2.2	424.7±9.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl isocyanide C_2H_5–**NC**	100.1±1.7	418.8±7.1	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
amonomethanenitrile H_2N–**CN**	118.8±3	497.1±12.6	Derived from $\Delta_f H^\circ$ in ref.	2001BIS/HOO
carboxamide **HC(O)**–NH_2	98.5	412.1	Derived from $\Delta_f H^\circ$ in ref.	1988LIA/BAR
acetamide $\mathbf{CH_3C(O)}$–NH_2	99.9	418.0	Derived from $\Delta_f H^\circ$ in ref.	1969BEN/CRU
N,N-dimethylformamide **HC(O)**–$N(CH_3)_2$	93.7±2	392.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
N,N-dimethylacetamide $\mathbf{CH_3C(O)}$–$N(CH_3)_2$	91.4	382 4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
N-(aminocarbonyl)acetamide **HC(O)**–$NHC(O)NH_2$	115.6±2	483.7±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
N-methylglycine or sarcosine $\mathbf{HO(O)CCH_2}$–$NHCH_3$	72.3±2	302.5±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
o-aminino-benzeneacetic acid $\mathbf{HO(O)CCH_2}$–NHC_6H_5	63.1±2	264 0+8 4	Derived from $\Delta_f H^\circ$ in ref.	1998NIST

续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
methanisothiocyanate CH_3-**NCS**	75.5	315.9	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
CH_3–**NHC$^\bullet$H$_2$**	20.6±3	86.2±12.6	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
CH_3–**N(CH$_3$)C$^\bullet$H$_2$**	12.9±3	54.0±12.6		
C_6H_5–**N(CH$_3$)C$^\bullet$H$_2$**	26.3±3	110.0±12.6		

8.4 N—S键能

表 8.4 N—S BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitrothiol HS–**NO**	33.2	138.9	Derived from $\Delta_f H^\circ$ in ref.	1984BLA/PAT
(nitrothio)methyl acetate $CH_3C(O)OCH_2S$–**NO**	19.1	80	AOP	2000LU/ZHU
methylnitrosothio CH_3S–**NO**	25±1	104.6±4 2	Review	1978BEN
(tert-butyl)nitrosothio t-BuS–**NO**	27.5	115.1	AOP	2001LU/WIT
(hexyl)nitrosothio $CH_3(CH_2)_5S$–**NO**	28.9±0.3	120.9±1.3	Pyrolysis	2001BAR/MAN
(cyclohexyl)nitrosothio c-$C_6H_{11}S$–**NO**	31.6±0.8	132.2±3.3	Pyrolysis	2001BAR/MAN
(benzyl)nitrosothio $PhCH_2S$–**NO**	28.8	120.5	AOP	2001LU/WIT
(triaryl)nitrosothio $(Ar)_3S$–**NO**	29±1	121.3±4.2	Review	1978BEN
(phenyl)nitrosothio, substituted 				
Y – H	(2) 19.4±1.3	81.2±5.4	AOP	(1) 2000LU/ZHU
2-Cl	(2) 19.3±1.5	80.8±6 3		(2) 2001LU/WIT
3-Cl	(2) 20.9±1.4	87.4±5.9		

续表

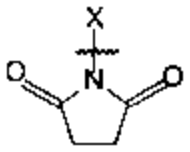
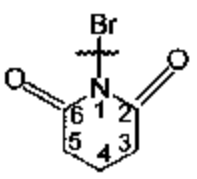
断裂键 (**黑体** - 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
4-Cl	(2) 19.2±1.4	80.3±5.9		
2-Me	(1) 17.2±1.4	72±5.9		
3-Me	(2) 19.9±1.2	83.3±5.0		
4-Me	(2) 21.4±1.2	89.5±5.0		
4-MeO	(2) 21.0±1.9	87.9±7.9		
4-NO_2	(2) 18.6±1.5	77.8±6.3		
thiazyl thifluoride **N**≡SF_3	93±3	389.1±12.6	Calorimetry	1970OHA/HUB
thiazyl fluoride **N**≡SF	71±5	297±21	Calorimetry	1970OHA/HUB
phenylphenylthiodiazene **Ph**N=N-SPh	29±1	121.3±4.2	Review	1978BEN
thiocyanogen **SCN**–SCN	61.1	255.6	Derived from $\Delta_f H^\circ$ in ref.	1998CHA

8.5 N—X(卤)键能

表 8.5 N—X(卤)BDEs

断裂键 (**黑体** = 离解原子)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitrosyl fluoride **F**–NO	56.23	235.26	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
nitryl fluoride **F**–NO_2	52.9	221.3	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
nitrogen trifluoride **F**–NF_2	(1) 60.7	254.0	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1998CHA
F–NF	(1) 58.8	246.0		
F–N	(2) 82.0	343.1	(2) Spectroscopy	(2) 1979HUB/HER
fluoroamine **F**–NH_2	68.5	286.6	Derived from $\Delta_f H^\circ$ in ref.	1994NIST
difluoroamine **F**–NHF	70.4	294.6	Derived from $\Delta_f H^\circ$ in ref.	1989GUR/VEY

续表

断裂键 (**黑体** = 离解原子)	BDEs (**黑体** = 推荐值. 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
nitrosyl chloride **Cl**–NO	38.0±0.2	158.8±0.8	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
nitryl chloride **Cl**–NO_2	33.9±0.3	141.8±1.3	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
nitrogen chlorofluoride **Cl**–NF_2	~ 32	~133.9	Kinetics	1967PET
chloramide **Cl**–NH_2	60.5	253.1	Derived from $\Delta_f H^\circ$ in ref.	1994NIST
chlorine azide **Cl**–N_3	51.7±2.3	216.1±9.6	Photolysis	2003HAN/WOD
nitrosyl bromide **Br**–NO	28.7±0.2	120.1±0.8	Derived from $\Delta_f H^\circ$ in ref.	2003NASA/JPL
nitryl bromide **Br**–NO_2	19.6±1.7	82.0±7.1	Resonance fluorescence	1991KRE/NIC
nitrogen bromofluoride **Br**–NF_2	<54.3	<227.2	Kinetics	1972CLY/CON
nitrosyl iodide **I**–NO	(1) 18.6±0.1 (2) 18.1±1	77.8±0.4 75.6±4	(1) UV spectrom. (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1981FOR/HIP (2) 2003NASA/JPL
nitryl iodide **I**–NO_2	(1) 18.3±1.0 (2) 19.0±1	76.6±0.4 79.6±4	(1) Spectroscopy (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1976VAN/TRO (2) 2003NASA/JPL
N-halogenosuccinimide 				
X = Cl	(1) 73±4	305.4±16.7	Electrochemical	(1) 1993LIN/JON
Br	(2) 66±2	276.1±8.4		(2) 1998LIN/MER
1-bromo-2,6-piperidione 	65±2	272.0±8.4	Electrochemical	1998LIN/MER

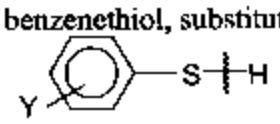
第 9 章　S—X 键能

9.1　S—H 键能

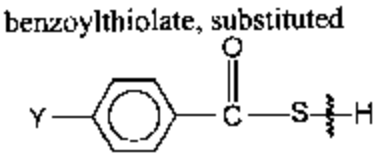
表 9.1　S—H BDEs

断裂键 (**黑体** = 离解原 *f*) $\Delta_f H^\circ$(R)/ kcal (kJ)	BDEs (**黑体** = 推荐值， 括号内数字 - 文献编号) kcal/mol	kJ/mol	方法	文献
oxythio radical **H**–SO	41.3	172.8	Kinetics	1978WIII/GAR
oxythio **H**–SOH	79±3.5	330.5±14.6	Ion flow tube	1993OHA/DEP
hydrogen sulfide **H**S–H $\Delta_f H^\circ$(R) = 34.2±0.2 (143.0±0.8)	(1) 91.1±1 (2) 91.2±0.7 (3) 91.2±0.7 (4) **91.2±0.1** (5) 91.10±0.01	381.2±4.2 381.6±2.9 381 6±2.9 **381.4±0.5** 381.18±0.05	(1) Iodination (2) Resonance fluorescence (3) Recommend (4) Photolysis (5) Spectroscopy	(1) 1979HWA/BEN (2) 1992STI/NIC (3) 1994BER/ELL (4) 1996WIL/HOW (5) 2000SHI/HU
S–H	(6) 83.4 (7) **84.4±0.7** (8) 82.3±2.3 (9) 84.6±1.0	349.1 **353.1±2.9** 344.3±9.6 353.9±4.3	(6) PIMS (7) Photodissoc. (8) Spectroscopy (9) Derived	(6) 1986GIB/GRE (7) 1991CON/BAL (8) 2002CRC (9) 2000REM/ERV
methylthiol **H** SCH_3 $\Delta_f H^\circ$(R) = 29.8±0.4 (124.7±1.7)	(1) 88.1 (2) 86.4±2.2 (3) 87.4 (4) **87.4±0.5** (5) 87.0±0.4	368.6 361.5±9.2 365.7 **365.7±2.1** 364.0±1 7	(1) VLPP (2) PFS (3) Resonance fluorescence (4) Recommend. (5) Photolysis	(1) 1977COL/BEN(b) (2) 1987MOR/ELL (3) 1992NIC/KRE (4) 1994BER/ELL (5) 1999BIS/CHO
H SCD_3	(6) 88.3±2	369 4±8.4	(6) Electron photodetach.	(6) 1980JAN/REE
ethene-1-thiol **H**–$SCHCH_2$	84±2	351.5±8.4	Review	1978BEN
ethylthiol **H**–SC_2H_5 $\Delta_f H^\circ$(R) = 24.1 (101)	(1) 88.6±2 (2) **87.3**	370.7±8.4 **365.3**	(1) Electron photodetach. (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1980JAN/REE (2) 1986PED/NAY

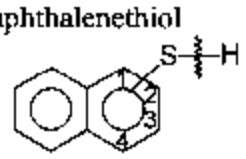
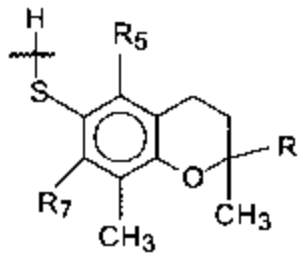
续表

断裂键 (黑体 = 离解原子) $\Delta_f H^\circ$(R)/ kcal (kJ)	BDEs (黑体 - 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
propylthiol **H**–SC_3H_7 $\Delta_f H^\circ$(R) = 19.1 (80)	(1) 88.6±2 (2) **87.4**	370.7±8.4 **365.7**	(1) Electron photodetach. (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1980JAN/REE (2) 1986PED/NAY
iso-propylthiol **H**–S–iC_3H_7 $\Delta_f H^\circ$(R) = 17.9±2 (74.9±8.4)	88.4±2	369.9±8.4	Electron photo-detach.	1980JAN/REE
tert-butylthiol **H**–S–tC_4H_9 $\Delta_f H^\circ$(R) = 10.5±2 (43.9±8.4)	(1) 88.6±2 (2) 86.6±2.2	370.7±8.4 362.3±9.2	(1) Electron photo-detach. (2) GPA	(1) 1980JAN/REE (2) 2003REE/HAR
alkyl thiol **H**–SR	87.4	365.7	Review	1992NIC/KRE
thioacetic acid **H**–$SCOCH_3$	88.6	370.7	Electrochemical	1999ZHA/LIN
thiobenzoic acid **H**–SCOPh	87	364.0	Pulse radiolysis	1998ZHA/LIN
methanedisulfide **H**–$SSCH_3$	79±3.5	330.5±14.6	Ion flow tube	1993OHA/DEP
benzenethiol PhS–**H** $\Delta_f H^\circ$(R) = 58.0±1 1 (242.7±4.6)	(1) 83.3±2 (2) 79.4 (3) 80 (4) 80.8 (5) **83.5±1.1**	348.5±8.4 332.2 334.7 338.1 **349.4±4.5**	(1) VLPP (2) AOP (3) AOP (4) Correlation (5) TR-PAC	(1) 1982MCM/GOL (2) 1992VEN/AMA (3) 1996ARM/SUN (4) 2000DEN/DEN (5) 2002SAN/MUR
benzenethiol, substituted 				
Y – 2-Cl	(1) 80.0	334.7	(1) AOP	(1) 1994BOR/ZHA(b)
3-Cl	(1) 80.1 (4) 80.3	335 1 335.8	(2) AOP (3) AOP	(2) 1992VEN/AMA (3) 1997ZHU/ZHA
4-Cl	(1) 79.2 (4) 79.9 (5) 86.1±0.8	331.4 334.1 360.4±3.5	(4) Correlation (5) TR-PAC	(4) 2000DEN/DEN (5) 2002SAN/MUR
4-Br	(1) 79.3 (2) 80.2	331.8 335.6		
4-NH_2	(1) 69.8 (2) 70.0	292.0 292.9		
2-Me	(1) 78.8	329.7		

续表

断裂键 (黑体　离解原子) $\Delta_f H^0$(R)/ kcal (kJ)	BDEs (黑体 = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
3-Me	(1) 78.9	330.1		
	(4) 80.8	338.1		
4-Me	(1) 78.3	327.6		
	(2) 77.8	325.5		
	(3) 78.4	328 0		
	(4) 80.0	334.8		
	(5) 84.8±1.0	354.9±4.1		
4-MeO	(1) 76 9	321.7		
	(2) 76.2	318.8		
	(3) 78.6	328.9		
	(4) 78.7	329.3		
	(5) 83.3±1.0	348.5±4.0		
3-CF_3	(4) 80.8	338.1		
4-CF_3	(1) 80.9	338.5		
	(5) 86.0±0.9	359.9±3.9		
2-$MeCO_2$	(1) 78.7	329.3		
4-NO_2	(1) 81 4	340.6		
	(2) 81.6	341.4		
4-OH	(2) 76.0	318.0		
4-EtO	(4) 78.8	329.6		
4-tBu	(4) 80.7	337.7		
2,4,6-Me_3	(4) 80.4	336.6		
benzoylthiolate, substituted 				
Y = H	**87.4**	365.7	AOP	2000ZHA/LIN
CH_3	87	364.0		
CH_3O	87	364.0		
CF_3	86	359.8		
CN	86	359.8		

续表

断裂键 (**黑体** = 离解原 f) $\Delta_f H^\circ$(R)/ kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 文献编号) kcal/mol	kJ/mol	方法	文献
phenylmethane-1-thiol $PhCH_2S$–**H** $\Delta_f H^\circ$(R) = 58.9 (246.4)	(1) 86.9 (2) 87.8	363.6 367.4	(1) AOP (2) Correlation	(1) 1994BOR/ZHA(b) (2) 1996DEN
naphthalenethiol  H-S at site 1	(2) 78.5	328.4	(1) AOP	(1) 1994BOR/ZHA(b)
2	(1) 77.9 (2) 78.1	325.9 326.8	(2) Correlation	(2) 2000DEN/DEN
thio-α-tocopherol  R = $CH_2(CH_2CH_2CH(CH_3))_3H$	80.0	334.7	Correlation	2000DEN/DEN
hydrogen disulfide radicals **H**–SS ·	55.2±4	231.0±16.7	Derived from $\Delta_f H^\circ$ in ref.	1993OHA/DEP
hydrogen disulfide **H**–SSH $\Delta_f H^\circ$(R) = 27.6±3.5 (115.5±14.6)	76±3.5	318.0±14.6	Ion flow tube	1993OHA/DEP
hydrogen alkyl disulfide **H**–SSR	70±1.5	292.9±6.5	Review	1978BEN
hydrogen trisulfide **H**–SSSH	70±1.5	292.9±6.5	Review	1978BEN
hydrogen polysulfide $H–S_{3-n}H$	70±1.5	292.9±6.5	Review	1978BEN
hydrogen alkyl polysulfide $H–S_{3-n}R$	70±1.5	292.9±6.5	Review	1978BEN
H–SCN	≤93.3±1.1	≤390.4±4.6	PIMS	1994RUS/BER(b)
H- $SC^{\bullet}H_2$	44.1±2.5	184.5±10.5	Derived from $\Delta_f H^\circ$ in ref.	1998NIST

9.2 S—S 键能

表 9.2 S—S BDEs

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
disulfur **S–S**	101.65	425.30	Spectroscopy	1979HUB/HER
trisulfur **S**–S_2	62.5±1.8, at 0 K	261.5±7.7	Derived	2003KRE/SCH
disulfur oxide **S**=SO	80.9	338.5	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
hydrogen disulfur **S**=SH_2	51±7	213.4±29	Review	1978BEN
difluoro disulfur **S**=SF_2	>57±8	>238.5±34	Review	1978BEN
dimethyl disulfur **S**=SMe_2	53±4	221.8±17	Review	1978BEN
hydrogen disulfide **HS**–SH	64.7±1	270.7±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
difluorodisulfane **FS**–SF	86.6	362.3	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
difluorodisulfane **ClS**–SCl	78.8	329.7	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
methanehydrodifulfide CH_3S–**SH**	65.0	272.0	Derived	1999ARM
alkylhydrodifulfide RS–**SH**	65.2	272.8	Derived	1999ARM
phenyl hydrodisulfide **PhS**–SH	61±1.5	255.2±6.3	Derived	1978BEN
dimethyl disulphide CH_3S-SCH_3	(1) 64 (2) 62.9±2.6 (3) **65.2±0.9**	267.8 263±11 **272.8±3.8**	(1) Electrochem. (2) Mol. beam (3) Resonance fluorescence	(1) 1992NUZ (2) 1988PEN/CAO (3) 1992NIC/KRE
diethyl disulphide C_2H_5S–SC_2H_5	66 1	276.6	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
dipropyl disulphide C_3H_7S–SC_3H_7	66.2	277.0	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
dibutyl disulphide *n*-C_4H_9S–S–*n*-C_4H_9	72	301	AOP	1991BAU/FAS
dialkyl disulphide **RS**–SR	66.2	277.0	Derived	1999ARM
methyl phenyl disulphide **MeS**–SPh	65±1.5	272.0±6.3	Derived	1978BEN

续表

断裂键 (**黑体** – 离解原子 或原子团)	BDEs (**黑体**：推荐值； 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
diphenyl disulphide C_6H_5S–SC_6H_5	(1) 47 (2) **51.2±3** (3) 55±2	196.6 **214.2±12.6** 230±8.4	(1) Electrochem. (2) Derived from $\Delta_f H^\circ$ in ref. (3) AOP	(1) 1992NUZ (2) 1986PED/NAY (3) 1991BAU/FAS
hydrogen trisulfide **HS**–SSH	50±2	209.2±8.4	Derived	1978BEN
methyl hydrotrisulfide CH_3S–SSH	54±2	225.9±8.4	Derived	1978BEN
alkyl hydrotrisulfide **RS**–SSH	54±2	225.9±8.4	Derived	1978BEN
phenyl hydrotrisulfide **PhS**–SSH	44±2	184.1±8.4	Derived	1978BEN
hydrogen tetrasulfide **HSS**–SSH	33.6±2	140.6±8.4	Derived	1978BEN
methyl methyl disulfanyl dissulfide **MeSS**–SSMe	32.9	137.7	Derived	1986HAW/GRI
ethyl ethyl disulfanyl dissulfide **EtSS**–SSEt	32.8	137.2	Derived	1986HAW/GRI
iso-propyl iso-propyl disulfanyl dissulfide **iPrSS**–SSiPr	32.0	133.9	Derived	1986HAW/GRI
tert-butyl tert-butyl disulfanyl dissulfide **tBuSS**- SStBu	32.4	135.6	Derived	1986HAW/GRI
dialkyl tetrasulfide **RSS**–SSR	33.6±2	140.6±8.4	Derived	1978BEN
dialkyl polysulfide RS_{2+n}–$S_{2-m}R$	33.6±2	140.6±8.4	Derived	1978BEN
hydro disulphide radicals **HS**–S ·	79±1	330.5±4.2	Derived	1978BEN
methyl disulphide radicals CH_3S–S ·	83±1	347.3±4.2	Derived	1978BEN
phenyl disulphide radicals **PhS**–S ·	74±1.5	309.6±6.3	Derived	1978BEN
alkyl trisulphide radicals **RSS**–S ·	63±1	263.6±4.2	Derived	1978BEN
alkyl tetrasulphide radicals **RSS**–S_2 ·	47.5±1	198.7±4.2	Derived	1978BEN
dialkyl disulfide ions (**RS**–SR′)$^{+\cdot}$ R = Me R′ = Me	(1) 26.5±0.5 (2) 27.5	(1) 111±2 (2) 115	(1) Equilibrium (2) FT-ICR	(1) 1995DEN/ILL (2) 1998VIS/BIC

续表

断裂键 (**黑体** = 离解原子 或原子团)		BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
		kcal/mol	kJ/mol		
Me	Et	(2) 26.8	112		
Et	Et	(1) 27.5±0.7 (2) 27.5 (3) 27.5±2.3	(1) 115±3 (2) 115 (3) 115±10	(3) FT-ICR	(3) 1996VIS/KON
Et	n-Pr	(2) 25.6	107		
n-Pr	n-Pr	(2) 24.6 (3) 23.3±2.3	(2) 103 (3) 97±10		
i-Pr	i-Pr	(2) 33.5	140		
n-Bu	n-Bu	(2) 23.2 (3) 21.2±2.3	(2) 97 (3) 89±10		
tetradialkyl disulfide ions (R_2SS-SSR_2')' R = Me R' = Me		27.5, at 0 K	115	Equilibrium	1996JAM/ILL
Me	Et	25.6, at 0 K	107		
Et	Et	28.7, at 0 K	120		
n-Pr	n-Pr	~29.4, at 0 K	~123		

9.3 S—C 键能

表 9.3 S—C BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** 推荐值; 括号内数字 - 文献编号)		方法	文献
	kcal/mol	kJ/mol		
carbon monosulfide S–C	170.7±0.3	714.1±1.2	MS	2002CRC
carbon disulfide S=CS	(1) 102.9±3, at 0K (2) 103.8±0.9, at 0 K (3) **94.2**	430.5±12.6 434.3±3.8 **394.1**	(1) MS (2) GIB MS (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1980MIL/ERE (2) 1991PRI/ARM (3) 2002CRC
carbon oxysulfide S=CO	73.7	308.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
thioformaldehyde $S=CH_2$	131.2	548.9	Derived from $\Delta_f H^\circ$ in ref.	1998NIST

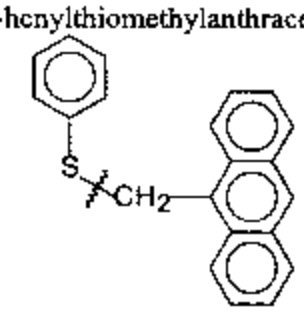
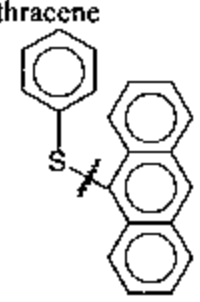
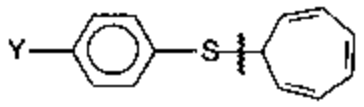
续表

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
(methylamino)methanethial **S**=CNCH$_3$	71	297	Review	1978BEN
methylthio radical **CH$_3$**–S •	70.2±0.3	293.8±1.4	Photodissoc.	1999BIS/CHO(b)
methanethiol HS–CH$_3$	(1) 75±1.5 (2) **74.7±1**	313.8±6.3 **312.5±4.2**	(1) Review (2) Resonance fluorescence	(1) 1978BEN (2) 1992NIC/KRE
ethene-1-thiol **HS**–C$_2$H$_3$	83±3	347.3+12.6	Review	1978BEN
ethanethiol **HS**–C$_2$H$_5$	73.6±0.5	307.9±2.1	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
1-propanethiol **HS**–nC$_3$H$_7$	74.2±0.7	310.5±2.9	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
2-propanethiol **HS**–iC$_3$H$_7$	73.4±0.9	307.1±3.8	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
1-butanethiol **HS**–nC$_4$H$_9$	73.9±0.7	309.2±2.9	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
2-butanethiol **HS**–sC$_4$H$_9$	73.5±0.7	307.5±2.9	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
2-methyl-1-propanethiol **HS**–iC$_4$H$_9$	74.1±1.1	310.0±4.6	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
2-methyl-2-propanethiol **HS**–tC$_4$H$_9$	72.0±0.9	301.2±3.8	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
cyclopentanethiol **HS**–c-C$_5$H$_9$	71.0±1.2	297.1±5.0	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
1-pentanethiol **HS**–nC$_5$H$_{11}$	73.5±1.5	307.5±6.3	Derived from $\Delta_f H°$ in ref.	2002CRC
2-methyl-2-butanethiol **HS**–C(CH$_3$)$_2$(C$_2$H$_5$)	71.6±1.5	299.6±6.3	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
2,2-dimethyl-1-propanethiol **HS**–neoC$_5$H$_{11}$	73.7±2.0	308.4±8.4	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
1-hexanethiol **HS**–nC$_6$H$_{13}$	73.2±1.5	306.3±6.3	Derived from $\Delta_f H°$ in ref.	2002CRC
benzenethiol **HS**–C$_6$H$_5$	86.2±1.5	360.7±6.3	Derived from $\Delta_f H°$ in ref.	1998NIST
cyclohexanethiol **HS**–cC$_6$H$_{11}$	72.9±1.4	305.0±5.9	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
benzenemethanethiol **HS**–CH$_2$C$_6$H$_5$	60.4±1.8	252.7±7.5	Derived from $\Delta_f H°$ in ref.	1986PED/NAY
methanethioic S-acid **HS**–C(O)H	74±2	309.6±8.4	Review	1978BEN
ethanethioic S-acid **HS**–C(O)CH$_3$	73.6±1.5	307.9±6.3	Derived from $\Delta_f H°$ in ref.	2002CRC

续表

断裂键 (**黑体** 离解原子 或原子团)	BDEs (**黑体** - 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
dimethyl sulphide **CH_3S** CH_3	(1) 77.2±2 (2) **73.6±0.8**	323.0±8 4 **307.9±3.3**	(1) Pyrolysis (2) Resonance fluorescence	(1) 1977COL/BEN (2) 1992NIC/KRE
ethyl methyl sulphide **CH_3S**–C_2H_5	72.4±1	302.9±4.2	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl methyl sulphide **C_2H_5S**–CH_3	73.4±1.5	307.1±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methyl propyl sulphide **CH_3S** C_3H_7	73.3±1.5	306.7±6.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methyl propyl sulphide **C_3H_7S**–CH_3	73.9±1.5	309.2±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
iso-propyl methyl sulphide **CH_3S**–iC_3H_7	72.4±1.5	302.9±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
butyl methyl sulphide **CH_3S**–C_4H_9	72.8±1.5	304.6±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
tert-butyl methyl sulphide **CH_3S**–tC_4H_9	70.4±1.5	294.6±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl propyl sulfide **C_2H_5S** C_3H_7	72.9±1.5	305.0±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
ethyl propyl sulfide **C_3H_7S**–C_2H_5	72.5±1.5	303.3+6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
ethyl isopropyl sulfide **C_2H_5S** iC_3H_7	73.4±1.5	307.1±6.3	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
cyclopentyl methyl sulphide **CH_3S**–c-C_5H_9	70.6±1.5	295.4±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methyl pentyl sulphide **CH_3S**–C_5H_{11}	71.9±1.5	300 8±6 3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
diethyl sulphide **C_2H_5S**–C_2H_5	72.5±1.5	303.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl butyl sulphide **C_2H_5S**-C_4H_9	73.0±1.5	305.4±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
tert-butyl ethyl sulphide **C_2H_5S**–tC_4H_9	71.1±1.5	297.5±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
dipropyl sulphide **C_3H_7S** -C_3H_7	72.8±1.5	304.6±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methyl phenyl sulphide **CH_3S**–C_6H_5	85.4±1.5	357.3±6.3	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methyl phenyl sulphide **C_6H_5S**–CH_3	(1) 69.4±2 (2) **66.5±2.5**	290.4±8.4 **278.2±10.5**	(1) VLPP (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1977COL/BEN (2) 1994PED
ethyl phenyl sulphide **C_2H_5S**–C_6H_5	84.6±2	354.0±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
ethyl phenyl sulphide C_2H_5–**SC_6H_5**	64.5±1.5	269.9±6.3	Derived from $\Delta_f H^\circ$ in ref.	1994PED

续表

断裂键 (黑体　离解原子 或原子团)	BDEs (黑体 · 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
benzyl methyl sulphide **CH_3S–CH_2Ph**	61.4±2	256.9±8.4	VLPP	1977COL/BEN
diphenyl sulphide **C_6H_5S–C_6H_5**	(1) 78.3±2.5 (2) 76±2	327.6±10.5 318±8.4	(1) Derived from $\Delta_f H^\circ$ in ref. (2) AOP	(1) 1986PED/NAY (2) 1991BAU/FAS
benzyl phenyl sulfide **C_6H_5S–$CH_2C_6H_5$**	54±2	225.9±8.4	AOP	1991BAU/FAS
9-henylthiomethylanthracene 	47±2	196.6±8.4	AOP	1991BAU/FAS
10-phenylthio-9-methyl-anthracene 	75±2	313.8±8.4	AOP	1991BAU/FAS
tropylium thiophenoxides, substituted 				
Y = H	24.6±0.2	102.9±0.8	AOP	1992VEN/AMA
Cl	24.0±0.3	100.4±1.3		
Br	25.7±0.3	107.5±1.3		
Me	23.7±0.3	99.2±1.3		
MeO	23.5±0.3	98.3±1.3		
NO_2	27.0±0.3	113.0±1.3		
methyl hydrodisulfide **CH_3–SSH**	57±1.5	238.5±6.3	Review	1978BEN

续表

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
dimethyl disulphide **CH_3**–$SSCH_3$	56.6	236.8	AE	1986HAW/GRI
ethyl methyl disulphide **C_2H_5**- $SSCH_3$	56.2	235.1	AE	1986HAW/GRI
iso-propyl methyl disulphide **iC_3H_7**–$SSCH_3$	54.5	228.0	AE	1986HAW/GRI
methyl tert-butyl disulphide **tC_4H_9**–$SSCH_3$	52.6	220.1	AE	1986HAW/GRI
alkyl ethyl disulfide **C_2H_5**–SSR	54±1.5	225.9±6.3	Review	1978BEN
alkyl phenyl disulfide **Ph**–SSR	69.5±1.5	290.8±6.5	Review	1978BEN
alkyl ethyl polysulfide **R**–S_nEt	54±1.5	225.9±6.3	Review	1978BEN
methanesulfenic acid HOS–**CH_3**	68.1±3	284.9±12.6	Derived from $\Delta_f H^\circ$ in ref.	1996HUN/SHE
dimethyl sulfoxide CH_3SO–**CH_3** $\Delta_f H^\circ(CH_3SO)$ = −16±2.4 (−67±10)	(1) 53±2, at 0 K (2) 55	221.8±8.4 230	(1) Photolysis (2) Derived	(1) 1997ZHA/CHE(b) (2) 2001IUPAC
methanesulfonic acid $HOSO_2$–**CH_3**	77.5±3	324.3±12.6	Derived from $\Delta_f H^\circ$ in ref.	2000GUT/GAL
dimethyl sulphone CH_3SO_2–**CH_3** $\Delta_f H^\circ(CH_3SO_2)$ = −57.2 (−239.3)	66.8	279.5	Iodination	1971SOL/BEN
methyl sulphone radical **CH_3** SO_2	21.4	89.5	Derived from $\Delta_f H^\circ$ in ref.	1971SOL/BEN
ethyl methyl sulphone CH_3SO_2–**C_2H_5**	68.9±2	288.3±8.4	Derived from $\Delta_f H^\circ$ in ref	1986PED/NAY
iso-propyl methyl sulphone CH_3SO_2–**iC_3H_7**	67.5±2	282.4±8.4	Derived from $\Delta_f H^\circ$ in ref	1986PED/NAY
allyl methyl sulphone H_3CSO_2–**C_3H_5**	55±2.5	230.1±10.5	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
butyl methyl sulphone H_3CSO_2–**C_4H_9**	71.3±2	298.3±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methyl tert-butyl sulphone H_3CSO_2–**tC_4H_9**	67.6±2	282.8±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
methyl phenol sulphone H_3CSO_2–**C_6H_5**	82.3±2	344.3±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY
benzyl methyl sulphone CH_3SO_2–**CH_2Ph**	56.2±2	235.1±8.4	Derived from $\Delta_f H^\circ$ in ref.	1986PED/NAY

续表

断裂键 (**黑体** – 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
methylthiocarbonitrile CH_3S–**CN**	97±2	405.8±8.4	Derived from Δ_fH° in ref.	1986PED/NAY
methylthiocarbonitrile **CH_3**–SC≡N	68.5	286.6	Derived from Δ_fH° in ref.	1978BEN
methanisothiocyanate CH_3NC=**S**	71	297	Review	1978BEN
S-ethyl thioacetate **C_2H_5S**–C(O)CH_3	76.2±2	318.8±8.4	Derived from Δ_fH° in ref.	2002CRC
S-propyl thioacetate **C_3H_7S**–C(O)CH_3	76.5±2	320.1±8.4	Derived from Δ_fH° in ref.	1994PED
pentafluorosulfur trifluoromethane **F_5S**–CF_3	93.7±10.3, at 0 K	392.0±43	Threshold photoelectron	2001CHI/KEN
methanedisulfur radical CH_3–**SS**	49.4	206.7	Derived from Δ_fH° in ref.	1986HOW/GRI
ethanedisulfur radicals C_2H_5–**SS**	48.7	203.8	Derived from Δ_fH° in ref.	1986HOW/GRI
propane-2-disulfur radical iC_3H_7–**SS**	48.4	202.5	Derived from Δ_fH° in ref.	1986HOW/GRI
2-methylpropane-2-disulfur radical tC_4H_9–**SS**	46.9	196.2	Derived from Δ_fH° in ref.	1986HOW/GRI
benzendisulfur radicals C_6H_5–**SS**	60±2	251.0±8.4	Review	1978BEN
CH_3–**SC$^\bullet$H$_2$**	30.7±2.5	128.4±10.5	Derived from Δ_fH° in ref.	1998NIST
C_6H_5–**SC$^\bullet$H$_2$**	43.0±4	179.9±16.7		

9.4 S—X(卤)键能

表 9.4 S—X(卤) BDEs

断裂键 (**黑体** – 离解原子)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
sulfur hexafluoride F-SF_5	(1) 91.1±3.2, at 0K	381.2±13.3	(1) Chemilumines-cent	(1) 1980KIA/ZAR
	(2) 92.2	385.8	(2) HP MS	(2) 1990SIE/AUS
	(3) 100.4±2.4	420±10	(3) SPST	(3) 1992TSA/HER
	(4) **93.6**	391.6	(4) Derived from Δ_fH° in ref.	(4) 1998CHA

续表

断裂键 (**黑体** = 离解原子)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
sulfur hexafluoride anion F–SF_5^-	≤42.5±2.9	≤178±12	CID	2003LOB/CHE
sulfur pentafluoride F-SF_4	(1) 53.1±6.0, at 0K (2) 53.7	222.2±25.1 224.7	(1) Chemilumines-cent (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1980KIA/ZAR (2) 1998CHA
sulfur pentafluoride anion SF_4- F^-	46.9±4.8	196.1±21	CID	2003LOB/CHE
sulfur tetrafluoride F SF_3	(1) 84.1±3.0, at 0K (2) 86.0±7.8 (3) 81.1	351.9±12.6 360±33 339.3	(1) Chemilumines-cent (2) Ion reactions (3) Derived from $\Delta_f H^\circ$ in ref.	(1) 1980KIA/ZAR (2) 1995MIL/MIL (3) 1998CHA
sulfur trifluoride F–SF_2	(1) 63.1±7.1 (2) 68.4	264±30 286.2	(1) Chemilumines-cent (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1980KIA/ZAR (2) 1998CHA
sulfur difluoride F -SF	(1) 91.7±4.3 (2) 93.0	383.7±18.0 389.1	(1) Chemilumines-cent (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1980KIA/ZAR (2) 1998CHA
sulfur fluoride F–S	(1) 81.2±1.6, at 0K (2) 82.1	339.7±6.7 343.5	(1) Chemilumines-cent (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1980KIA/ZAR (2) 1998CHA
sulfur dichloride Cl–SCl	70.6	295.4	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
sulfur chloride Cl–S	57.8	241.8	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
chloromethylthio Cl–SCH_3	70±3	292.9±12.6	Review	1978BEN
chlorophenylthio Cl-SC_6H_5	31+2.5	129.7±10.5	Review	1978BEN
dichloro disulfide Cl–SSCl	51±2	213.4±8.4	Review	1978BEN
methyl hydrodisulfide Cl–$SSCH_3$	51±2.5	213.4±10.5	Review	1978BEN
chloromethylsulfone Cl–SO_2CH_3	(1) 70.3 (2) 70	294 293	PAC	(1) 1994CHA/GRI (2) 1999LAA/MUL
chlorophenylsulfone Cl–SO_2Ph	(1) 70.5 (2) 71	295 297	PAC	(1) 1994CHA/GRI (2) 1999LAA/MUL
chloro disulfide radicals Cl–SS •	42±2	176±8	Review	1978BEN

续表

断裂键 (**黑体** = 离解原子)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
sulfur dibromide **Br** SBr	62±4	259±17	Review	1978BEN
sulfur bromide **Br**–S	52±4	218±17	Review	1978BEN
dibromo disulfide **Br**–SSBr	42±4	176±17	Review	1978BEN
iodothio **I**–SH	49.4±2	206.7±8.4	Kinetics	1979HWA/BEN(b)
iodomethylthio **I**–SCH_3	49.3±1.7	206.3±7.1	VLPP	1983SHU/BEN

9.5 S—P, S—As 和 S—Sb 键能

表 9.5 S—P, S—As 和 S—Sb BDEs

断裂键 (**黑体** = 离解原子 或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
trifluorophosphino-1-thione **S**=PF_3	100	418.4	Review	1973BEN
trichlorophosphino-1-thione **S**=PCl_3	68	284.5	Review	1973BEN
tribromophosphino-1-thione **S**=PBr_3	94	393.3	Review	1973BEN
tricyclohexylphino-1-thione **S**=PCy_3	98	410	Calorimetry	1998CAP/WIX
tributylhosphino-1-thione **S**=PBu_3	96	402	Calorimetry	1998CAP/WIX
trimethylhosphino-1-thione **S**=PMe_3	94	393	Calorimetry	1998CAP/WIX
dimethylphenylphosphino-1-thione **S**=PMe_2Ph	93	389	Calorimetry	1998CAP/WIX
methyldiphenylphosphino-1-thione **S**=$PMePh_2$	91	381	Calorimetry	1998CAP/WIX
triphenylphosphino-1-thione **S**=PPh_3	88	368	Calorimetry	1998CAP/WIX
triphenylarsono-1-thione **S**=$AsPh_3$	70	293	Calorimetry	1998CAP/WIX
triphenylantimono-1-thione **S**=$SbPh_3$	67	280	Calorimetry	1998CAP/WIX
(also see Section 10.1)				

第 10 章　Si—, Ge—, Sn— 和Pb—X 键能

10.1　Si—X 键能

表 10.1　Si—X BDEs

断裂键 (**黑体** = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDFs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
silane	(1) 90.3 ±1.2	377.8±5.0	(1) Iodination	(1) 1981DON/WAL
SiH_3–**H**	(2) 91.8±0.5	384.1±2.1	(2) PIMS detect.	(2) 1991SEE/FEN
$\Delta_f H^\circ$(R) = 47.9±0.6	(3) **91.7±0.5**	**383.7±2.1**	(3) Recommended	(3) 1994BER/ELL
(200.4±2.5)	(4) 91.5±2	382.8±8.4	(4) Review	(4) 1995CHA
	(5) 91.8±0.5	384±2	(5) Review	(5) 1998BEC/WAL
SiH_2–**H**	(5) 71.0±2	297±8		
SiH **H**	(5) 76.7	321		
Si-**H**	(5) 69.8	292		
	(6) **70.1±0.5**, at 0 K	**293.3±1.9**	(6) Re-anal.	(6) 2004HIR/YAN
Si–**D**	(7) 72.3	302.5	(7) Spectroscopy	(7) 1979HUB/HER
methyl silane	(1) 89.6±2	374.9±8.4	(1) Iodination	(1) 1989WAL
$MeSiH_2$–**H**	(2) 92.3±3	386.2±12.6	(2) Review	(2) 1995CHA
$\Delta_f H^\circ$(R) = 33.7±1.5 (141±6)	(3) **92.7±1.2**	**388±5**	(3) Revised	(3) 1998BEC/WAL
dimethylsilane				
Me_2SiH–**H**	(1) 89.4±2	374.0±8.4	(1) Iodination	(1) 1989WAL
$\Delta_f H^\circ$(R) = 18.6±1.5 (78±6)	(2) **93.5±1.2**	**391±5**	(2) Revised	(2) 1998BEC/WAL
trimethylsilane	(1) 90.3±1.4	377.8±5.9	(1) Iodination	(1) 1989WAL
Me_3Si–**H**	(2) 95.0±0.5	397.5±2.1	(2) Flash photolysis	(2) 1994KAL/GUT
$\Delta_f H^\circ$(R) = 3.6±1.7 (15±7)	(3) 92.0	385	(3) VLPP	(3) 1994BUL/WAL
	(4) **94.6±1.7**	**396±7**	(4) Revised	(4) 1998BEC/WAL
Me_3Si–**D**	(5) 93.0	389.1	(5) Kinetics	(5) 1981ELL/POT
disilane	(1) 86.3±2	361.1±8.4	(1) Iodination	(1) 1989WAL
H_5Si_2–**H**	(2) **89.1±2**	**373±8**	(2) Revised	(2) 1998BEC/WAL
$\Delta_f H^\circ$(R) = 55.9±2 (234±8)				
3-ethyl-silapentane	(1) 90.1	377.0	(1) PAC	(1) 1987KAM/HAW
$(C_2H_5)_3Si$–**H**	(2) 95.1	397.9	(2) Review	(2) 1995CHA
	(3) 96.0	401.7	(3) PAC, revised	(3) 1999LAA/MUL
	(4) **94.6±1**	**396±4**	(4) Review	(4) 1998BEC/WAL

续表

断裂键 (**黑体** = 离解原子或原子团) $\Delta_f H°$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
pentamethyl disilane $(CH_3)_3Si(CH_3)_2Si$–**H**	(1) 85.3±2 (2) 90.3 (3) 91.0 (4) **89.9±1**	356.9±8.4 377.8 380.7 **376±4**	(1) PAC (2) Review (3) PAC, revised (4) Review	(1) 1987KAM/HAW (2) 1995CHA (3) 1999LAA/MUL (4) 1998BEC/WAL
3(1,1-dimethyl-1-silaethyl)- 2,2,4,4,-tetramethyl-2,3,4- trisilapentane $((CH_3)_3Si)_3Si$–**H**	(1) 79.0 (2) 83.9 (3) 84 (4) **83.7±1**	330.5 351.0 351.5 **350±4**	(1) PAC (2) Review (3) PAC, revised (4) Review	(1) 1987KAM/HAW (2) 1995CHA (3) 1999LAA/MUL (4) 1998BEC/WAL
2,2,3,4,4-pentamethyl-3- silapentane $(tBu)_2MeSi$–**H**	89.1	372.8	Correlation	1998DEN
3-(tert-butyl)-2,2,4,4- tetramethyl-3-silapentane $(tBu)_3Si$–**H**	86.6	362.3	Correlation	1998DEN
1-phenyl-silaethane $C_6H_5SiH_2$–**H** $\Delta_f H°$(R) = 62.1 (260)	(1) 88.2±1.2 (2) 90.1 (3) **91.3±1.2**	369.0±5 377.0 **382±5**	(1) Iodination (2) Review (3) Revised	(1) 1989WAL (2) 1995CHA (3) 1998BEC/WAL
trimethylthiosilamethane $(CH_3S)_3Si$–**H**	(1) 82.5 (2) 87.4 (3) **87.0**	345.2 365.7 **364.0**	(1) PAC (2) Review (3) PAC, revised	(1) 1992CHA/GUE (2) 1995CHA (3) 1999LAA/MUL
triisopropylthiosilamethane $(iPrS)_3Si$–**H**	(1) 85.6 (2) **90.0**	358.2 **376.6**	(1) PAC (2) PAC, revised	(1) 1991CLA/GRI (2) 1999LAA/MUL
phenyl methyl silamethane, substituted R_1R_2MeSi–**H**				
R_1 = Ph R_2 = H	(1) 91.3±3.1	382.0±13	(1) ICR	(1) 1989WET/SAL
Ph F	(2) 92.1	385.4	(2) Correlation	(2) 1998DEN
Ph Cl	(2) 90.0	376.6		
Ph C_6F_5	(2) 89.7	375.5		
Ph Ph_3Si	(2) 83.1	347.7		
Ph $tBuCH_2$	(2) 87.5	366.2		
Me 3-CF_3–C_6H_4	(2) 87.1	364.2		
1-Np C_6H_5	(2) 87.2	365.0		
1-Np 3-F–C_6H_4	(2) 88.2	369.2		
1-Np 3-MeO–C_6H_4	(2) 87.5	366.2		

续表

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1-Np 3-CF_3-C_6H_4	(2) 88.3	369.6		
1-Np 3-Me C_6H_4	(2) 86.9	363.6		
1-Np 4-CF_3–C_6H_4	(2) 88.6	370.7		
1-Np 4-MeO–C_6H_4	(2) 86.6	362.4		
dimethyl phenyl silamethane $PhMe_2Si$–**H**	(1) 84.6 (2) 88.7 (3) **90.1±1.7**	354.0 371.0 **377±7**	(1) PAC (2) Correlation (3) Review	(1) 1990DIA/DIO (2) 1998DEN (3) 1998BEC/WAL
diphenyl silamethane Ph_2SiH–**H**	(1) 86.0 (2) 87.7 (3) **90.6±1.7**	359.8 366.8 **379±7**	(1) PAC (2) Correlation (3) Review	(1) 1990DIA/DIO (2) 1998DEN (3) 1998BEC/WAL
diphenyl methyl silamethane Ph_2MeSi–**H**	(1) 81.7 (2) 87.5 (3) **86.3±2.4**	341.8 366.2 **361±10**	(1) PAC (2) Correlation (3) Review	(1) 1990DIA/DIO (2) 1998DEN (3) 1998BEC/WAL
triphenyl silamethane, substituted R_3Si–**H** R = C_6H_5 3-CF_3–C_6H_4	(1) 84.1 (2) 86.4 (3) **88.7±0.5** (2) 89.3	351.9 361.8 **371±2** 373.6	(1) PAC (2) Correlation (3) Review	(1) 1990DIA/DIO (2) 1998DEN (3) 1998BEC/WAL
trifluorosilane SiF_3-**H** $\Delta_f H^\circ$(R) = - 235.9±4.8 (–987±20)	(1) 100.1±1.2 (2) **103.2±1.2**	418.8±5 **432±5**	(1) Iodination (2) Revised	(1) 1989WAL (2) 1998BEC/WAL
trichlorosilane $SiCl_3$–**H** $\Delta_f H^\circ$(R) = –77±2 (–322±8)	(1) 91.3±1.2 (2) **94.4±1.2**	382.0±5 **395±5**	(1) Iodination (2) Revised	(1) 1989WAL (2) 1998BEC/WAL
tribromosilane $SiBr_3$–**H**	79 8±2	334±8	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
silicon clusters $Si(Si)_x$–**Si** x = 0 1 2	(1) 74.1 (1) 96.6 (2) 105.2	310 404 440	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived	(1) 1998CHA (2) 1997GIN/VIS
disilane SiH_3 **SiH_3**	(1) ≤82.7, at 0 K (2) **76.7±1**	≤346 **321±4**	Derived	(1) 1991RUS/BER(c) (2) 1998BEC/WAL

续表

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 - 推荐值; 括号内数字 文献编号)		方法	文献
	kcal/mol	kJ/mol		
disilene SiH_2=**SiH_2**	63.3±1.2	264.8±5.0	Derived	1991RUS/BER(c)
trisilane **SiH_3**–Si_2H_5	74.8±2	313±8	Derived	1998BEC/WAL
tetrasilane **H_5Si_2**–Si_2H_5	73.1	306	Derived	1998BEC/WAL
hexamethyl disialne **Me_3Si**–$SiMe_3$	(1) 80.5 (2) **79.3±2.9**	336.8 **332±12**	(1) Pyrolysis (2) VLPP	(1) 1975DAV/HOW (2) 1994BUL/WAL
hexaphenyl disilane **Ph_3Si**–$SiPh_3$	88.0	368.2	Derived	1981WAL
disilicon hexafluoride **F_3Si**–SiF_3	108.3±6	453.1±25	Derived from $\Delta_f H^\circ$ in ref.	2001LYM/NOD
methyl silane SiH_3–**CH_3**	89.6±1.2	375±5	Derived	1998BEC/WAL
2-silapropane $MeSiH_2$–**CH_3**	90.1±1.7	377±7	Derived	1998BEC/WAL
trimethylsilane Me_2SiH–**CH_3**	92 5±1 7	387±7	Derived	1998BEC/WAL
tetramethylsilane Me_3Si–**CH_3**	(1) 91.6 (2) **94.2±2**	383 **394±8**	(1) VLPP (2) Derived	(1) 1994BUL/WAL (2) 1998BEC/WAL
trifluoromethylsilane SiF_3–**CH_3**	85	355.6	Derived	1990ALL/MCM
methyl silane-1,1,1-triol $(OH)_3Si$–**CH_3**	103.5	433	Derived	2003BRA/NES
trimethyl sec-butylsilane Me_3Si–**sBu**	99	414.2	Pyrolysis	1980DAV/WOO
trimethyl allylsilane Me_3Si–**C_3H_5**	70	292.9	Pyrolysis	1980DAV/WOO
phenyl silane-1,1,1-triol $(OH)_3Si$–**C_6H_5**	126.9	531	Derived	2003BRA/NES
silicon oxide $Si(O)_x$–**O** x = 0 1	 (1) 191.1±3.2 (2) 188.7±3.9, at 0 K (1) 108.6	 799.6±13.4 789.3±16.4 454.2	 (1) Derived from $\Delta_f H^\circ$ in ref (2) Spectroscopy	 (1) 1998NIST (2) 1999RED/AHA
3-oxa-disilapropane H_3Si–**$OSiH_3$**	131.0	548.1	Derived	2001SCH/BER
2-methyl-2-silapropan-2-ol Me_3Si–**OH**	132.6±2.0	555±8	Derived	1998BEC/WAL
silane-1.1,1,1-tetraol $(OH)_3Si$–**OH**	144.4	604	Derived	2003BRA/NES

续表

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值， 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1-methyl-1,1-dimethyl-1-silaethane Me_3Si **OMe**	122.6±2.6	513±11	Derived	1998BEC/WAL
1-ethoxy-1,1-dimethyl-1-silaethane Me_3Si–**OEt**	122.4±2.6	512±11	Derived	1998BEC/WAL
2,2,6,6-tetramethyl-4-oxa-3,5-disilapentane Me_3Si–**OSiMe$_3$**	136	569	Derived	1998BEC/WAL
nitrososilane H_3Si–**NO** D_3Si–**NO**	37.8±1.4 38.4±1.4	158.2±5.7 160.8±5 7	Laser photolysis, MS detect	1997KRA/KAL
nitroso trimethylsilane Me_3Si **NO**	44.8±1.0	187.4±4.2	Laser photolysis, MS detect.	1995KRA/NII
(1,1-dimethyl-1-silaethyl)-methylamine Me_3Si–**NHMe**	100.1±2	412±8	Derived	1998BEC/WAL
(1,1-dimethyl-1-silaethyl)-dimethylamine Me_3Si–**NMe$_2$**	97.5±2	408±8	Derived	1998BEC/WAL
tri(1,1-dimethyl-1-silaethyl)-amine Me_3Si–**N(SiMe$_3$)$_2$**	108.7	455	Derived	1998BEC/WAL
phosphino silane H_3Si–**PH$_2$**	79.2	331.4	Derived from $\Delta_f H^\circ$ in ref.	1990PIL
fluorosilane SiH_3–**F**	152.5±1.2	638±5	Derived	1998BEC/WAL
trimethyl fluorosilane Me_3Si -**F**	159.9±4.8	669±20	Derived	1989WAL
tetrafluorosilane SiF_3–**F** SiF_2–**F** SiF–**F** Si–**F**	(1) 166.6±1.5 (2) 102.4±4 (2) 166.7±2 (2) 131.3±2	697±6 428±17 697.5±8.4 549.4±8.4	Derived	(1) 1998BEC/WAL (2) This volume
OSi F **OFSi**–F	31.3 36.1	131 151	Derived	2001HIL/LAU
fluorosilane-1,1,1-triol $(OH)_3Si$–**F**	166.1	695	Derived	2003BRA/NES

续表

断裂键 (**黑体** = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 · 文献编号)		方法	文献
	kcal/mol	kJ/mol		
chlorosilane SiH_3–**Cl**	109.5±1.7	458±7	Derived	1998BEC/WAL
trimethyl chlorosilane Me_3Si–**Cl**	112.8±2.0	472±8	Derived	1989WAL
tetrachlorosilane $SiCl_3$–Cl	(1) 110.4±2.2 (2) **111.3±1**	462±9 **465.7±4.2**	Derived	(1) 1998BEC/WAL (2) 2003HIL/LAU
$SiCl_2$ -**Cl**	(3) 67.0±1	280.3±4.2		(3) This volume
SiCl–**Cl**	(3) 104.0±1.5	435.1±6.3		
Si–**Cl**	(3) 99.6±1.5	416.7±6.3		
OSi–Cl	22.0	92	Derived	2001HIL/LAU
OClSi–Cl	26.3	110		
chlorosilane-1,1,1-triol $(OH)_3Si$- **Cl**	118.3	495	Derived	2003BRA/NES
bromosilane SiH_3–**Br**	89.9±2.2	376±9	Derived	1998BEC/WAL
trimethyl bromosilane Me_3Si–**Br**	96.0±2.0	402±8	Derived	1989WAL
tetrabromosilane $SiBr_3$–**Br**	(1) 89.9±5 3 (2) **88.1±2**	376±22 **368.6±8.4**	Derived	(1) 1998BEC/WAL (2) 2003HIL/LAU
$SiBr_2$ **Br**	(3) 53.7±2	224.7±8 4		(3) This volume
SiBr–**Br**	(3) 88.7±2	371.1±8.4		
Si-**Br**	(3) 85.6±2	358.2±8.4		
bromosilane-1,1,1-triol $(OH)_3Si$–**Br**	102.5	429	Derived	2003BRA/NES
iodosilane SiH_3–**I**	71.5±2.0	299±8	Derived	1998BEC/WAL
trimethyl iodosilane Me_3Si–**I**	(1) 76.9 (2) **76.7±2.0**	321.7 **320.9±8.4**	(1) UV spectrom. (2) Derived	(1) 1979DON/WAL (2) 1989WAL
tetraiodosilane SiI_3–**I**	(1) 67.9±6.2	284±26	Derived	(1) 1998BEC/WAL
SiI_2–I	(2) 39.1±2	163.6±8.4		(2) This volume
SiI–**I**	(2) 78.5±2	328.4±8.4		
Si–I	(2) 58.1±2	243.1±8.4		

续表

断裂键 (**黑体** = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 文献编号) kcal/mol	kJ/mol	方法	文献
OSi(I)$_x$–I x = 0 1	≤24 ≤80	≤100 ≤335	MS	2001HIL/LAU
2-silaeth-1-ene **SiH$_2$=CH$_2$**	34.9±1	146±4	Review	1998BEC/WAL
2-silapro-1-ene **MeHSi=CH$_2$**	36.8±2.9	154±12	Review	1998BEC/WAL
2-methyl-2-silapro-1-ene **Me$_2$Si=CH$_2$**	(1) 39±6 (2) **38.5±2.9**	163±25 **161±12**	(1) ICR (2) Review	(1) 1990ALL/MCM (2) 1998BEC/WAL
disilene **SiH$_2$=SiH$_2$**	27.0±2	113±8	Review	1998BEC/WAL
difluoro-2-silaeth-1-ene **SiF$_2$=CH$_2$**	50±5	209±21	ICR	1990ALL/MCM
fluoro-2-silapro-1-ene **MeFSi=CH$_2$**	45±5	188±21	ICR	1990ALL/MCM
Si(Si)$_x$–C x = 0 1	106.8 110.2	447 461	Derived from $\Delta_f H^\circ$ in ref.	1998CHA
silaforaldehyde **SiH$_2$=O**	61.2±6	256±25	Review	1998BEC/WAL
silaketene **H$_2$Si=CO**	21.3	89	Kinetics	2001BEC/CAN
Si–Si$_2$N	69.6±4.1	291±17	Derived from $\Delta_f H^\circ$ in ref.	1997BAB/VIS
Si–N	(1) 101.0, at 0 K (2) 103.6	422.6 433.4	Spectroscopy	(1) 1989RAJ (2) 2000RED/AHA
Si$_3$–**N** –**B**	141.7 121.7	593 509	Derived	1997GIN/VIS
Si–**P**	86.9	363.6	MS	1972SMO/DEP
Si$_2$B–**Si** Si$_2$N–**Si**	103.3 68.6	432 287	Derived	1997GIN/VIS
Si(S)$_x$–S x = 0 1	(1) 147.9 (2) 148.4 (3) 147.5±1.2 (1) 80.6	619 621 617±5 337	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Derived from $\Delta_f H^\circ$ in ref. (3) Derived	(1) 1991GUR/VEY (2) 1998NIST (3) 1997TOM/HOP

续表

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
$Si(Se)_x$–Se				
$x = 0$	128.6±3.1	538±13	Review	1994TOM/SUS
1	75.5±4.3	316±18		
$Si(Te)_x$–Te				
$x = 0$	92.6±2	448±8	Review	1994TOM/SUS
1	46.8±3 8	196±16		
(SiO) –SiO	53±10	222±42	Review	1967DRO/GOL

10.2 Ge—X 键能

表 10.2 Ge—X BDEs

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
germane	(1) 78.0±1	326.4	(1) VLPP	(1) 1987AGR/SET
	(2) 82.6±2.4	345.6±10.0	(2) VLPP	(2) 1983NOB/WAL
GeH_3–**H**	(3) **83.4±2**	**348.9±8.4**	(3) Recommend.	(3) 1994BER/ELL
$\Delta_f H^\circ$(R) = 53±2 (221.8±8.4)	(4) 85.6±2.1	358.2±8.8	(4) FT-ICR	(4) 1993DEC/GAL
	(5) 82.5	345.2	(5) EA	(5) 2001MOR/RIV
GeH_2–**H**	(6) 59	247	(6) PIMS	(6) 1990RUS/SCH
GeH–**H**	(6) 66	276		
Ge–**H**	(6) 63	**264**		
	(7) **62.9±1.2**	**263.2±4.8**	(7) Spectroscopy	(7) 2000RAJ/RAJ(c)
Ge–**D**	(8) <65.2	< 272.8	(8) Spectroscopy	(8) 1971KRO/LAG
trimethyl germane	(1) 81.7±2.4	341.8±10.0	(1) VLPP	(1) 1979DON/WAL
	(2) 82	343.1	(2) AE	(2) 1979JAC
Me_3Ge **H**	(3) 81.6±0.5	341.4±2.1	(3) PAC	(3) 1991CLA/GRI
	(4) 79.8±3.5	333.9±14.6	(4) Electron photodetach.	(4) 1995BRI/SAL
	(5) **87.0**	**364.0**	(5) PAC, revised	(5) 1999LAA/MUL
triethyl germane	(1) 82 3	344.3	(1) PAC	(1) 1991CLA/GRI
$(C_2H_5)_3Ge$–**H**	(2) **86.0**	**359.8**	(2) PAC, revised	(2) 1999LAA/MUL
tri-tert-butyl germane	(1) 82.6	345.6	(1) PAC	(1) 1991CLA/GRI
$(tBu)_3Ge$–**H**	(2) **88.0**	**368.2**	(2) PAC, revised	(2) 1999LAA/MUL

续表

断裂键 (**黑体** 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** · 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
3-(1,1-dimethyl-1-silaethyl)-3-germa-2,2,4,4-tetramethyl-2,4-disilapentane $(Me_3Si)_3Ge$-**H**	73.1	305.8	Correlation	2002DRO/DEN
phenylgermane, substituted $(2,4,6\text{-}Me_3\text{-}C_6H_2)GeH_2$–**H**	80.7	337.5	Correlation	2002DRO/DEN
diphenylgermane, substituted $(2,4,6\text{-}Me_3\text{-}C_6H_2)_2GeH$–**H**	80.5	336.8	Correlation	2002DRO/DEN
2-germa-1-phenylfromtane $(PhCH_2)(C_2H_5)GeH$-**H**	81.6	341.6	Correlation	2002DRO/DEN
2-germa-1,3-diphenyl-2-benzylpropane $(PhCH_2)_3Ge$–**H**	77.7	324.9	Correlation	2002DRO/DEN
phenyl germane PhH_2Ge–**H**	(1) 79.2 (2) **86.0**	331.4 **359.8**	(1) PAC (2) PAC, revised	(1) 1991CLA/GRI (2) 1999LAA/MUL
diphenyl germane Ph_2HGe–**H**	(1) 79.5 (2) **85.0**	332.6 **355.6**	(1) PAC (2) PAC, revised	(1) 1991CLA/GRI (2) 1999LAA/MUL
triphenyl germane Ph_3Ge–**H**	(1) 80.2 (2) **86.0** (3) 77.1	335.6 **359.8** 322.5	(1) PAC (2) PAC, revised (3) Correlation	(1) 1991CLA/GRI (2) 1999LAA/MUL (3) 2002DRO/DEN
methoxygermane $H_2Ge(OMe)$–**H**	81.5	341.0	EA	2001MOR/RIV
dimethoxygermane $HGe(OMe)_2$-**H**	82.6	345.6	EA	2001MOR/RIV
germanium clusters **Ge(Ge)$_x$** –Ge				
$x = 0$	(1) 64 (2) 64.5±5, at 0 K (3) 63.0±1.7 (4) **62.3±1.6**	268 269.9±20.9 263.5±7.0 **260.7±6.8**	(1) MS (2) MS (3) MS (4) MS	(1) 1959DRO/MAR (2) 1972NEC/SOD (3) 1986KIN/NAG (4) 2002SHI/BAB
1	(1) 89 (5) **77.7±5.2**	372 **325±22**	(5) Derived from $\Delta_f H^\circ$ in ref.	(5) 2000GIN/BAB
2	(1) 128 (5) **90.0±7.5**	537 **377±32**		
Ge_2 –Ge_2	112	469	MS	1959DRO/MAR
digermane **H_3Ge**–GeH_3	67.2±3	281.2±8.4	Derived from $\Delta_f H^\circ$ in ref.	2002CRC
Ge–C	(1) 109±5 (2) 110 (3) **108.9±2.6**	456±21 460 **455.7±11**	(1) MS (2) Review (3) Re-evaluated	(1) 1959DRO/MAR (2) 1970DAR (3) 1998SHI/BAB

续表

断裂键 (**黑体** 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
Ge(Ge)$_x$–C				
x = 1	175	732	MS	1959DRO/MAR
2	155	649		
3	148	619		
Cl_3Ge–CH_3	66.4±4.6	278±19	Derived	1972TAM/CZI
$(CH_3)_3Ge$–CH_3	67.8±3.2	284±14		
Cl_3Ge–CCl_3	55.6±4.6	233±19		
GeSi–C	173	724	MS	1959DRO/MAR
Ge_2Si–C	155	649		
Ge(Ge)$_x$–Si				
x = 0	71	297	MS	1959DRO/MAR
1	99	414		
2	99	414		
GeC–Si	128	537	MS	1959DRO/MAR
Ge_2C–Si	100	418		
C_2–Ge	146	611	MS	1959DRO/MAR
GeSi–Ge	93	389		
Ge_2C–Ge	84	352		
Ge_2Si–Ge	93	389		
GeSiC–Ge	79	331		
Ge–Sn	55.0±3.1	230.1±13	Derived from $\Delta_f H^\circ$ in ref.	1998SCH/GIN
Ge(Sn)–Sn	79.8±6.3	333.9±26		
Ge(O)$_x$–O				
x = 0	(1) 157.6	659	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1991GUR/VEY
	(2) **156.0±2**	**652.7**	(2) MS	(2) 1996KAZ/BOL
1	(1) 75.9	318		

续表

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 推荐值, 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
$Ge(S)_x$–S				
$x = 0$	(1) 133.0	556	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1991GUR/VEY
	(2) 127.9±0.7	535±3	(2) Evaluation	(2) 1995OHA/CUR
	(3) 127.6±0.7	534±3	(3) Derived	(3) 1997TOM/HOP
1	(1) 60.0	251		
	(2) 64.3±4.8	269±20		
Ge–Sc	114.9±0.4	480.6±1.7	Review	1996OHA/ZYW
$Ge(Te)_x$–Te				
$x = 0$	94.8±0.8	396.7±3.3	MS	1995OHA
1	50.2±2	210±8		
$Ge(F)_x$–F				
$x = 0$	125±3	523±13	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
1	139±5	582±21		
2	75±12	314±50		
3	111±12	464±50		
$Ge(Cl)_x$ –Cl				
$x = 0$	(1) 101±5	423±21	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1991GUR/VEY
	(2) 92.5±2.3	387.0±9.6	(2) MS	(2) 1996HIL/LAU
1	(1) 86±5	360±21		
	(2) ~93	~389		
2	(1) 52±12	218±50		
3	(1) **84±12**	**352±50**		
	(3) 64.1±4.6	310±19	(3) MS	(3) 1972TAM/CZI
$(CH_3)_3Ge$–Cl	107±4.6	448±19	MS	1972TAM/CZI
$Ge(Br)_x$ Br				
$x = 0$	83±2	347±8	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
1	74±3	310±13		
2	40.5±12	170±50		
3	68±12	285±50		

续表

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 - 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
$Ge(I)_x$–I				
$x = 0$	64±6	268±25	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
1	64±6	268±25		
2	27.5±12	115±50		
3	51±12	213±50		
triphenylgermane, , substituted Ph_3Ge–**X**				
X – O	108.7	455	Derived	1992CAR
C_2CH_3	92.0	385		
Ph	86.0	360		
C≡CPh	125	523		
$GePh_3$	61.4	257		
Ge–Y	65.7±2.6, at 0 K	275±11	MS	1989CHA/GIN
Ge–Ni	(1) 66.4±2.9	278±12	(1) Review	(1) 1985GIN/SHI
	(2) 68.5±2.6	286.8±10.9	(2) MS	(2) 1988SHI/KIN
–Pd	(1) 62.9±2.4	263±10		
	(3) 60 2±2.5	252.0±10.5	(3) MS	(3) 1986SHI/KIN
(GeO)–GeO	45±3	188.3±12.6	Review	1967DRO/GOL

10.3 Sn—X 键能

表 10.3 Sn—X BDEs

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
trimethylstannane	(1) 74	309.6	(1) PAC	(1) 1991CLA/GRI
Me_3Sn–**H**	(2) 75±3.5	313.8±14.6	(2) Electron photodetach.	(2) 1995BRI/SAL
	(3) **78.0**	**326.4**	(3) PAC, revised	(3) 1999LAA/MUL
	(4) 76.1	318.5	(4) Correlation	(4) 2002DRO/DEN
	(5) 77±4	322±17	(5) Derived	(5) 2002BEC/BOG
tributylstannane	(1) 73.7±2	308.4±8.4	(1) PAC	(1) 1986BUR/MAJ
$(nBu)_3Sn$–**H**	(2) **78.0**	**326.4**	(2) PAC, revised	(2) 1999LAA/MUL

续表

断裂键 (**黑体** = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
triphenylstannane	70.4	294.6	Correlation	2002DRO/DEN
Ph_3Sn–**H**	71.3	298.3		
Sn–H	63±4	264±17	Review	1968GAY
tin dimer	(1) 45.8±4	191.6±16.7	(1) MS	(1) 1962ACK/DRO
Sn–Sn	(2) **44.7±0.1**	**187.1±0.3**	(2) Spectroscopy	(2) 1988PAK/CAI
Sn(Sn)$_x$ –Sn				
x = 3	58.4±6.2	244.3±26	Derived from $\Delta_f H^\circ$ in ref.	2000MEL/SCH
4	86.1±8.5	360.2±36		
5	70.4±11	294.6±46		
Sn–Ge	55.0±3.1	230.1±13	Derived from $\Delta_f H^\circ$ in ref.	1998SCH/GIN
–Ge(Sn)	79.8±6.3	333.9±26		
–Sn(Ge)	63.7±7.6	266.5±32		
Sn(F)$_x$ –F				
x = 0	(1) 111.5±3 (2) 113.7±2	466.5±12.5 476±8	(1) MS (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1968ZMB/HAS (2) 1991GUR/VEY
1	118.4±3	495±13		
2	51±12	213±50		
3	109±17	456±71		
Sn(Cl)$_x$–Cl				
x = 0	(1) 98±4 (2) **82.7±1**	410±17 **346±8**	(1) Review (2) Spectroscopy	(1) 1974GUR/KAR (2) 1993RAJ/PON
1	(3) 85.7±4	359±17	(3) Derived from $\Delta_f H^\circ$ in ref.	(3) 1991GUR/VEY
2	(3) 50.5±13	211±55		
3	(3) 73±13	305±55		
Sn(Br)$_x$ –Br				
x = 0	80.6±3	337±13	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
1	73.3±3	307±13		
2	36.2±12	151±50		
3	66.3±12	277±50		

续表

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^0$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
$Sn(I)_x$–I				
x = 0	56.2±3	235±3	Derived from $\Delta_f H^0$ in ref.	1991GUR/VEY
1	68.7±3	287±13		
2	25.5±12	107±50		
3	52±12	218±50		
$Sn(Bi)_x$ –Bi				
x = 0	46.2±3	193±13	Derived from $\Delta_f H^0$ in ref.	2002MEL/GIN
1	26.8±4.5	112±19		
2	45.3±5.6	190±23		
trimethylstannane, substituted Me_3Sn–**X**				
X = Cl	(1) 107 (2) **101.6±4**	448 **425±17**	Derived	(1) 1998GAL/PAU (2) 2002BEC/BOG
Br	(1) 91.3 (2) 91±4	382 381±17		
I	(1) 76.7 (2) 76.5±4	321 320±17		
OH	(2) 116.6±4	488±17		
CH_3	(2) **70.5±4** (3) 64.0 (4) 60.5	**295±17** 267.8 253		(3) 1988GRI/KAM (4) 1992CAR
2,2-dimethyl-2-stannabutane Me_3Sn–**Et**	60.0	251.0	Derived	1988GRI/KAM
2,2,3-trimethyl-2-stanna-butane Me_3Sn–**iPr**	55.4	231.8	Derived	1988GRI/KAM
2,2,3,3-tetramethyl-2-stanna-butane Me_3Sn–**tBu**	50.4	210.9	Derived	1988GRI/KAM
Sn–Au	60.4±1.7	252.6±7.2	MS	1986KIN/GIN

续表

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
triphenylstannane, substituted Ph_3Sn–**X**				
X = O	81.0	338.9	Derived	1992CAR
OH	90.6	379.1		
C_2CH_3	67.4	282		
Ph	65.5	274		
C≡CPh	102.1	427		
$SnPh_3$	45.2	189.1		
Sn(O)$_x$–O				
x= 0	(1) 126.1±3.0 (2) 126.3	528±13 528	(1) Review (2) Derived from $\Delta_f H^\circ$ in ref.	(1) 1983PED/MAR (2) 1991GUR/VEY
1	(2) 62.0	259		
Sn(S)$_x$–S				
x= 0	111.6	467	Derived from $\Delta_f H^\circ$ in ref.	1991GUR/VEY
1	57.0	238		
Sn–Se	95±1.4	397.5±5.9	MS	1964COL/DRO
–Te	79.9±1.5	334.3±6.3		
(SnO)–SnO	67±4	280.0±16.7	Review	1967DRO/GOL

10.4 Pb—X 键能

表 10.4 Pb—X BDEs

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
lead dimer **Pb**–Pb	(1) 18.2 (2) **19.8±0.2**, at 0 K	76 **83±1**	MS	(1) 1976GIN/COC (2) 1981PIT
Pb–H	≤37.5	≤157	Spectroscopy	1979HUB/HER
Pb(F)$_x$–F x = 0	(1) 84.8±3	355±13	Derived from $\Delta_f H^\circ$ in ref.	(1) 1998NIST
1	(1) 103.8±3	434±13		
2	(2) 30±15	126±63		(2) 1991GUR/VEY
3	(2) 93±19	389+79		

续表

断裂键 (**黑体** = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号) kcal/mol	kJ/mol	方法	文献
Pb(Cl)$_x$–Cl				
x = 0	(1) 72.0±12	301±50	Derived from $\Delta_f H^\circ$ in ref.	(1) 1998NIST
1	(1) 74.2±12	310±50		
2	(2) 29.5±20	123±84		(2) 1991GUR/VEY
3	(2) 64.8±20	271±84		
Pb(Br)$_x$–Br				
x = 0	(1) **59.4±3.5**	**248.5±14.6**	(1) Laser-induced fluorescence	(1) 1995DRA/SIM
	(2) 56.4±10	236±42	(2) Derived from $\Delta_f H^\circ$ in ref.	(2) 1998NIST
1	(1) **66.5±3.5**	**278.2±14.6**		
	(2) 68.6±11	287±46		
2	(3) 26.8±19	112±80	(3) Derived from $\Delta_f H^\circ$ in ref.	(3) 1991GUR/VEY
3	(3) 45 4±27	190±113		
Pb(I)$_x$–I				
x = 0	(1) 46.4±9	194±38	Derived from $\Delta_f H^\circ$ in ref.	(1) 1998NIST
1	(1) 52.0±10	218±42		
2	(2) 17.8±19	75±80		(2) 1991GUR/VEY
3	(2) 40.6±27	170+113		
Pb–Li	18.7±2	78.2±8	MS	1980NEU/IHL
Pb–O	(1) 89.4	374	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1998NIST
	(2) **56±3**	**234.3±12.6**	(2) MS	(2) 2000HIL/LAU
Pb–O$_2$	(1) 43.3	181	(1) Derived from $\Delta_f H^\circ$ in ref.	(1) 1991GUR/VEY
	(2) < 37	< 155	(2) Photodissoc.	(2) 2003CAM/PLA
Pb(S)$_x$–S				
x = 0	(1) 81.8±0.4	342.3±1.7	(1) MS	(1) 1969UY/DRO
	(2) 95.2	398	(2) Derived from $\Delta_f H^\circ$ in ref.	(2) 1991GUR/VEY
1	(2) 38.5	161		
Pb–Se	71.5±1.0	299.1±4.2	MS	1969UY/DRO
–Te	58.8±2.5	246.1±10.5		

续表

断裂键 (黑体 = 离解原子或原子团) $\Delta_f H^\circ$(R)/kcal (kJ)	BDEs (黑体 = 推荐值; 括号内数字 - 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Pb–Sb	(1) 38.6±2.5	161.5±10.5	MS	(1) 1981ZMB/NEU
–Bi	(2) 33.0	138.1		(2) 1967ROV/DRO
(PbO)–PbO	63±5	263.6±21	Review	1967DRO/GOL
tetramethylead $\mathbf{(CH_3)_3Pb}$–CH_3	57±5	238±21	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
tetraethyllead $\mathbf{(C_2H_5)_3Pb}$–C_2H_5	55±5	230±21	Derived from $\Delta_f H^\circ$ in ref.	1998NIST

第 11 章　P—, As—, Sb—, Bi—, Se—, Te— 和 Po—X 键能

11.1　P—X 键能

表 11.1　P—X BDEs

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号) kcal/mol	 kJ/mol	方法	文献
phosphine				
H_2P-**H**	(1) 82.5±0.5, at 0K (2) **83.9±0.5**	346.2±2.1 **351.0±2.1**	(1) PIMS (2) Recommend.	(1) 1986BER/CUR (2) 1994BER/ELL
HP–**H**	(1) 74.7±0.5, at 0K (3) **75.3**	312.5±2.1 **315.1**	(3) Derived from $\Delta_f H^\circ$ *in ref.*	(3) 1998NIST
P–**H**	(1) 71.0±0.5	297.0±2.1		
P-**D**	(4) 71.5	299.0	(4) Review	(4) 1979HUB/HER
methylphosphine CH_3PH–**H**	77±3	322.2±12.6	GPA	1994SUN/PAN
octylphosphine $CH_3(CH_2)_7PH$–**H**	89.7	375.3	PAC	1999LAA/MUL
ethylphosphine C_2H_5PH–**H**	89 7	375.3	MS	1969BOG/GRI
α-CN-proyulphosphine $NC(CH_2)_3PH$–**H**	89.2	373.4	Correlation	2002DRO/DEN
di(α-CN-proyul)phosphine $(NC(CH_2)_3)_2P$–**H**	88.3	369.5	Correlation	2002DRO/DEN
dibutylphosphine $(CH_3(CH_2)_3)_2P$–**H**	89.6	375.0	Correlation	2002DRO/DEN
diethylphosphine $(CH_3CH_2)_2P$–**H**	90.3	377.8	Correlation	2002DRO/DEN
dicyclohexylphosphine (cyclo-$C_6H_{11})_2P$–**H**	85.5 86.9	357.6 363.6	Correlation	2002DRO/DEN
phosphorus clusters **P(P)**$_x$ P				
$x = 0$	116.0	485.3	Review	1992YOO/RUS(b)
1	59.0	246.9		
2	110.8	463.6		

续表

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
$\mathbf{P_2}$–P_2	54.7	228.7	PIMS	1977SME/COP
diphosphine $\mathbf{H_2P}$–PH_2	61.2	256.1	MS	1969MCA/LOS
tetrachlorodiphosphine $\mathbf{Cl_2P}$–PCl_2	58	242.7	MS	1963SAN/MOS
tetraiododiphosphine $\mathbf{I_2P}$–PI_2	73.9	309	MS	1969FIN/HAM
(diethylphosphino)diethyl-phosphine $\mathbf{(C_2H_5)_2P}$–$P(C_2H_5)_2$	86	359.8	MS	1968GRI/BOG
phosphino fluoride $\mathbf{H_2P}$ -F	110.3±2.5	461.5±10.5	Derived from $\Delta_f H^\circ$ in ref.	2000FER/ALC
phosphorus fluorides $\mathbf{F_2P}$–F $\mathbf{FP}$ F P–F	(1) 131.3 (1) 123.2 (1) 107.1 (2) ≤96.7	549 515 448 ≤405	(1) Derived from $\Delta_f H^\circ$ in ref. (2) IR chemilumi	(1) 1998NIST (2) 1995ZHA/SET
phosphorus chlorides $\mathbf{Cl_2P}$–Cl ClP–Cl P–Cl	(1) 85.0±2 (2) ≤77.7 (3) 72.8±3 (1) 73.8 (4) ≤89.8	356±8 ≤325 305±13 309 ≤376	(1) Derived from $\Delta_f H^\circ$ in ref. (2) Spectrometry (3) Derived from $\Delta_f H^\circ$ in ref (4) IR chemilumin	(1) 1998CHA (2) 1979KOL/VEL (3) 1989GUR/VEY (4) 1995ZHA/SET
phosphorus tribromides $\mathbf{Br_2P}$ Br P–Br	(1) <62 (2) ≤78.7	<259 ≤329	IR chemilumin.	(1) 1980MAL/SET (2) 1995ZHA/SET
phosphorus triiodide $\mathbf{I_2P}$- I	51.9	217	MS	1969FIN/HAM
phosphino silane H_3Si–$\mathbf{PH_2}$	79.2	331.4	Derived from $\Delta_f H^\circ$ in ref.	1990PIL
$\mathbf{P(O)_x}$–O $x = 0$ 1	(2) 140.8 (2) 129.1	589 540	Derived from $\Delta_f H^\circ$ in ref.	1998NIST
phosphoryl fluoride $\mathbf{O}$=PF_3	(1) 130±5 (2) 129	544±21 534	Review	(1) 1966KER (2) 1973BEN
phosphoryl chloride $\mathbf{O}$=PCl_3	(1) 122±5 (2) 124	510±21 519	Review	(1) 1966KER (2) 1973BEN

续表

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
phosphoryl bromide **O=PBr_3**	(1) 119±5 (2) 122	498±21 510	Review	(1) 1966KER (2) 1973BEN
phosphoryl iodide **O=$P(CH_3)_3$**	139	582	Review	1973BEN
ethyl ethylphosphate **O=$P(OC_2H_5)_3$**	148	619	Review	1973BEN
phosphinotris(dimethylamino)-1-one **O=$P(N(CH_3)_2)_3$**	128	536	Review	1973BEN
triphenylphosphino-1-one **O=PPh_3**	130	544	Review	1973BEN
phosphorus monosulfide **S–P**	(1) 104.7±2.4 (2) **110.7±5.7**	438±10 **463±24**	(1) MS (2) Review	(1) 1973DRO/MYE (2) 2004LOD
trifluorophosphino-1-thione **S=PF_3**	100	418	Review	1973BEN
trichlorophosphino-1-thione **S=PCl_3**	68	285	Review	1973BEN
tribromophosphino-1-thione **S=PBr_3**	94	393	Review	1973BEN
tricyclohexylphino-1-thione **S=PCy_3**	98	410	Calorimetry	1998CAP/WIX
tributylhosphino-1-thione **S=PBu_3**	96	402	Calorimetry	1998CAP/WIX
trimethylhosphino-1-thione **S=PMe_3**	94	393	Calorimetry	1998CAP/WIX
dimethylphenylphosphino-1-thione **S=PMe_2Ph**	93	389	Calorimetry	1998CAP/WIX
methyldiphenylphosphino-1-thione **S=$PMePh_2$**	91	381	Calorimetry	1998CAP/WIX
triphenylphosphino-1-thione **S=PPh_3**	88	368	Calorimetry	1998CAP/WIX
Se–P	86.0±2.4	360±10	MS	1973DRO/MYE
Se=PBu_3 **=PCy_3** **=Ph_3**	75 75 67	314 314 280	Calorimetry	1998CAP/WIX
Te–P	70.3±24	294±10	MS	1973DRO/MYE
Te=PBu_3	52	218	Calorimetry	1998CAP/WIX
$(CH_3)_3P$–$Al(CH_3)_3$	21	88	Re-anal.	1989HAA
C–P	122.7±2	513.4±8	MS	1971SMO/MYE
Si–P	86.9	363.6	MS	1972SMO/DEP

续表

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Tl–P	50±3	209±13	MS	1978PIA/BAL
Sb–P	85.3±1.0	356.9±4.2	MS	1972KOR/GIN
$B(CH_3)_3$ –$PH(CH_3)_2$	11.4	47.7	Equilibrium	1956BRO
–$P(CH_3)_3$	16.5	69.0		
BF_3 –$PH(CH_3)_2$	14.7	61.5	Equilibrium	1956BRO
–$P(CH_3)_3$	18.9	79.1		

11.2 As—X 键能

表 11.2 As—X BDEs

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
arsenic clusters				
$As(As)_x$–As				
$x = 0$	91.3	382.0	Review	1992YOO/RUS(b)
1	52	217.6		
2	93.3	390.4		
$As(H)_x$–H				
$x = 0$	(1) 63.9±2.8, at 0K	267.3±11.6	(1) Spectroscopy	(1) 1968DIX/LAM
	(2) 64.6±0.7, at 0K	270.3±2.9	(2) PIMS	(2) 1988BER
1	(2) 66.5±0.2, at 0K	278.2±0.8		
	(3) 52.1	218.0	(3) Derived from $\Delta_f H^\circ$ in ref.	(3) 1998NIST
2	(2) 74.9±0.2	313.4±0.8		
	(4) 76.3±0.2	**319.2±0.8**	(4) Recommend.	(4) 1994BER/ELL
	(5) 73.5±3.0	307.5±12.6	(5) GPA	(5) 1994SUN/PAN
	(6) 72.6	303.9	(6) Photoionization	(6) 1998RAN/SHU
As–D	(7) 63.6, at 0 K	266.3	(7) Spectroscopy	(7) 1979HUB/HER
As–F	(1) 96.8, at 0 K	405.2	(1) Spectroscopy	(1) 1979HUB/HER
–Cl	(2) 107	448	(2) Review	(2) 1970DAR

续表

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
I	(3) 70.0±5.8	293±24	(3) MS	(3) 1979RUN/ZHU
As–O	(1) 114.8, at 0 K	480	(1) Review	(1) 1983PED/MAR
–S	(2) 89.8±1.5, at 0 K	375.7±6.3	(2) MS	(2) 1982LAU/BRI
–Se	(3) 22.2	92.7	(3) MS	(3) 1966PEL/MIL
O=**AsPh**$_3$	102.6±7.3	429±31	Calorimetry	1988BAR/BUR
S=**AsPh**$_3$	70	293	Calorimetry	1998CAP/WIX
As–N	(1) 116±0.5, at 0 K	485±2.1	(1) Spectroscopy	(1) 1991RAJ/SEN
–P	(2) 102.7±3	429.7±12.6	(2) MS	(2) 1974GIN/COC
–Sb	(3) 79.0±1.3	330.5±5.4	(3) MS	(3) 1978DRO/SMO
As–Al	(1) 47.6±1.7	199±7	(1) MS	(1) 1979PIA
–Ga	(2) 48.4±1.2	202.5±4.8	(2) Spectrometry	(2) 1990LEM/BIS
–In	(3) 47.3±2.4	198±10	(3) MS	(3) 1982PIA/GIG
–Tl	(4) 46.4±3.6	194±15	(4) MS	(4) 1972PIA/MAL

11.3 Sb—X 键能

表 11.3 Sb—X BDEs

断裂键 (黑体 = 离解原子或原子团)	BDEs (黑体 = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
antimony clusters				
Sb(Sb)$_x$–Sb				
x = 0	71.2	297.9	Review	1992YOO/RUS(b)
1	53.9	225.5		
2	88.7	371.1		
Sb(H)$_x$–H				
x = 0	(1) 56.4±1.0, at 0 K	236.0±4.2	(1) Photoioniz	(1) 1993RUS/BER(c)
1	(1) 58.3±0.6, at 0 K	243.9±2.5		
2	(2) 68.9±0.5	288.3±2.1	(2) Recommend	(2) 1994BER/ELL
Sb–Li	40.4±2.4, at 0 K	169.0±10.0	MS	1982NEU/ZMB

续表

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值， 括号内数字 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Sb–O	102.8±10, at 0 K	430±42	Review	1983PED/MAR
S=**SbPh**$_3$	67	280	Calorimetry	1998CAP/WIX
Sb–S	90.5	378.7	MS	1972FAU/MIT
Sb–Te	(1) 60.0 (2) 65.4±0.9	250.9 273.6±3.8	MS	(1) 1960POR/SPE (2) 1974SUL/ZEH
Sb–Pb	38.6±2.5	161.5±10.5	MS	1981ZMB/NEU
Sb–N	110±20	460±84	Review	1974GUR/KAR
Sb–P –Bi	(1) 85.3±1.0 (2) 60.4±0.9	356.9±4.2 252.7±3.9	MS	(1) 1972KOR/GIN (2) 1968KOH/CAR
Sb–In	35.4	148.1	MS	1959MAR/DRO
Sb–C_3H_5 **Sb**–C_3H_7	21.6 30.8	90.4 128.9	Pyrolysis	1991LI/LAR

11.4 Bi—X 键能

表 11.4 Bi—X BDEs

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** - 推荐值； 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
bismuth clusters **Bi(Bi)**$_x$–Bi x = 0 1 2	 47 22 61	 196.6 92.0 255.2	Review	1992YOO/RUS(b)
Sn(Bi)$_x$ –**Bi** x = 0 1 2	 46.2±3 26.8±4.5 45.3±5.6	 193±13 112±19 190±23	Derived from $\Delta_f H^\circ$ in ref.	2002MEL/GIN
Pb–**Bi**	33.0	138.1	MS	1967ROV/DRO
Bi–H –D	≤67.7 67.8	≤283.3 283.7	Spectroscopy	1975LIN/NIL
Bi(F)$_x$ –F x = 0	86.7±3	363±13	Photoionization	1992YOO/RUS

续表

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值, 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
1	80.7±3.5	338±15		
2	104±4.6	435±19		
Bi(Cl)$_x$–Cl				
x = 0	71.8	300.4	Derived	1967CUB
1	<58	<242.7		
2	>71	>297.1		
Bi–Br	(1) 63.9	267.4	(1) Calorimetry	(1) 1968CUB(b)
	(2) 57.4	240.2	(2) Spectroscopy	(2) 2000RAJ/RAJ
Bi–I	(1) 51.5	215.5	(1) Calorimetry	(1) 1968CUB
	(2) 44.9	188.0	(2) Spectroscopy	(2) 1982RAO/RAO
Bi–Li	(1) 33.2±1.4	138.9±6	MS	(1) 1980NEU/IHL
	(2) 34.8, at 0 K	145.7		(2) 1981PIT
Bi O	(1) 81.0±1.4	338.9±5.9	(1) MS	(1) 1969UY/DRO
	(2) **79.7±3.0**, at 0 K	**333±13**	(2) Review	(2) 1983PED/MAR
–S	(1) 74.5±1.1	311.8±4.6		
–Se	(1) 66.1±1.4	276.5±5.9		
–Te	(1) 54.6±2.7	228.5±11.3		
Bi–P	(1) 66.4±3.0, at 0 K	278±13	MS	(1) 1974GIN/COC
–Sb	(2) 59.5±0.9, at 0 K	248.9±3.9		(2) 1968KOH/CAR
Bi–Ga	(1) 37±4, at 0 K	154.8±16.7	MS	(1) 1973PIA/DES
–In	(2) 36.7±0.4	153.6±1.7		(2) 1981RIE/HAR
–Tl	(3) 28±3	117.2±12.6		(3) 1972MAR/MAL
Bi–Pb	33.0	138.1	MS	1967ROV/DRO

11.5 Se—X 键能

表 11.5 Se—X BDEs

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Se–Se	(1) 71.2±2	297.9±8	MS	(1) 1966BER/CHU
	(2) 73.6±2.0	307.9±8.4		(2) 1968COL/DRO

续表

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
	(3) 78.6±0.1 (4) **78.1**	329.0±0.3 **326.8**		(3) 1969UY/DRO (4) 1977DRO/SMO
PhSe–SePh	66.9±4.5	280±19	Calorimetry	1980MOR/WAT
$Se(H)_x$–H $x = 0$	(1) 75.16±0.23 (2) 73.8	314.47±0.96 308.7	(1) Photoioniz. (2) Est. by exp.	(1) 1986GIB/GRE (2) 2004HIR/YAN
1	(1) 79.88±0.18 (3) **80.05±0.18**	334.22±0.75 **334.93±0.75**	(3) Recommend	(3) 1994BER/ELL
C_6H_5Se–H	78±4	326.4±16.7	ICR	1996LEE/LI
$Se(F)_x$–F $x = 0$	(1) 80.7±4 6	337.7±19.3	(1) MS	(1) 1970OHA/WAH
4	(2) 64.6±4.6	270.2±19.3	(2) Collision ionization	(2) 1978COM/REI
5	(2) 72.6±4.6	303.9±19.3		
Se–F	81±10	339±42	Review	1974GUR/KAR
–Cl	77	322		
–Br	71±20	297±84		
Se–O	(1) **111.1±5**, at 0 K (2) 101.9±1.5, at 0 K	**465±21** 426.4±6.3	(1) Review (2) MS	(1) 1983PED/MAR (2) 1984SMO/DRO
Se–C	140.2±1.4	586.6±5.9	MS	1977SMO/DRO
Se_2–C	225.4±1.7	943.1±7.1		
$Se=PBu_3$	75	314	Calorimetry	1998CAP/WIX
$Se=PCy_3$	75	314	Calorimetry	1998CAP/WIX
$Se=Ph_3$	67	280	Calorimetry	1998CAP/WIX
Se–S	87.8	367.4	MS	1977DRO/SMO
–Te	70.1	293.3		

11.6 Te—X 键能

表 11.6 Te—X BDEs

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Te–Te	(1) 55.9±2.0 (2) 62.3±0.2	233.9±8.4 260.7±0.8	MS	(1) 1868COL/DRO (2) 1969UY/DRO

续表

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
	(3) **61.6±1**	**257.6±4.1**		(3) 1994VIS/BAB
Te(H)$_x$–H x = 0	(1) 61.2±1.6	256.1±6.7	(1) FT-ICR	(1) 1989GAL/MAR
1	(2) 66.2±1.2	277.0±5.0	(2) Recommend	(2) 1994BER/ELL
Te–I	46±10	192±42	Review	1974GUR/KAR
Te–O	89.1±5	373±21	Review	1983PED/MAR
Te–S	80±10	335±42	Review	1974GUR/KAR
Te–Se	70.1	293.3	MS	1977DRO/SMO
Te=PBu_3	52	218	Calorimetry	1998CAP/WIX
Te–Sb	(1) 60.0 (2) 65.4±0.9	250.9 273.6±3.8	MS	(1) 1960POR/SPE (2) 1974SUL/ZEH

11.7 Po—X 键能

表 11.7 Po—X BDEs

断裂键 (**黑体** = 离解原子或原子团)	BDEs (**黑体** = 推荐值; 括号内数字 = 文献编号)		方法	文献
	kcal/mol	kJ/mol		
Po–Po	44.7	187.0	Spectroscopy	2002CRC

第三篇　原子和自由基生成热的数据库

第 12 章　原子、无机和有机自由基的生成热

12.1　气相原子

表 12.1　气相原子的生成热

原子	$\Delta_f H^\circ$		文献
	kcal/mol	kJ/mol	
Ag	68.1±0 2	284.9±0.8	1984COX/WAG
Al	78.8	329.7	1998NIST
As	72.3 ± 3.1	302.5±13	2002CRC
Au	88.0±0.5	368 2±2.1	2002CRC
B	133.84	560.00	1998NIST
Ba	42.80	179.08	1998NIST
Be	77.4±1.2	324±5	1984COX/WAG
Bi	50.1± 0.5	209.6±2.1	2002CRC
Br	26.74	111.86	1998NIST
C	171.29±0.11	716.68±0.45	1984COX/WAG
Ca	42.5±0.2	177.8±0.8	1984COX/WAG
Cd	28.25 ± 0.05	111.80±0.20	1998NIST
Ce	100.4±0.5	420.1±2.1	1989CHA/GIN
Cl	28.992 ± 0.002	121.301±0.008	1984COX/WAG
Co	101.98	426.68	1998NIST
Cr	95.0	397.48	1998NIST
Cs	18.28±0.24	76.5±1	1984COX/WAG
Cu	80.688	337.60	1998NIST
Dy	69.4±0.5	290.4±2.1	1989CHA/GIN
Er	75.6±0.5	316.4±2.1	1989CHA/GIN
Eu	42.4±0.5	177.4±2.1	1989CHA/GIN
F	18.97 ± 0.07	79.38±0.30	1984COX/WAG
Fe	99.30	415 47	1998NIST
Ga	65.0	271.96	1984COX/WAG
Gd	95.0±0.5	397 5±2.1	1989CHA/GIN
Ge	88.9±0 7	372±3	1984COX/WAG
H	52.103 ± 0.001	217.998±0 006	1984COX/WAG

续表

原子	$\Delta_f H^\circ$		文献
	kcal/mol	kJ/mol	
Hf	147.80	618.40	1998NIST
Hg	14.67 ± 0.01	61.38±0.04	1984COX/WAG
Ho	71.8±0.5	300.6±2.1	1989CHA/GIN
I	25.52 ± 0.01	106.76±0.04	1984COX/WAG
In	58 1±1	243+4	2002CRC
Ir	159.9±1	669±4	2002CRC
K	21.27±0.2	89.0±0.8	1984COX/WAG
La	103.0± 0.5	431.0±2.1	1989CHA/GIN
Li	38.07±	159.3±1.0	1984COX/WAG
Lu	102.2±0.5	427.6±2.1	1989CHA/GIN
Mg	35.16±0.2	147.1±0.8	1984COX/WAG
Mn	67.70	283 26	1998NIST
Mo	157.50	658.98	1998NIST
N	112.97 + 0 096	472.68±0.40	1984COX/WAG
Na	25.65	107.30	1998NIST
Nb	175.20	733.04	1998NIST
Nd	78.1±0.5	326.9±2.1	1989CHA/GIN
Ni	102.80	430.12	1998NIST
O	59.555 ± 0.02	249.18±0.10	1984COX/WAG
Os	188±1.5	787±6 3	2002CRC
P	75 619	316.39	1998NIST
Pb	46.65±0.2	195.2±0.8	1984COX/WAG
Pd	90.0±0.5	376.6±2.1	2002CRC
Pr	85.3±0.5	356.9±2.1	1989CHA/GIN
Pt	135.2±0.3	565.7±1.3	2002CRC
Pu	87.1±4.1	364.4±17	2003CRC
Rb	19.3±0.2	80.9±0.8	1984COX/WAG
Re	185±1 5	774±6.3	2002CRC
Rh	132.9±1	556±4	2002CRC
Ru	155 5±1.5	650.6÷6.3	2002CRC
S	66.20	276 98	1998NIST
Sb	63.2+0.6	264.4±2.5	2002CRC
Sc	90.3±1	377.8±4	2002CRC
Se	54.3±1	227.2±4	2002CRC
Si	107.55±2	450.0±8	1984COX/WAG
Sm	49.4±0.5	206.7±2.1	1989CHA/GIN
Sn	71.99 ± 0.36	301.2±1.5	1984COX/WAG
Sr	39.2	164 0	1998NIST
Ta	186.9±0.6	782.0±2.5	2002CRC
Th	92.9±0.5	388 7±2.1	1989CHA/GIN

续表

原子	$\Delta_f H^\circ$		文献
	kcal/mol	kJ/mol	
Te	47.0±0.5	196.6±2.1	1989CHA/GIN
Th	143.9±1.4	602±6	1998NIST
Ti	113.20	473.63	1998NIST
Tl	43.55±0.1	182.21±0.4	2002CRC
Tm	55.5±0.5	232.2±2.1	1989CHA/GIN
U	127.4±2	533±8	1998NIST
V	123.20	515.47	1998NIST
W	203.40	851.03	1998NIST
Y	101.5± 0.5	424.7±2.1	1989CHA/GIN
Yb	37.2±0.5	155.6±2.1	1989CHA/GIN
Zn	31.17±0.10	130.4±0.40	1984COX/WAG
Zr	145.80	610.03	1998NIST

12.2 气相无机自由基

12.2.1 含金属的无机自由基

表 12.2.1 含金属的无机自由基的生成热

含金属的无机自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
AlH	62±5	260±20	1998CHA
AlH_2	66.2±5	277±20	1996GUR/VEY
AlF	63.5+0.8	265.7±3.4	1998CHA
AlF_2	- 166±10	–695±40	1998CHA
AlHF	–43.7±7	–183±30	1996GUR/VEY
AlFCl	–117±15	–490±63	1998CHA
AlCl	–12.3±1.5	–51.5±6.3	1998CHA
$AlCl_2$	–67±5	–280±20	1998CHA
AlHCl	2.5±7	10.5±30	1996GUR/VEY
AlBr	3.8±3	15.9±12 6	1998CHA
$AlBr_2$	–33.6±12	–141±50	1996GUR/VEY
AlI	16 2+1 0	68±4.2	1998CHA
AlI_2	–8.1±12	–34±50	1996GUR/VEY
AlC	164.8±2.4	689.5±10	1998CHA
AlO	16.0±2	67±8	1998CHA
AlOH	–43.0±3	- 180±13	1998CHA
$Al(OH)_2$	-121.3±12	–508±50	1996GUR/VEY
Al(OH)Cl	–89.3±10	–374±40	1996GUR/VEY
AlN	125±9	523±38	1998CHA
AlS	57.0±2	238.5±8.4	1998CHA

续表

含金属的无机自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
BaH	50.1±1.4	209.5±5.9	1996GUR/VEY
BaOH	–53.6±3.6	–224.3±15	1996GUR/VEY
BaF	–77.0±2	–322.2±8.4	1998CHA
BaCl	–34.0±3	–1142.3±13	1998CHA
BaBr	–26.4±10	–110.6±42	1998CHA
BaI	10.1±20	–42.4±84	1998CHA
BeH	76.7±6.9	321±29	1998CHA
BeF	40.6±2	–170±8	1998CHA
BeCl	14.5±3	60.7±12.6	1998CHA
BeBr	28.7±10	120±42	1998CHA
BeI	40.6±10	170±42	1998CHA
BeOH	–27.4+9	–115±38	1998CHA
BeN	102	427	1998CHA
CaH	54.8±0.5	229.4±2.0	1996GUR/VEY
CaF	–65±2	–272±8	1998CHA
CaCl	–25±3	–104.6±13	1998CHA
CaBr	11.8±10	–49±42	1998CHA
CaI	1.2±20	–5.0±84	1998CHA
CaOH	–46.3±5	–194±21	1998CHA
CoF_2	–85.2±3	–356.5±12.6	1998CHA
CoCl	46±3	193±12.6	1998CHA
$CoCl_2$	–22.4±2	–93.7±8	1998CHA
CuF	–3.0±4	–12.6±16.7	1998CHA
CuCl	21.8±0.4	91.1±1.7	1998CHA
FeF	11.2±5	46.7±20.9	1998CHA
FeCl	60±20	251±84	1998CHA
GaH	51.2±1.1	214±5	1996GUR/VEY
GaO	35.1±5	147±20	1996GUR/VEY
GaOH	–34.3±2.4	–144±10	1996GUR/VEY
GaF	–55.6±2.6	233±11	1996GUR/VEY
$\bullet GaF_2$	–123.5±12	–517±50	1996GUR/VEY
GaCl	–16.7±1	–69.9±4	1996GUR/VEY
$\bullet GaCl_2$	–52.8±12	–221±50	1996GUR/VEY
GaBr	–4.3±2.4	18±10	1996GUR/VEY
$\bullet GaBr_2$	35.6±12	–149±50	1996GUR/VEY
GaI	10.7±0.7	44.9±3	1996GUR/VEY
$\bullet GaI_2$	–6.9±12	–29±50	1996GUR/VEY
$\bullet GeH_3$	53.0±2	221 8±8.4	1994BER/ELL
GeF_2	–137.2±4.8	–574±20	1991GUR/VEY

续表

含金属的无机自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
•GeF_3	−192.9±12	−807±50	1991GUR/VEY
GeCl	16.5±4.3	69±18	1991GUR/VEY
$GeCl_2$	−40.9±1.2	−171±5	1991GUR/VEY
•$GeCl_3$	−64.0±12	−268±50	1991GUR/VEY
GeBr	32.8±1.2	137±5	1991GUR/VEY
$GeBr_2$	−14.6±1.2	−61±5	1991GUR/VEY
•$GeBr_3$	−28.4±12	−119±50	1991GUR/VEY
GeI	50.4±6	211±25	1991GUR/VEY
GeI_2	12.0±1	50.2±4	1991GUR/VEY
•GeI_3	10±12	42±50	1991GUR/VEY
HgH	57.0±4	238.5±16.7	1998CHA
HgF	0.7±12	2.9±50	1998CHA
HgCl	18.7±2.3	78.5±9.6	1998CHA
HgBr	24.9±9	104.2±38	1998CHA
HgI	31.9±1.1	133.5±4.6	1998CHA
InH	51.4±0.5	215±2	1996GUR/VEY
InO	34.9±6	146±25	1996GUR/VEY
InOH	29.7±3.6	124.4±15	1996GUR/VEY
InF	−46.2±2.4	−193.4±10	1996GUR/VEY
•InF_2	−109.2±12	−457±50	1996GUR/VEY
InCl	−17.2±1.2	−72.1±5	1996GUR/VEY
•$InCl_2$	−48.0±12	−201±50	1996GUR/VEY
InBr	−12.9±2	−54.1±8.5	1996GUR/VEY
•$InBr_2$	−35.8±12	−150±50	1996GUR/VEY
InI	6.3±0.3	26.3±1.4	1996GUR/VEY
•InI_2	−9.3±12	−39±50	1996GUR/VEY
KO	17±10	71.1±41.8	1998CHA
LiO	20.1±5	84.1±20.9	1998CHA
LiN	80±40	334.7±167	1998CHA
MgH	40.4±11.5	169±48	1998CHA
MgF	−56.6±2	−236.8±8.4	1998CHA
MgCl	10.4±10	−43.5±42	1998CHA
MgBr	−8.4±10	−35.3±41.8	1998CHA
MgI	5.9±10	24.6±41.8	1998CHA
MgN	69±6	288.7±25.1	1998CHA
MoF	67.6±3	282.8±12.6	1998CHA
MoF_2	−38.9±4	162.8±16.7	1998CHA
MoF_3	−145±4	−607±16.7	1998CHA
MoF_4	−226.5±4	−947.7±16.7	1998CHA
MoF_5	−296.7±1	1241.4±4.2	1998CHA
$MoCl_4$	−92.0±3	−384.9±12.6	1998CHA

续表

含金属的无机自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$MoCl_5$	−107.0±1	−447.7±4.2	1998CHA
MoBr	109.3±10	457 3±42	1998CHA
$MoBr_2$	40±20	167.4±84	1998CHA
$MoBr_3$	−2.0±7.9	−8.4±33	1998CHA
$MoBr_4$	−40.9±2	−171.1±8	1998CHA
MoI	119.2±10	498 7±41.8	1998CHA
MoI_2	61 6±10	257.7±41.8	1998CHA
MoI_3	43.7±10	182.8±41.8	1998CHA
MoI_4	29.8±10	124.7±41.8	1998CHA
NaO	20±10	83.7±41.8	1998CHA
NiCl	43.5±1	182.0±4 2	1998CHA
NiS	85.4±4	357.4±16.7	1198CHA
PbH	56.5±4.6	236.2±19.2	1998CHA
PbF	−19.2±2.5	-80.3±10.5	1998CHA
PbF_2	104±2	−435.1±8.4	1998CHA
PbF_3	−117±14.3	490±60	1991GUR/VEY
PbCl	3.6±12	15.1±50	1998CHA
$PbCl_2$	−41.6±0.3	−174.1±1.3	1998CHA
$PbCl_3$	-42.5±19	−178±80	1991GUR/VEY
PbBr	16.9±10	70.9±42	1998CHA
$PbBr_2$	-25.0±1.5	−104.4±6.3	1998CHA
$PbBr_3$	-24.9±19	−104±80	1991GUR/VEY
PbI	25.7±9	107.4±37.7	1998CHA
PbI_2	−0.76±1	−3.2±4.2	1998CHA
PbI_3	5.2±19	22±80	1991GUR/VEY
SnF	−22.7±1.7	−95±7.2	1991GUR/VEY
SnF_2	−122.1±2.2	−511±9.2	1991GUR/VEY
SnF_3	−154.6±12	-647±50	1991GUR/VEY
SnCl	8.4±2.9	35±12	1991GUR/VEY
$SnCl_2$	−48.4±1.7	−202.6±7.1	1991GUR/VEY
$SnCl_3$	−69 8+12	−292±50	1991GUR/VEY
SnBr	18.2±2.9	76±12	1991GUR/VEY
$SnBr_2$	-28.4±0.7	−119±2.8	1991GUR/VEY
$SnBr_3$	−38±12	−159±50	1991GUR/VEY
SnI	41.3±2.9	173±12	1991GUR/VEY
SnI_2	−1.9±1	−8.1±4.2	1991GUR/VEY
SnI_3	−1.9±12	−8±50	1991GUR/VEY
SrH	52.4±0.7	219.2±3.1	1996GUR/VEY
SrOH	-46.4±2.4	−194.1±10	1996GUR/VEY
SrF	−70.4±2	- 294.6±8.4	1998CHA
SrCl	-29.6±2	−123.9±8.4	1998CHA

续表

含金属的无机自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
SrBr	-21.3±10	-89.1±42	1998CHA
SrI	-7.3±20	-30.5±83.7	1998CHA
TiF	-16±10	-66.9±41.8	1998CHA
TiF_2	-164.5±10	-688.3±41.8	1998CHA
TiF_3	-284.1±10	-1188.7±41.8	1998CHA
TiCl	36.9±10	154.4±41.8	1998CHA
$TiCl_2$	-56.7±4	237.2±12.6	1998CHA
$TiCl_3$	-128.9±1.5	539.3±6.3	1998CHA
TiBr	50.8±10	212.5±42	1998CHA
$TiBr_2$	-42.8±5	-179.1±20.9	1998CHA
$TiBr_3$	-89.6±3	-374.9±10.5	1998CHA
TiI	65.5±10	274.1±41.8	1998CHA
TiI_2	4.7±8	-19.7±33.5	1998CHA
TiI_3	-35.9±8	-150.2±33.5	1998CHA
TlH	49.0±0.4	204.8±1.5	1996GUR/VEY
TlOH	26.3±7	-110±30	1996GUR/VEY
TlF	44.7±0.8	-186.9±3.4	1996GUR/VEY
TlCl	16.0±0.3	-66.9±1.1	1996GUR/VEY
TlBr	8.2±0.1	34.3±0.6	1996GUR/VEY
TlI	3.8±0.1	15.9±0.5	1996GUR/VEY
WF	92.3±15	386.2±62.8	1998CHA
WCl	132.3±10	553.5±41.8	1998CHA
WCl_2	-3±25	-12.6±105	1998CHA
WBr	140±20	586±84	1998CHA
ZrH	123.4	516.3	1998CHA
ZrF	19.8±5	82.8±20.9	1998CHA
ZrF_2	-133.4±5	-558.1±20.9	1998CHA
ZrF_3	-264.2±5	-1105.4±21	1998CHA
ZrCl	49.1±5	205.4±20.9	1998CHA
$ZrCl_2$	44.5±5	-186.2±20.9	1998CHA
$ZrCl_3$	-125.3±5	-524.3±20.9	1998CHA
ZrBr	72±10	301.2±42	1998CHA
$ZrBr_2$	41.7±10	-174.5±42	1998CHA
$ZrBr_3$	-103	-431	1998CHA
ZrI	141.3±10	591.2±41.8	1998CHA
ZrI_2	-15.9	-66.6	1998CHA
ZrI_3	-53	-221.8	1998CHA
ZrN	170.5	713.4	1998CHA

12.2.2 含非金属的无机自由基

表 12.2.2 含非金属的无机自由基的生成热

含非金属的无机自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
AsH	40.1	167.8	1988BER
AsH_2	40.1±0.3	167.8±1.3	1994BER/ELL
BH	105.8±2	442.7±8.4	1998CHA
BH_2	48±15	201±63	1998CHA
BF	–27.7±3.3	--116±14	1998CHA
BF_2	–141±3	- 590±13	1998CHA
BCl	33.8	141.4	1998CHA
BCl_2	–19±3	-79.5±12.6	1998CHA
BBr	56±10	234±42	1998CHA
BBrF	–57.5±2.4	- 240.6±10	1998CHA
BBrCl	–2.5	–10.5	1998CHA
BBr_2	15±3.6	62.8±15	1998CHA
BI	72.9±10	305±42	1998CHA
BI_2	58±15	243±63	1998CHA
BC	198±10	828.4±41	1998CHA
BO	0±2	0±8	1998CHA
BS	–166±6	–695±25	1998CHA
C_2	195.3±2	817±8	1994GIN/FIN
C_3	198.6±3	831±13	1994GIN/FIN
C_4	251.4±3.8	1052±16	1994GIN/FIN
C_5	258.4±3.8	1081±16	1994GIN/FIN
C_6	313.6±4.3	1312±18	1994GIN/FIN
C_7	316.7±4.3	1325±18	1994GIN/FIN
NO	21.58±0.04	90.29±0 17	1998CHA
NO_2	7.91±0.2	33.10±0.8	1998CHA
ONOO	19.8	82.8	1993DAV/KIM
sym–NO_3	15 8	66.1	1976BEN
N_2O	19.61±0.1	82.05±0.4	1998CHA
NH	85.3±0.3	357±1	1999AND
NH_2	44.5±0.3	186±1	1999AND
N_3	112±5	468.6±20.9	1982MCM/GOL
N_2H_3	58.2	243.5	1988GRE/COL
(Z) N_2H_2	50.9±2.6	213.0±10.9	1998CHA
NF_2	10 1±2	42 3±8	1998CHA
NF	50.0	209.2	1979HUB/HER
NHF	26.8±3.6	112±15	1989GUR/VEY
HNO	25.6±0.6	107.1±2.5	1999AND

续表

含非金属的无机自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
FNO	−15.7±0.4	65.7±1.7	1998CHA
ClNO	12.36±0.10	51.71±0.42	1998CHA
NBr	71.9±5	301±21	1998CHA
BrNO	19.63±0.2	82.13±0.8	1998CHA
INO	26.8±5	112.1±20.9	1998CHA
NCN	111.1±0.7	464.8±2.9	1999BIS/CHO
NSi	89±15	372.4±62.8	1998CHA
OH	8.91±0.07	37.28±0.29	2002RUS/WAG
OOH	3.3±0.8	13.8±3.3	1998LIT/RUS
OF	26.0±2.4	109±10	1998CHA
OCl	24.29±0.02	101.63±0.1	1998CHA
OBr	30.2±0.4	126.2±1.7	2001IUPC
OI	27.7±1.2	115.9±5	2001IUPC
OP	5.6±1	−23.3±4.2	1998CHA
PH	55.8±8	233.6±33.5	1998CHA
PH_2	33.1±0.6	138.5±2.5	1994BER/ELL
PF	−12.5±5	−52.3±20.9	1998CHA
PF_2	−116.7±5	−488.3±20.9	1998CHA
PCl	30.8	129	1998CHA
PCl_2	−13.0±1.4	54.3±6	1989GUR/VEY
PFCl	−67.6±7	283±30	1989GUR/VEY
PBr	38.9	162.6	1998CHA
SH	34.18±0.68	143.01±2.85	1994BER/ELL
SSH	27.6±3.5	115.5±14.6	1993OHA/DEP
SO	1.2±0.3	5.0±1.3	1998CHA
SO_2	−70.95±0.05	−296.84±0.21	1998CHA
SO_3	−94.59±0.17	−395.77±0.7	1998CHA
S_2O	−13.5±8	−56.48±33.5	1998CHA
HSO	1.5±0.7	6.1±2.9	1993BAL/CAS
HSO_2	53.0	221.8	1980BOY/GUP
$HOSO_2$	92	385	1984MAR
SF	3.1±1.5	13.0±6.3	1998CHA
SF_5	−70.9±4	−296.7±16.7	1998CHA
SF_3	−120.2±8	−503.0±33.5	1998CHA
SF_4	−182.415	763.2±20.9	1998CHA
SF_5	−210.3±3.6	−879.9±15.1	1998CHA
SCl	37.4±4	156.5±16.7	1998CHA
HSe	34.6±0.5	144.8±2.1	1994BER/ELL
SP	33.1±10	138.6±41.8	1998CHA

续表

含非金属的无机自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
SbH_2	51.5±0.6	215.5±2.5	1994BER/ELL
HPO	−13.6±10	−57±42	1989GUR/VEY
HTe	37.9±1.2	158.6±5.0	1994BER/ELJ

12.3 气相有机自由基

12.3.1 C-中心自由基

表 12.3.1 C-中心自由基的生成热

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
CH	142.77±0.3	597.37±1.3	1991GUR/VEY
CH_2 (triplet)	93.31±0.20	390.41±0.84	1999RUC/LIT
CH_2 (singlet)	102.31±0.20	428.07±0.84	1999RUC/LIT
$^\bullet CH_3$, methyl	35.06±0.1	146.69±0.42	1987DOB/BEN
$^\bullet C_2H$, acetenyl, CH≡C$^\bullet$	135.6±0.5	567.4±2.1	1994MOR/ASH
$^\bullet C_2H_2$, CH$_2$–C$^{\bullet\bullet}$	100.3±4	419.7±16.7	1999AHM/PET
$^\bullet C_2H_3$, vinyl, CH$_2$=C$^\bullet$H	71.6±0.8	299.6±3.3	1994BER/ELL
$^\bullet C_2H_5$, ethyl, CH$_3$C$^\bullet$H$_2$	28.4±0.3	118.8±1.3	1997DOB/BEN
$^\bullet C_3H_3$, propargyl, CH≡CC$^\bullet$H$_2$	81.0±1.0	339.0±4.2	1996TSA
$^\bullet C_3H_3$, CH$_3$C≡C$^{\bullet\bullet}$	121±3.0	506.3±12.6	2000SHI/ERV
$^\bullet C_3H_3$, CH$_2$=C=CH$^\bullet$ ↔ CH≡CC$^\bullet$H$_2$	81.0±1.0	339.0±4.2	1996TSA
$^\bullet C_3H_3$, cyclopro-2-en-1-yl	105.1±4.1	439.7±17.2	1980DEF/MCI
$^\bullet C_3H_5$, allyl, CH$_2$=CHC$^\bullet$H$_2$	40.9±0.7	171.0±3.0	1996TSA
$^\bullet C_3H_5$, CH$_3$CH–C$^\bullet$H	63.8±1.5	267±6	1999TSA
$^\bullet C_3H_5$, CH$_3$C$^\bullet$–CH$_2$	55.3	231.4	1990TAK
$^\bullet C_3H_5$, cyclopropyl	66.9±2.5	279.9±10.5	1979BAG/BEN
n-$C_3H_7^\bullet$, n-propyl, CH$_3$CH$_2$C$^\bullet$H$_2$	23.9±0.5	100±2	1996TSA
i-$C_3H_7^\bullet$, i-propyl, CH$_3$C$^\bullet$HCH$_3$	21.0±0.7	88±3	1988RUS/SEE(b)
$^\bullet C_4H_5$, CH$_3$C≡CC$^\bullet$H$_2$	70.2±2	293.7±8.4	1982NGU/KIN
$^\bullet C_4H_5$, CH≡CC$^\bullet$HCH$_3$	70.5±2.2	295.0±9.2	1981NGU/KIN
$^\bullet C_4H_7$, CH$_3$CH=CHC$^\bullet$H$_2$	34.9±2.0	146±8	1999TSA
$^\bullet C_4H_7$, CH$_2$=CHCH$_2$C$^\bullet$H$_2$	46.0	192.5	1984SCH/HOU
$^\bullet C_4H_7$, CH$_2$=C(CH$_3$)C$^\bullet$H$_2$	30.6±0.6	128.0±2.5	1991ROT/BAU
$^\bullet C_4H_7$, CH$_2$=CHC$^\bullet$HCH$_3$	31.8±1.5	133.1±6.5	1987LIA/AUS
$^\bullet C_4H_7$, cyclopropylmethyl	51.1±1.6	213.8±6.7	1971MCM/GOL
$^\bullet C_4H_7$, cyclobutyl	51.4±1.0	215.1±4.2	1972MCM/GOL

续表

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
n-$C_4H_9^\bullet$, n-butyl, $CH_3CH_2CH_2C^\bullet H_2$	18.6±0.5	77.8±2.1	1990WAL/TSA
i-$C_4H_9^\bullet$, i-butyl, $(CH_3)_2CHC^\bullet H_2$	16.7±1.0	70±4	1999TSA
s-$C_4H_9^\bullet$, s-butyl, $CH_3C^\bullet HCH_2CH_3$	16.2+0.5	67.8+2.1	1992SEA/PIL
t-$C_4H_9^\bullet$, t-butyl, $(CH_3)_3C^\bullet$	11.5±0.7	48±3	1996TSA
$^\bullet C_5H_4$, cyclo-penta-1,3-dinyl	252.4±11	1056±46	2000SZT/BAE
$^\bullet C_5H_5$, CH_2=CHC≡$CC^\bullet H_2$	84.0	351.5	1992STA/KIN
$^\bullet C_5H_5$, CH_2=CH-$C^\bullet H$-C≡CH	89	372.4	1988LIA/BAR
$^\bullet C_5H_5$, cyclopenta-1,3-dien-5-yl	62.5±1	261.5±4.2	2001ROY/BRA
$^\bullet C_5H_7$, CH_3C≡$CC^\bullet HCH_3$	65.2±2.2	272.8±9.2	1981KIN/NGU
$^\bullet C_5H_7$, CH≡$CC^\bullet HC_2H_5$	66.2±2	277.0±8.4	1976LOS/TRA
$^\bullet C_5H_7$, CH≡$CC^\bullet(CH_3)_2$	61.5±2.2	257.3±9.2	1977KIN
$^\bullet C_5H_7$, CH_2=CHCH=$CHC^\bullet H_2$	49±3	205.0±12.6	1982MCM/GOL
$^\bullet C_5H_7$, $(CH_2$=$CH)_2C^\bullet H$	49.7±1.0	208.0±4.2	1991CLA/CUL
$^\bullet C_5H_7$, CH_3CH=C=$CHC^\bullet H_2$	66.9	278.0	2001TUM/DEN
$^\bullet C_5H_7$, spiropentyl	91.0±1.0	380.7±4.2	1971FER/WHI
$^\bullet C_5H_7$, cyclopent-1-en-3-yl	38.4±1.0	160.7±4.2	1970FUR/GOL(b)
$^\bullet C_5H_9$, cyclopentyl	25.3±1.0	105.9±4.2	1982CAS/GRI
$^\bullet C_5H_9$, CH_2=$CHC^\bullet HCH_2CH_3$	26.2±2	109.6±8.4	1976LOS/TRA
$^\bullet C_5H_9$, CH_3CH=$CHC^\bullet H(CH_3)$	22	92	1988LIA/BAR
$^\bullet C_5H_9$, CH_3CH=$C(CH_3)C^\bullet H_2$	22.0	92.0	2001TUM/DEN
$^\bullet C_5H_9$, CH_2=$CHC^\bullet(CH_3)_2$	20.8±2	87.0±8.4	1970EGG/JOL
$^\bullet C_5H_9$, CH_2=$C(CH_3)C^\bullet H(CH_3)$	22.4	93.7	2001TUM/DEN
$^\bullet C_5H_9$, CH_2=$C(C^\bullet H_2)CH_2CH_3$	27.3	114.2	2001TUM/DEN
$^\bullet C_5H_9$, CH_2=$CH(CH_2)_2C^\bullet H_2$	42.9	179.5	1996CAM/AUT
n$C_5H_{11}^\bullet$, $CH_3CH_2CH_2CH_2C^\bullet H_2$	13	54.4	1988LIA/BAR
$^\bullet C_5H_{11}$, $(C_2H_5)_2C^\bullet H$	11.2	47.0	1996CAM/AUT
$^\bullet C_5H_{11}$, $(nC_3H_7)(CH_3)C^\bullet H$	12	50.2	1988LIA/BAR
$^\bullet C_5H_{11}$, $(CH_3)_3C^\bullet CH_2$	8.7±2	36.4±8.4	1969LAR/HAR
$^\bullet C_5H_{11}$, $(C_2H_5)(CH_3)_2C^\bullet$	6.9	29	1999TSA
$^\bullet C_6H_5$, phenyl	78.9±0.8	330.1±3.3	1994BER/ELL
$^\bullet C_6H_7$, cyclohexa-1,3-dien-5-yl	47.6	199.2	1991STE/BRO
$^\bullet C_6H_7$, cyclohexa-1,4-dien-3-yl	48.2±1.2	201.7±5.0	1986TSA
$^\bullet C_6H_9$, CH_3C≡$CC^\bullet(CH_3)_2$	53.0±2.2	221.8±9.2	1981KIN/NGU
$^\bullet C_6H_9$, $(CH_2$=$CH)_2C^\bullet(CH_3)$	46.3	193.7	1999LAA/MUL
$^\bullet C_6H_9$, cyclohexa-1-en-3-yl	28.6	119.7	1988BOR/CHE
$^\bullet C_6H_{11}$, CH_2=$CH(CH_2)_3C^\bullet H_2$	37.9	158.6	1996CAM/AUT
$^\bullet C_6H_{13}$, CH_2=$CHC^\bullet H(CH_3)_2CH_3$	21.3	89.0	2001TUM/DEN
$^\bullet C_6H_{11}$, CH_2=$C(CH_3)C^\bullet(CH_3)_2$	9.0±1.5	37.7±6.3	1973ROD/WU
$^\bullet C_6H_{11}$, $(CH_3)_2C$=$C(CH_3)C^\bullet H_2$	9.5±1.5	39.7±6.3	1973ROD/WU

续表

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$^\bullet C_6H_{11}$, $(CH_3)_2C{=}CHC^\bullet H(CH_3)$	11.3	47.3	2001TUM/DEN
$^\bullet C_6H_{11}$, (Z)-$CH_3CH{-}CHC^\bullet(CH_3)_2$	13.0	54.4	2001TUM/DEN
$^\bullet C_6H_{11}$, cyclohexyl	18±1.5	75.3±6.3	1981TSA
$nC_6H_{13}^\bullet$, $CH_3CH_2CH_2CH_2CH_2C^\bullet H_2$	8	33.5	1988LIA/BAR
$^\bullet C_6H_{13}$, $(nC_4H_9)(CH_3)C^\bullet H$	7	29.3	1988LIA/BAR
$^\bullet C_6H_{13}$, 2-methyl-2-pentyl	0.8±2	3.3±8.4	1983SER/GOR
$^\bullet C_6H_{13}$, 3-methyl-3-pentyl	3.4	14.2	1996CAM/AUT
$^\bullet C_6H_{13}$, 2,3-dimethyl-2-butyl	0.7±2.4	3.1±10	2000KIR/KOR
$^\bullet C_7H_3$, $(CH{\equiv}C)_3C^\bullet$	187.5	784.5	1990TAK
$^\bullet C_7H_7$, benzyl, $C_6H_5C^\bullet H_2$	48.4±1.5	202.5±6.3	1994BER/ELL
$^\bullet C_7H_7$, quadricyclolan-5-yl	138.3±1.3	578.6±5.4	1996LEE/DEP
$^\bullet C_7H_7$, quadricyclolan-4-yl	140.4±1.3	587.4±5.4	1996LEE/DEP
$^\bullet C_7H_7$, norborna-2,5-dien-7-yl	122.3±1.9	511.7±7.9	1996LEE/DEP
$^\bullet C_7H_7$, cyclohepta-1,3,5 trien-7-yl	68.2±3	285.3±12.6	1980DEF/MCI
$^\bullet C_7H_9$, $CH_2{=}CH(CH{=}CH)_2CC^\bullet H_2$	60	251.0	1996CAM/AUT
$^\bullet C_7H_9$, $(CH_2{=}CH)_3C^\bullet$	65.5	274.0	1990TAK
$^\bullet C_7H_{11}$, norborn-1-yl	32.6±2.5	136.4±10.5	1970ONE/BAG
$^\bullet C_7H_{11}$, cycloheptenyl	28.5	119.2	2001TUM/DEN
$^\bullet C_7H_{13}$, cycloheptyl	12.1±1	50.6±4.2	1971FER/WHI
$^\bullet C_7H_{13}$, cyclo-[$C^\bullet(CH_3)(CH_2)_5$]	5.4	22.6	2001TUM/DEN
$^\bullet C_7H_{13}$, cyclo-[$C^\bullet(CH_2CH_3)(CH_2)_4$]	11.2	47.0	2001TUM/DEN
$^\bullet C_7H_{15}$, $(nC_5H_{11})(CH_3)CH^\bullet$	2	8.4	1988LIA/BAR
$^\bullet C_8H_7$, cubyl	198.6±4	831.0±16.7	1997HAR/EMR
$^\bullet C_8H_7$, $C_6H_5C^\bullet{-}CH_2$	74	309.6	1997PON/TAK
$^\bullet C_8H_7$, $C_6H_5CH{-}CH^\bullet$	92.5	387.0	1997PON/TAK
$^\bullet C_8H_9$, $C_6H_5C^\bullet H(CH_3)$	40.4	169.0	1982MCM/GOL
$^\bullet C_8H_9$, 1-phenyl-eth-2-yl	55.9	234.0	1989FRE/OLM
$^\bullet C_8H_9$, p-$CH_3C_6H_4C^\bullet H_2$	40	167.4	1986HAY/KRU
$^\bullet C_8H_9$, m-$CH_3C_6H_4C^\bullet H_2$	40	167.4	1986HAY/KRU
$^\bullet C_8H_9$, o-$CH_3C_6H_4C^\bullet H_2$	40	167.4	1986HAY/KRU
$^\bullet C_8H_{11}$, $C_6H_5C^\bullet(CH_3)_2$	32.0	134.0	1997LAA/BOR
$^\bullet C_8H_{13}$, $CH_2{-}CHCH{-}CHC^\bullet H(CH_2)_3CH_3$	31.2	130.5	2001TUM/DEN
$^\bullet C_8H_{13}$, $CH_2{=}CHC^\bullet H(CH_2)_3CH{=}CH_2$	31.2	130.5	2001TUM/DEN
$^\bullet C_8H_{13}$, bicyclooct-1-yl	22.0	92.0	1971DAN/TIP
$^\bullet C_8H_{15}$, $CH_2{=}CHC^\bullet H(CH_2)_4CH_3$	11.9	49.8	2001TUM/DEN
$^\bullet C_8H_{15}$, (E)-$CH_3CH{=}C^\bullet(CH_2)_4CH_3$	7.1	29.7	2001TUM/DEN
$^\bullet C_8H_{15}$, (Z)-$(CH_3)_2C^\bullet CH{=}CHCH(CH_3)_2$	2.2	9.2	2001TUM/DEN
$^\bullet C_8H_{15}$, cyclooctanyl	14.2	59.4	2001TUM/DEN

续表

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$^{\bullet}C_8H_{15}$, cyclo-[$C^{\bullet}(CH_2CH_3)(CH_2)_5$]	2.4	10.0	2001TUM/DEN
$^{\bullet}C_8H_{15}$, (E)-cyclo-[$C^{\bullet}(CH_3)CH(CH3)(CH_2)_4$]	−2.1	−8.8	2001TUM/DEM
$^{\bullet}C_8H_{15}$, (Z)-cyclo-[$C^{\bullet}(CH_3)CH(CH3)(CH_2)_4$]	1.5	6.3	2001TUM/DEM
$^{\bullet}C_9H_7$, indenyl	71	297.1	1982MCM/GOL
$^{\bullet}C_9H_9$, indanyl-1	48.8±2	204.2±8.4	2000DEN/DEN
$^{\bullet}C_9H_{11}$, 2,6-dimethylbenzyl	29 8	124.7	1980BAR/STE
$^{\bullet}C_9H_{11}$, 3,6-dimethylbenzyl	29.8	124.7	1980BAR/STE
$^{\bullet}C_9H_{11}$, 3,5-dimethylbenzyl	29.8	124 7	1980BAR/STE
$^{\bullet}C_9H_{11}$, $C_6H_5C^{\bullet}(CH_3)_2$	32.0±1.0	133 9±4.2	1997LAA/BOR
$^{\bullet}C_9H_{17}$, cyclononanyl	12.5	52.3	2001TUM/DEN
$^{\bullet}C_{10}H_7$, naphth-1-yl	96.0±1.3	401.7±5.4	2000REE/KAS
$^{\bullet}C_{10}H_7$, naphth-2-yl	95.7±1.4	400.4±5.9	2000REE/KAS
$^{\bullet}C_{10}H_{11}$, tetralin-1-yl	37±1.2	154.8±5.0	1997LAA/MUL
$^{\bullet}C_{10}H_{13}$, 1-phenyl-but-4-yl	45.9	192.0	1989FRE/OLM
$^{\bullet}C_{10}H_{13}$, $(C_6H_5CH_2)(C_2H_5)C^{\bullet}H$	44.1	184.5	1989FRE/OLM
$^{\bullet}C_{10}H_{13}$, $(C_6H_5CH_2CH_2)(CH_3)C^{\bullet}H$	44.1	184.5	1989FRE/OLM
$^{\bullet}C_{10}H_{13}$, $C_6H_5C^{\bullet}HCH_2CH_2CH_3$	32.2	134.7	1989FRE/OLM
$^{\bullet}C_{10}H_{15}$, 1-adamantyl	12.3	51.5	1986KRU/BEA
$^{\bullet}C_{10}H_{15}$, 2 adamantyl	14.8	61.9	1986KRU/BEA
$^{\bullet}C_{10}H_{19}$, cyclodecanyl	7.7	32.2	2001TUM/DEN
$^{\bullet}C_{11}H_9$, 1-naphthylmethyl	60.4	252.7	1982MCM/GOL
$^{\bullet}C_{11}H_{21}$, cycloundecanyl	1.8	7.5	2001TUM/DEN
$^{\bullet}C_{12}H_{23}$, cyclododecanyl	−9.2	−38.5	2001TUM/DEN
$^{\bullet}C_{13}H_9$, 9-fluorenyl	71.1	297.5	1994RAK/VER
$^{\bullet}C_{13}H_{11}$, $(C_6H_5)_2C^{\bullet}H$	72.2±1.0	302.1±4.2	1991PAR/HAN
$^{\bullet}C_{14}H_{11}$, 9-methyl-9-fluorenyl	64.1	268.2	1994RAK/VER
$^{\bullet}C_{14}H_{11}$, 9,10-dihydroanthracen-9-yl	62.4	261.0	1991STE/BRO
$^{\bullet}C_{15}H_{11}$, 9-anthracenylmethyl	80.7	337.6	1991PAK/HAN
$^{\bullet}C_{15}H_{11}$, 9-phenanthrenylmethyl	74.4	311.3	1982MCM/GOL
$^{\bullet}C_{16}H_{31}$, $CH_2{=}CHC^{\bullet}H(CH_2)_{13}CH_3$	−28.4	−118.8	2001TUM/DEN
$^{\bullet}C_{19}H_{15}$, trityl, $(C_6H_5)_3C^{\bullet}$	93.7±2	392.0±8.4	1991PAR/HAN
$^{\bullet}C_{34}H_{25}$, pentamethylcyclopentadienyl	16.1	67.4	1995ROT/HUN
CF	61.0±2	255 2±8	1998CHA
CF_3	-43.5±1.5	−182.0±6.3	1998CHA
$FC^{\bullet}(O)$	−38 5±2.0	-161.2±8.4	1997KNY/BEN
CHF	34.2±3.0	143.0±12.6	1997POU/PAU
CClF	7.4±3.2	31.0±13.4	1997POU/PAU
CCl	105.9±3.1	443.1±13.0	1999JES/SQU
CCl_2	54.0	226	2000BOR/ING

续表

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
ClC•(O)	−5.2±0.6	−21.8±2.5	1990NIC/KRE
CHCl	78.0±2.0	326.4±8.4	1997POU/PAU
CClBr	63.8	267	2000BOR/ING
CBr	122±15	510±63	1998CHA
CBr_2	77.4	324	2000BOR/ING
CI	136.3±8.4	570±35	1991GUR/VEY
Cl_2	112±14	468±60	1991GUV/VEY
$•CF_3$	−111.3±0.5	−465.7±2.1	1998RUS/MIC
$•CHF_2$	−57 1±1	−238.9±4.2	1983PIC/ROD
$•CH_2F$	-7.6±1	−31.8±4.2	1983PIC/ROD
$•CClF_2$	−66.7±2	279.0±8.4	1992MIY/TSC
$•CCl_2F$	−21.3±2	−89.0±8.4	1992MIY/TSC
•CBrClF	−8.5±1.5	-35.5±6.3	2003OWE/NAU
•CHClF	−14.5±2.4	−60.7±10.0	1987TSC/PAD
$•CBrF_2$	-53.7±3	-224.7±12.6	1993BAU/HUB
$•CCl_3$	17.0±0.6	71.1±2.5	1991HUD/JON
$•CHCl_2$	22.3±1.0	93.3±4.2	1997POU/PAU
$•CH_2Cl$	28.0±0.7	117.2±2.9	1996SEE
•CHBrCl	34.2+1 4	143±6	2003SEE
$•CHBr_2$	45.0±2.2	188.3±9.2	1987TSC/PAD
$•CBr_2Cl$	39±2	163±8	2000SEE
$•CBrCl_2$	29.6±2	124±8	2000SEE
$•CBr_3$	49.0±2	205.0±8.4	1988HOL/LOS
$•CH_2Br$	40.9±0.6	171.1±2.7	2003SEE
$•CI_3$	101.6±0.7	424.9±2.8	2002SEE
$•CHI_2$	75.1±0.8	314 4±3.3	2002SEE
$•CH_2I$	54.9±2	229.7±8.4	1988HOL/LOS
$•C_2F$, FC≡C•	110±5	460.0±21.0	1996ZAR/WES
$•C_2Cl$, ClC≡C•	135.7±6.2	568±26	2002ZHU/BOZ(b)
$•C_2F_3$, CF_2=C•F	−45.9±2	192.0±8.4	1983SPY/SAU
$•C_2F_2H$, CF_2=C•H	−22.2±2	−92.9±8.4	1981STE/ROW
$•C_2F_2H$, CHF−C•F	−12.1±2	−50.6±8.4	1981STE/ROW
$•CCl_2H$, CHCl−C•Cl	56.1±2	234 7±8.4	1981STE/ROW
$•CClH_2$, CH_2=C•Cl	> 60	>251	1989RUS/SEN
$•C_2F_5$, $CF_3C•F_2$	−213.4±1	−892.9±4.2	1981EVE/WHI
$•C_2HF_4$, $CF_3C•HF$	−162.7±2.3	−680.8±9.6	1983MAR/PAR
$•C_2HF_4$, $CHF_2C•F_2$	−158.9	−664.8	1996ZAR/WES
$•C_2H_2F_3$, $CF_3C•H_2$	−123.6±2	−517.1±8.4	1974WU/ROD
$•C_2H_2F_3$, $CHF_2C•HF$	−109	456.0	1996ZAR/WES

续表

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$^\bullet C_2H_2F_3$, $CH_2FC^\bullet F_2$	−107.5	−449.8	1996ZAR/WES
$^\bullet C_2H_2F_2Cl$, $CF_2ClC^\bullet H_2$	−74.3±1.7	−310.9±7.0	1994PAD/CHE
$^\bullet C_2H_3F_2$, $CH_3C^\bullet F_2$	−72.3±2	−302.5±8.4	1977PIC/ROD
$^\bullet C_2H_3F_2$, $CHF_2C^\bullet H_2$	−68.3	−285.8	1996ZAR/WES
$^\bullet C_2H_3F_2$, $CH_2FC^\bullet HF$	−57.0	238.5	1996ZAR/WES
$^\bullet C_2H_4F$, $CH_3C^\bullet HF$	−16.8±2	70.3±8.4	1996MIY/OZA
$^\bullet C_2H_4F$, $CH_2FC^\bullet H_2$	−14.2±2	−59.4±8.4	1996MIY/OZA
$^\bullet C_2F_4Cl$, $CF_2ClC^\bullet F_2$	−164	686.0	1972FOO/TAI
$^\bullet C_2F_3ClBr$, $CF_2C^\bullet ClBr$	−120.5±2	504.2±8.4	1982MCM/GOL
$^\bullet C_2HF_3Cl$, $CClF_2C^\bullet HF$	107.7±3	−450.6±12.6	1998SKO/DYM
$^\bullet C_2Cl$, $ClC{\equiv}C^\bullet$	127.6±12	534±50	1991GUR/VEY
$^\bullet C_2Cl_3$, $CCl_2{=}C^\bullet Cl$	45.4±12	190±50	1991GUR/VEY
$^\bullet C_2Cl_5$, $CCl_3C^\bullet Cl_2$	8.4±1.3	35.1±5.4	1969FRA/HUY
$^\bullet C_2HCl_4$, $CHCl_2C^\bullet Cl_2$	5.6±2	23.4±8.4	1976LEW
$^\bullet C_2HCl_4$, $CCl_3C^\bullet HCl$	12.2	51.0	1994FRE/KAB
$^\bullet C_2H_2Cl_3$, $CH_2ClC^\bullet Cl_2$	6.3	26.4	1994FRE/KAB
$^\bullet C_2H_2Cl_3$, $CHCl_2C^\bullet HCl$	11.1	46.4	1994FRE/KAB
$^\bullet C_2H_2Cl_3$, $CCl_2C^\bullet H_2$	17.1±2	71.5±8	1988ROD/JER
$^\bullet C_2H_3Cl_2$, $CH_3C^\bullet Cl_2$	10.2±0.4	42.5±1.7	1996SEE
$^\bullet C_2H_3Cl_2$, $CH_2ClC^\bullet ClH$	15.6	65.3	1994FRE/KAB
$^\bullet C_2H_3Cl_2$, $CHCl_2C^\bullet H_2$	21.5±0.2	90.1±0.8	2000SEE
$^\bullet C_2H_4Cl$, $CH_3C^\bullet HCl$	18.3±0.4	76.5±1.6	1996SEE
$^\bullet C_2H_4Cl$, $CH_2ClC^\bullet H_2$	22.2±0.6	93.0±2.4	1998SEE
$^\bullet C_2H_3Br_2$, $CH_3C^\bullet Hr_2$	33.5±1.3	140.2±5.4	1999MIY/TSC
$^\bullet C_2H_4Br$, $BrCH_2C^\bullet H_2$	32.3	135.1	1988HOL/LOS
$^\bullet C_2H_4Br$, $CH_3C^\bullet HBr$	30.3	126.8	1990MIY/TSC
n-$C_3F_7^\bullet$, $CF_3CF_2C^\bullet F_2$	104±2	435.1±8.4	1982MCM/GOL
i-$C_3F_7^\bullet$, $CF_3C^\bullet FCF_3$	103.6±0.6	433.5±2.5	1983EVE/WEE
$^\bullet C_3H_6Cl$, $CH_3CH_2C^\bullet HCl$	13.5	56.6	1998SEE
$^\bullet C_3H_6Cl$, $CH_3C^\bullet ClCH_3$	7.1±0.2	29.9±0.6	2000SEE
$^\bullet C_3H_6Br$, $C^\bullet H_2CH_2CH_2Br$	28.7±0.3	120.1±1.3	2003GAR
$^\bullet C_3H_6Br$, $CH_3C^\bullet HCH_2Br$	23.1±1.4	96.7±5.9	2003GAR
$^\bullet C_3H_6Br$, $CH_3CH_2C^\bullet HBr$	25.7±0.6	107.5±2.5	2003GAR
$^\bullet C_5H_2Cl_3$, 1,3,4-trichlorocyclopentadiene-1-yl	36.8±5	154±21	2003BUR/KHA
$^\bullet C_6F_5$	−130.9±2	−547.7±8.4	1974KRE/PRI
$^\bullet CH_3O$, $HOC^\bullet H_2$	4.08±0.8	−17.07±3.35	1994BER/ELL
$^\bullet CH_2ClO$, $HOC^\bullet ClH$	−14.5±1.8	−60.7±7.5	2001SUN/BOZ
$^\bullet CHCl_2O$, $HOC^\bullet Cl_2$	−22.5±1.8	−94.1±7.5	2001SUN/BOZ
$^\bullet CH_2ClO$, $ClOC^\bullet H_2$	32.4±2.2	135.6±9.2	2001BOZ/JUN

续表

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$^\bullet CH_2BrO$, $BrOC^\bullet H_2$	36.1±3.9	151±16	2000ESP
$^\bullet C_3H_5O$, $C^\bullet H$=CHOH	28.9±2.6	121±11	1997FUL/HAM
$^\bullet C_2H_5O$, $CH_3C^\bullet HOH$	−13.3±0.8	−55.6±3.5	2001SUN/BOZ
$^\bullet C_2H_4ClO$, $CH_3C^\bullet ClOH$	−25.9±2.1	108.4±8.8	2001SUN/BOZ(b)
$^\bullet C_2H_4ClO$, $C^\bullet H_2CHClOH$	−17.5±2.1	−73.2±8.8	2001SUN/BOZ(b)
$^\bullet C_2H_3Cl_2O$, $C^\bullet H_2CCl_2OH$	−23.8±2.1	99.6±8.8	2001SUN/BOZ(b)
$^\bullet C_2H_5O$, $C^\bullet H_2CH_2OH$	−7.5±1.7	−31±7	1997FUL/HAM
$^\bullet C_2H_3O$, oxiran-2-yl	35.8±1.5	149.8±6.3	1984BAL/KEE
$^\bullet C_3H_5O$,CH_2=$CHC^\bullet HOH$	0±2	0±8.4	1973ALF/GOL
$^\bullet C_3H_7O$, $CH_3CH_2C^\bullet HOH$	−19.4±1.0	−81±4	1999TSA
$^\bullet C_3H_7O$, $(CH_3)C^\bullet HCH_2OH$	−18.8±2	−78.7±8.4	1992HOL
$^\bullet C_3H_7O$, $HOCH_2CH_2C^\bullet H_2$	16.0±2	−66.9±8.4	1992HOL
$^\bullet C_3H_7O$, $(CH_3)_2C^\bullet OH$	−26.6±1	−110.0±4.2	1982MCM/GOL
$^\bullet C_3H_7O$, $^\bullet CH_2CH(OH)CH_3$	−15.0±2.8	−62.8±11.7	2002SUN/BOZ
$^\bullet C_4H_9O$, $^\bullet CH_2C(OH)(CH_3)_2$	−35.2±2	−147.3±8.4	1992HOL
$^\bullet C_5H_7O$, $(CH_2$=$CH)_2C^\bullet OH$	22.1±2	92.5±8.4	1991CLA/CUL
$^\bullet C_2H_3O_3$, $C^\bullet H_2OCH_2OOH$	−26.2±1	109.6±4.2	2000YAM/BOZ
$Ph_2C^\bullet OH$	36.4±1.5	152.3±6.3	1973TRE
$^\bullet C_2H_5O$, $CH_3OC^\bullet H_2$	0±1	0±4.2	1999ATK/BAU
$^\bullet C_3H_7O$, $CH_3OC^\bullet HCH_3$	-13.8±2	−57.7±8.4	1984HOL/LOS
$^\bullet C_3H_7O$, $CH_3CH_2OC^\bullet H_2$	−10.8±2	−45.2±8.4	1991HOL/LOS
$^\bullet C_3H_7O$, $C^\bullet H_2CH_2OCH_3$	1.7±1.0	−7.1±4.2	2003CHE/BOZ
$^\bullet C_4H_9O$, $(CH_3)_2CHOC^\bullet H_2$	16.8±1.7	-70.3±7.1	2003CHE/BOZ
$^\bullet C_4H_9O$, $CH_3CH_2OC^\bullet HCH_3$	−19.4±1.0	−81.2±4.2	1986BUR/MAJ
$^\bullet C_4H_9O$, $C^\bullet H_2CH(CH_3)OCH_3$	−10.1±0.9	−42.3±3.8	2003CHE/BOZ
$^\bullet C_4H_9O$, $(CH_3)_2C^\bullet OCH_3$	−17.3±2.4	−72.4±10	2003CHE/BOZ
$^\bullet C_5H_{11}O$, $(CH_3)_3COC^\bullet H_2$	-24.5±2.0	102.5±8.4	2003CHE/BOZ
$^\bullet C_2H_5O_2$, $HOCH_2C^\bullet HOH$	−52.6±2	−220.1±8.4	1992HOL
$C^\bullet H$=C=O	42.2±0.7	176.6±2.9	1997OSB/MOR
$HC^\bullet(O)$	10.2±0.1	42.5±0.5	1996TER/KAB
$CH_3C^\bullet(O)$	−2.4±0.2	−10.0±0.8	1994BER/ELL
$CH_2ClC^\bullet(O)$	−5±3	−21±12.6	2002ZHU/BOZ
$CHCl_2C^\bullet(O)$	4.2±5.5	17.6±23	2002ZHU/BOZ
$CCl_3C^\bullet(O)$	−5.2±5.6	−21.8±23.4	2002ZHU/BOZ
$CF_3C^\bullet(O)$	128.4	537.2	1995TAK/PAS
$CH_3CH_2C^\bullet(O)$	−7.7±1	−32.3±4.2	2000ATK/BAU
$CH_3CHC^\bullet(O)$	19.3±2	80.8±8.4	1995LUN/DAA
$C_6H_5C^\bullet(O)$	27.8±2.6	116.3±10.9	1989SIM/GRI
$HC(O)CH_2^\bullet$	2.5±2.2	10.5±9.2	1994BER/ELL

续表

C-中心自由基	$\Delta_f H^0$(R)		文献
	kcal/mol	kJ/mol	
$ClC(O)CH_2^•$	-12.6±3.1	-52.7±13	2002ZHU/BOZ
E-$C^•HClC(O)H$	-6.5±2.5	-27.2±10.5	2002ZHU/BOZ
Z-$C^•HClC(O)H$	-5.6±2.5	-23.4±10.5	2002ZHU/BOZ
$C^•Cl_2C(O)H$	-13.3±3.4	-55.6±14.2	2002ZHU/BOZ
E-$C^•HClC(O)Cl$	-21.2±3.6	-88.7±15.1	2002ZHU/BOZ
Z-$C^•HClC(O)Cl$	-20.3±3.3	-84.9±13.8	2002ZHU/BOZ
$C^•Cl_2C(O)Cl$	-24.3±3.7	-101.7±15.5	2002ZHU/BOZ
$CH_3C(O)CH_2^•$	-8.1±0.7	-34±3	2001BOU/CHA
$CH_3C(O)C^•HCH_3$	-16.8±1.7	-70.3±7.1	1970SOL/BEN
$CH_3C(O)C^•-CH_3$	27.1	113.4	1990TAK
$C_2H_5C(O)C^•HCH_3$	-25.7±5	-107.5±20.9	1990BOR/HAR
$iPrC(O)C^•(CH_3)_2$	-41.5±5	-173.6±20.9	1990BOR/HAR
$tC_4H_9C(O)C^•H_2$	-27.6±3	-115.5±12.6	1990BOR/HAR
$PhC(O)C^•H_2$	20.2±3	84.5±12.6	1990BOR/HAR
$PhC(O)C^•HCH_3$	9.9±5	41.4±20.9	1990BOR/HAR
$PhC^•HC(O)CH_2Ph$	32.1±3	134.3±20.9	1990BOR/HAR
$PhC(O)OC^•H_2$	-16.7	-69.9	1970SOL/BEN
$^•C(O)OH$-trans	-46.5±0.7	-194.6±2.9	1994BER/ELL
$^•C(O)OH$-cis	-52.5	-219.7	1989RUS/SCH(b)
$^•C(O)OCH_3$	-40.5±2	-169.5±8.4	1991HOL/LOS
$C^•H_2C(O)OH$	-59.5±2.9	-248.9±12.0	1994WEN/SQU(b)
$C^•H(CH_3)C(O)OH$	-70.0±0.7	-293±3	2002LAG/DIO
$C^•H_2C(O)OCH_3$	-56.6±2	-236.8±8.4	1991HOL/LOS
$C^•H$-$C(O)OCH_2CH_3$	-62.2±3	-260.2±12.6	1995BOR/ZHA
$C^•H_2C(O)OPh$	-6.7	-28.0	1973ALF/GOL
$^•C_4H_7O$, tetrahydrofuran-2-yl	-4.3±1.5	-18.0±6.3	1982MCM/GOL
$^•C_4H_6O$, cyclopentanon-2-yl	-10±3	-41.8±12.6	1991BOR/GAL
$^•C_4H_7O_2$, 1,4-dioxan-2-yl	-31.5±3	-131.8±12.6	2000KRA/CIR
$^•C_7H_5O_2$, 2-C(O)OH-$^•C_6H_4$	-7.9	-33.0	1998NAS/SQU
$^•C_7H_5O_2$, 3-C(O)OH-$^•C_6H_4$	-8.4	-35.0	1998NAS/SQU
$^•C_7H_5O_2$, 4-C(O)OH-$^•C_6H_4$	-8.6	-36.0	1998NAS/SQU
$^•CH_2O_2$, $C^•H_2OOH$	4.1	17	2001TYN/COX
$^•C_2H_3O_2$, $C^•H_2CH_2OOH$	11.0±1.1	46.0±4.6	2000CHE/BOZ
$^•C_2H_3O_2$, $CH_3CH^•OOH$	0.5	2	2001TYN/COX
$^•C_3H_5O_2$, $CH_3CH^•CH_2OOH$	2.6±1.3	10.9±5.4	2000CHE/BOZ
$^•C_3H_5O_2$, $C^•H_2CH(OOH)CH_3$	0.7±1.5	2.9±6.3	2000CHE/BOZ
$^•C_4H_9O_2$, $(CH_3)_3C^•CH_2OOH$	-7.2±1.3	-30.1±5.4	2000CHE/BOZ
$^•C_4H_9O_2$, $C^•H_2C(CH_3)_2OOH$	-6.4±1.3	-26.8±5.4	2000CHE/BOZ
$^•C_2H_3O_3$, $C^•H_2C(O)OOH$	-33.0	-137.9	2002LEE/CHE

续表

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$^\bullet C_6H_5O$, 2,4-cyclohexadiene-1-one-2-yl	27.0	113.0	2003BUR/KHA
$^\bullet C_6H_4ClO$, 2,5-cyclohexadiene-2-chloro-1-one-4-yl	16.2±15	67.8±63	2003BUR/KHA
$^\bullet C_6H_4ClO$, 2,4-cyclohexadiene-6-chloro-1-one-2-yl	55±30	230±126	2003BUR/KHA
$^\bullet C_6HCl_3OH$, 2,4,6-trichlorophenol-5-yl	16.9±5	70.7±21	2003BUR/KHA
$^\bullet C_6H_2Cl_3O_2$, 2,4,6-trichlorobicyclo-2-hexene-1-one-4,6-peroxy-5-yl	2.1	–8.7	2003BUR/KHA
$^\bullet C_{12}H_5Cl_4O_3$, 1,3-dichloro-1-ol-2-yl-3,5-hexadiene-p-dioxin-6,8-dichlobenzen radical	-103.4±5	-432.6±21	2003BUR/KHA
$^\bullet C_{12}H_5Cl_4O_3$, 1,3-dichloro-2-ol-3-yl-1,4-hexadiene-p-dioxin-6,8-dichrobenzene radical	-77±15	322±63	2003BUR/KHA
$^\bullet CHN_2$	118.2	494.5	1996FUL/HIP
$^\bullet CH_2N{=}CH_2$	63±3	263.6+12.6	1993LAZ/PAP
$^\bullet CH_2NH_2$	36.3±2	151.9±8.4	1983BUR/CAS
$CH_3C^\bullet HNH_2$	26.7±2	111.7±8.4	1983BUR/CAS
$(CH_3)_2C^\bullet NH_2$	16.7±2	69.9±8.4	1983BUR/CAS
$^\bullet CH_2NHCH_3$	30.5±2	127.6±8.4	1981GRI/LOS
$^\bullet CH_2N(CH_3)_2$	33.2±2	139.0±8.4	1999LAA/MUL
$(C_2H_5)_2NC^\bullet HCH_3$	16.4±0.5	68.6±2.1	1990DOM/DIN
$^\bullet CH_2N(CH_3)Ph$	63.6±3	266.0±12 6	1999DOM/DIN
$^\bullet CN$	105.0±0.7	439.3±2.9	2000COO/LAN
$^\bullet CH_2CN$	60.4±1	252.6±4	2000LAF/SZA
$CH_3C^\bullet HCN$	54.2±3	226.7±12.6	1999SEN/IKE
$^\bullet CH_2CH_2CN$	58.7±3	245.4±12.6	1999SEN/IKE
$(CH_3)_2C^\bullet CN$	45.5±3	190.4±12.6	1998BRO/BEC
$Ph(CH_3)C^\bullet CN$	59.4±2	248.5±8.4	1982MEO
$NCC^\bullet HCH_2CN$	91.3±3	381.8±12.6	1999SEN/IKE
$^\bullet CH_2NC$	80±4	334.7±16.7	2002NIM/DAV
$^\bullet CCN$	133±30	556±126	1998CHA
$^\bullet C(O)NC$	50.2±2.4	210.0±10	2001DOR/NOV
$^\bullet C(O)NH_2$	-3.6±1	–15.1±4	2003NASA/JPL
$C^\bullet NN$	136±5	569±21	1998CLI/WEN(b)
$HC^\bullet NN$	110±2	460±8	1998CLI/WEN(b)
$H_2C^\bullet NN$	69.9±0.5	292.5±2.1	2000BIS/HOO
$^\bullet CH_2NO$	37.5±1	157±4	2003NASA/JPL
$^\bullet CH_2NO_2$	27.5±3	115.1±12.6	1994BOR/SAT
$CH_3C^\bullet HNO_2$	14.8±3	61.9±12.6	1994BOR/SAT
$(CH_3)_2C^\bullet NO_2$	1.5±3	6.3±12.6	1994BOR/SAT
$PhC^\bullet HNO_2$	40.4±3	169.0±12.6	1995BOR/ZHA(c)
$^\bullet C_6H_6N$, 3-NH_2-C_6H_4	76.5	320.1	1975MAT/NAS

续表

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$^{\bullet}C_6H_6N$, 4-NH_2-C_6H_4	78.3	327.8	1975MAT/NAS
$^{\bullet}C_6H_4NO_2$, 3-NO_2-C_6H_4	81.4±2.4	340.6±10.0	1985GON/LAR
$^{\bullet}C_6H_4NO_2$, 4-NO_2-C_6H_4	72.3	302.7	1975MAT/NAS
$^{\bullet}C_6H_4CH_3$, 2-Me-C_6H_4	75.3±2.5	315.1±10.5	1985GON/LAR
$^{\bullet}C_6H_4CH_3$, 4-Me-C_6H_4	70.9±2.3	296.6±9.6	1985GON/LAR
$^{\bullet}C_6H_3N_2O_4$, 3,5-$(NO_2)_2$-C_6H_3	73.0	305.4	1975MAT/NAS
$^{\bullet}C_7H_6NO_2$, 2-Me-4-NO_2-C_6H_3	70.6±2	295.4±8.4	1985GON/LAR
$^{\bullet}C_4H_3N$, pyrrol-2-yl	92.2	385.8	1994BLA/NOR
$^{\bullet}C_4H_3N$, pyrrol-3-yl	92.2	385.8	1994BLA/NOR
$^{\bullet}C_4H_8N$, pyrrolidin 2-yl	34.1±3	142.7±12.6	2000KRA/CIR
$^{\bullet}C_5H_4N$, pyrid-2-yl	86.5	362.0	1997KIE/ZHA
$^{\bullet}C_5H_4N$, pyrid-3-yl	93.5	391.0	1997KIE/ZHA
$^{\bullet}C_5H_4N$, pyrid-4-yl	93.5	391.0	1997KIE/ZHA
$^{\bullet}C_4H_7N_2$, piperad-2-yl	28.6	119.7	1997WAY/CLA
$^{\bullet}C_4H_3N_2$, pyrimid-2-yl	92.7	388.0	1997KIE/ZHA
$^{\bullet}C_4H_3N_2$, pyrimid-4-yl	97.7	409.0	1997KIE/ZHA
$^{\bullet}C_4H_3N_2$, pyrimid-5-yl	106.7	446.4	1997KIE/ZHA
$^{\bullet}CH(NO_2)_2$	33.2	139.1	2001ORL
$^{\bullet}C(NO_2)_3$	48.1	201.2	2001ORL
$^{\bullet}CH_2C(NO_2)_3$	36.0	150.6	2001MIR/KOS
$^{\bullet}CH_2CH(NO_2)_2$	24.7	103.3	2001MIR/KOS
$^{\bullet}CH_3CH_2C(NO_2)_3$	32.0	133.9	2001MIR/KOS
$^{\bullet}CH_2N(NO_2)CH_2C(NO_2)_3$	41.5	173.6	2001MIR/KOS
$^{\bullet}CH_3N(NO_2)CH_2CH(NO_2)_2$	30.2	126.4	2001MIR/KOS
$^{\bullet}CH_2N(NO_2)(CH_2)_2(NO_2)NCH_2C(NO_2)_3$	47.2	197.5	2001MIR/KOS
$^{\bullet}CH_2N(NO_2)(CH_2)_2(NO_2)NCH_2CH(NO_2)_2$	35.9	150.2	2001MIR/KOS
$(NO_2)_3CCH_2N(NO_2)CH_2C^{\bullet}H-N(NO_2)CH_2C(NO_2)_3$	46.9	196.2	2001MIR/KOS
$(NO_2)_2CHCH_2N(NO_2)CH_2C^{\bullet}HN(NO_2)CH_2CH(NO_2)_2$	24.3	101.7	2001MIR/KOS
$^{\bullet}CH_2CH_2N(NO_2)CH_2C(NO_2)_3$	40.3	168.6	2001MIR/KOS
$^{\bullet}CH_2CH_2N(NO_2)CH_2CH(NO_2)_2$	29.0	121.3	2001MIR/KOS
$^{\bullet}CH_2CH_2ONO_2$	9.0	37.7	2001KOS/MIR(a)
$^{\bullet}CH_2(ONO_2)CHCH_2ONO_2$	−6.1	−25.5	2001KOS/MIR(a)
$^{\bullet}CH(CH_2ONO_2)_2$	−13.7	−57.3	2001KOS/MIR(a)
$^{\bullet}CH_2C(CH_2ONO_2)_3$	−37.8	−158.2	2001KOS/MIR(a)
$^{\bullet}CH_2NHNO_2$	39.4	164.8	2001KOS/MIR(b)
$^{\bullet}CH_2N(NO_2)CH_3$	35.7	149.4	2001KOS/MIR(b)
$^{\bullet}CH_2N(NO_2)_2$	50.3	210.5	2001KOS/MIR(b)

续表

C-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$^\bullet CH_2CH_2N(NO_2)CH_3$	34.5	144.3	2001KOS/MIR(b)
$^\bullet CH_2N(NO_2)CH_2N(NO_2)CH_3$	48.3	202.1	2001KOS/MIR(b)
$^\bullet CH_2N(NO_2)(CH_2)N(NO_2)CH_3$	41.4	173.2	2001KOS/MIR(b)
CS	55.9	233.9	2002CRC
$C^\bullet(S)H$	71.8±2	300.4±8.4	1994BER/ELL
$^\bullet CH_2SH$	36.3±2	151.9±8.4	1994BER/ELL
$^\bullet CH_2SCH_3$	32.7±1.4	136.8±5.9	1994JEF/NIC
$^\bullet CH_2SPh$	64.2±3	268.6±12.6	1993ZHA/BOR
$^\bullet CH_2SOCH_3$	5.7±3	23.8±12.6	1998BOR/LIU
$HOC^\bullet(S)S$	26.4	110.5	1990MUR/LOV
$^\bullet CH_2SO_2CH_3$	−42.3±3	−177.0±12.6	1992BOR/HAR
$^\bullet CH_2SO_2Ph$	−13.7±3	−57.3±12.6	1992BOR/HAR
$PhC^\bullet HSO_2CH_3$	−26.1±3	−109.2±12.6	1992ZHA/BOR
$PhC^\bullet HSO_2Ph$	1.7±3	7±12.6	2001ORL/TUR
$Ph_2C^\bullet SO_2Ph$	24.4±3	102±12.6	2001ORL/TUR
$Ph_2C^\bullet SPh$	104.1±3	435.6±12.6	2001ORL/TUR
$NC^\bullet(O)$	30.4	127.2	1996ZYR/DRO
$^\bullet CNH$	49.7±2.9	207.9±12.1	2000WEN
$^\bullet CNO$	77.2±7.2	323±30	2002SAI/PAL
$^\bullet CH_2SiMe_3$	−7.6±1.5	−32±6	1998BEC/WAL
$^\bullet CH_2C(CH_3)_2SiMe_3$	-29.9	−125	1998BEC/WAL
$^\bullet CP$	107.6±2.2	450±9	1998CHA

12.3.2 O-中心自由基

表 12.3.2 O-中心自由基的生成热

O-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$HO^\bullet$	8.91±0.07	37.28±0.29	2002RUS/WAG
$FO^\bullet$	26±3	109±10	2003NASA/JPL
$ClO^\bullet$	24.29±0.03	101.63±0.1	2003NASA/JPL
$BrO^\bullet$	30.2±0.4	126.2±1.7	2003NASA/JPL
$IO^\bullet$	27.7±1.2	115.9±5.0	2003NASA/JPL
$HOO^\bullet$	3.2±0.5	13.4±2.1	2002RAM/BLA
$FOO^\bullet$	6.1±0.5	25.4±2	1998CHA
$ClOO^\bullet$	23.4±1	98.0±4	1998CHA
$BrOO^\bullet$	25.8±9.6	108±40	1998CHA
$IOO^\bullet$	23±4	96.6±15	2001IUPC
$OFO^\bullet$	90.5±4.8	378.6±20	1998CHA

续表

O-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$OClO^\bullet$	22.8	95.4	1994NIC/FRI
$ClOOClO^\bullet$	33.9±2.9	142±12	1989HAY/COX
$ClClO^\bullet$	22±7	90±30	1998CHA
$NCO^\bullet$	44.0	184.1	1990TAK
$HONNO^\bullet$	41.1	172	2004POS/SHA
sym-ClO_3	51.9±5	217.2±21	1992COL/SAN
$HSOO^\bullet$	26.8	112	1999ARM
$CH_3SOO^\bullet$	18.2	76	1999ARM
$CF_3SO_2O^\bullet$	−218	−912	1995TAK/PAS
O_3	34.1±0.4	142.7±1.7	1998CHA
$NCO^\bullet$	44.0	184.0	1990TAK
$O_2NO^\bullet$	17.0	71.1	1998NIST
$ONOO^\bullet$	19.8	82.8	1993DAV/KIM
$CH_3O^\bullet$	4.5±0.7	18.8±2.9	2002ERV/DET
$CH_2ClO^\bullet$	5.1±2.2	−21.3±9.2	2001SUN/BOZ
$CHCl_2O^\bullet$	−7.7±2.2	−32.2±9.2	2001SUN/BOZ
$CCl_3O^\bullet$	−9.1±2.2	−38.1±9.2	2001SUN/BOZ
$CH_2=CH-O^\bullet$	4.4±0.3	18.4±1.3	2002SEB/BOC
$CF_3CHFO^\bullet$	203.4	−851.0	2003WU/CAR
$C_2H_5O^\bullet$	−3.6±0.8	−15.1±3.3	2002ERV/DET
$CH_3CHClO^\bullet$	−14.8±2.9	−61.9±12.1	2001SUN/BOZ(b)
$CH_3CCl_2O^\bullet$	−21.9±2.8	−91.6±11.7	2001SUN/BOZ(b)
$nC_3H_7O^\bullet$	−7.2±2.0	−30.1±8.4	1973BEN/ONE
$iC_3H_7O^\bullet$	−11.6±0.8	−48.5±3.3	2002ERV/DET
$(CH_3)_2CClO^\bullet$	−25.9±2.0	108.4±8.4	2002SUN/BOZ
$nC_4H_9O^\bullet$	−15	−62.8	1974BAT/CHR
$sC_4H_9O^\bullet$	−16.6	−69.5	1974BAT/CHR
$tC_4H_9O^\bullet$	−20.5±0.9	−85.8±3.8	2002ERV/DET
$CH_2=CHCH_2O^\bullet$	20.8	87.0	2002LEE/CHE
$C_6H_5O^\bullet$	12.9±1.5	54±6	1996TSA
o-OH-$C_6H_4O^\bullet$	−44.5	−186.3	1991PON/TAK
p-OH-$C_6H_4O^\bullet$	−34.3	−143.6	1991PON/TAK
o-CH_3O-$C_6H_4O^\bullet$	−30.0	−125.5	1991PON/TAK
p-CH_3O-$C_6H_4O^\bullet$	−19.4	81.1	1991PON/TAK
$C_6H_5CH_2O^\bullet$	25.6±3	107.1±12.6	1996BOR/LIU
$C_{10}H_7O^\bullet$, naphthoxy-1	39.5	165.3	1975MAH/DAR
$C_{10}H_7O^\bullet$, naphthoxy-2	41.6	174.1	1975MAH/DAR
$CF_3O^\bullet$	−151.8±1.7	−635.1±7.1	2000REI/PRA
$HC(O)O^\bullet$	−30±3	−125.5±12.6	2003BLA/ELL

续表

O-中心自由基	$\Delta_f H°$(R)		文献
	kcal/mol	kJ/mol	
$FC(O)O^•$	–88	368.0	1995TAK/PAS
$CH_3C(O)O^•$	–43±3	–179.9±12.6	2003BLA/ELL
$CF_3C(O)O^•$	–190.5	–797.0	1995TAK/PAS
$C_6H_5C(O)O^•$	-12±4	–50.2±16.7	2003BLA/ELL
$CH_3OO^•$	4.8±1.2	20.1±5.1	2001BLA/RAM
$C_2H_3OO^•$, $CH_2=CHOO^•$	24.3±0 4	101 7±1 7	2002SEB/BOC
$C_2H_5OO^•$	–6.8±2.3	-28.5±9.6	2001BLA/RAM
$C_3H_5OO^•$, $CH_2=CHCH_2OO^•$	21.2	88.7	2002LEE/CHE
$iC_3H_7OO^•$	-15.6±2.7	–65.4±11.3	1998KNY/SLA(b)
$C_4H_7OO^•$, $CH_3CH=CHCH_2OO^•$	19.7±1.3	82.6±5.3	1998KNY/SLA
$tC_4H_9OO^•$	–24.3±2.2	-101.5±9.2	1998KNY/SLA(b)
neo-$C_5H_{11}OO^•$	–27.6	–115.5	2004SUN/BOZ
$HOCH_2OO^•$	–38.7	162.1	1992LIG/COX
$HOOCH_2CH_2OO^•$	23.9	100	2002BOZ/SHE
$C_6H_5CH_2OO^•$	27.4±1	114.6±4.2	1993ELM/MIN
c-$C_6H_7OO^•$, R = cyclohexadienyl	36.2±3	151.6±12.6	2000KRA/CIR
c-$C_6H_{11}OO^•$	–6±2.5	–25.0±10.5	2000KRA/CIR
c-$C_4H_8NOO^•$, R = pyrrolidin-2-yl	24.2±3	101.3±12.6	2000KRA/CIR
$(C_2H_5)N(CH3)CHOO^•$	8.6±3	–36.0±12.6	2000KRA/CIR
$CF_3OO^•$	–146.7±3.7	–614.0±15.4	1992LIG/COX
$CF_2ClOO^•$	–97.2±3.5	–406.7±14.6	1992LIG/COX
$CFCl_2OO^•$	–51.1	-213.7	1992LIG/COX
$CH_2ClOO^•$	–1.2±3.3	–5.1±13.6	1998KNY/SLA(b)
$CHCl_2OO^•$	-4.6±2.7	–19.2±11.2	1998KNY/SLA(b)
$CCl_3OO^•$	–5.0±2.1	20.9±8.9	1998KNY/SLA(b)
$CH_3CHClOO^•$	–13.1±0.8	54.7±3.4	1998KNY/SLA(b)
$CH_3CCl_2OO^•$	-15.2±2.3	–63.8±9.8	1998KNY/SLA(b)
$CH_3OCH_2OO^•$	–34.0±1.0	–142.2±4.2	2000YAM/BOZ
$CH_3C(O)CH_2OO^•$	–38.7	–162	2001TYN/COX
$CH_3C(O)OO^•$	- 36.9±1.4	154.4±5.8	2003NASA/JPL
$HOOO^•$	7.1±2	29.7±8.4	2002DEN/KIE
$CH_3OOO^•$	8±3	33.4±12.6	1996JUN/SEI
$C_2H_5OOO^•$	1.3±3	5.4±12.6	1996JUN/SEI
$C_4H_7O–OO^•$, R = tetrahydrofuran-2-yl	–36.3±4	–152.0±16.7	2000KRA/CIR
$C_4H_7O_2–OO^•$, R = dioxan-2-yl	–65.5±4	–274 0±16.7	2000KRA/CIR
$C_6H_2Cl_3O^•$, 2,4,6-trichlorophenoxy radical	–7.8±3	–32.6±12.6	2003BUR/KHA
$C_6H_4ClO^•$, o-chlorophenoxy radical	4.3±1	18.0±4.2	2003BUR/KHA
$C_6H_2Cl_3O_2^•$, 2,4.6-trichlorobicyclo-2,5-hexadiene-1,4-peroxyl-1phenoxy radical	30.7	128.4	2003BUR/KHA

续表

O-中心自由基	Δ_fH°(R)		文献
	kcal/mol	kJ/mol	
$C_{12}H_4Cl_5O_2^\bullet$, 2,4-dichlorophenoxy-1',3',5'-trichlorophenyl-6-2' ether radical	-30.6±6	-128±25	2003BUR/KHA
$C_{12}H_5Cl_4O_2^\bullet$, 2,4-dichlorophenoxy-1',3'-dichloro-phenyl 6,6'-ether radical	-20.4	85.4	2003BUR/KHA

12.3.3 N-中心自由基

表 12.3.3 N-中心自由基的生成热

N-中心自由基	Δ_fH°(R)		文献
	kcal/mol	kJ/mol	
ON	21.58±0.04	90.29±0.17	1998CHA
NO_2	7.91±0.2	33.10±0.8	1998CHA
N_2O	19.61±0.1	82.05±0.4	1998CHA
NH	85.3±0.2	357±1	1999AND
$^\bullet NH_2$	44.5±0.2	186±1	1999AND
$^\bullet NNH$	59.64	249.5	2000SMI/GOL
$^\bullet NCO$	31.5	131.8	2000SMI/GOL
$^\bullet N_3$	112±5	486.6±20.9	1981PEL/JAC
$^\bullet N_2H_3$	58.2	243.5	1988GRE/COL
(Z)-N_2H_2	50.9±2.6	213.0±10.9	1998CHA
NF	50	209.2	1979HUB/HER
$^\bullet NF_2$	10.1±2	42.3±8	1998CHA
$^\bullet NHF$	26.8±3.6	112±15	1989GUR/VEY
NBr	71.9±5	301±21	1998CHA
HNO	25.6±0.6	107.1±2.5	1999AND
FNO	-15.7±0.4	-65.7±1.7	1998CHA
ClNO	12.36±0.10	51.71±0.42	1998CHA
BrNO	19.63±0.2	82.13±0.8	1998CHA
INO	26.8±5	112.1±20.9	1998CHA
NCO	31.3	131	1999ARM(b)
NCN	111.1±0.7	464.8±2.9	1999BIS/CHO
NSi	89±15	372.4±62.8	1998CHA
$NH_2C(O)N^\bullet H$	0.2±3	0.8±12.6	1991BOR/JI(b)
$CH_3C(O)N^\bullet H$	-1.6±3	-6.7±12.6	1991BOR/JI(b)
$NH_2C(S)N^\bullet H$	46.4±3	194±12.6	2001ORL/TUR
$CH_3C(S)N^\bullet H$	41.3±3	173±12.6	2001ORL/TUR
$PhC(S)N^\bullet H$	73.4±3	307±12.6	2001ORL/TUR
$HCON^\bullet H$	11.9±3	49.8±12.6	1995BOR/ZHA
$NH_2C(NH)N^\bullet H$	59.9±3	250.6±12.6	1991BOR/JI(b)

续表

N-中心自由基	$\Delta_f H^\circ(R)$		文献
	kcal/mol	kJ/mol	
$^{\bullet}NHCN$	79.4	332.2	1993ESP/COR
$HN^{\bullet}CN$	76.3±0.7	319.2±3.0	2001BIS/HOO
$CH_2N^{\bullet}H$	25.0±3	104.6±12.6	1988GRE/COL
$CH_3N^{\bullet}H$	44.0±2	184.1±8.4	1988COL
$tBuN^{\bullet}H$	22.8±3	95.4±12.6	1998BOR/LIU
$C_6H_5CH_2N^{\bullet}H$	68.9±3	288.3±12.6	1998BOR/LIU
$C_6H_5N^{\bullet}H$	58.4±1	244.3±4.2	1997MAC/WAY
$(CH_3)_2N^{\bullet}$	37.8±2	158.2±4.2	1988COL
$(C_6H_5)(CH_3)N^{\bullet}$	57.6±1.5	241.0±6.3	1993BOR/ZHA
$(C_6H_5)_2N^{\bullet}$	87.5±1.5	366.0±6.3	1997MAC/WAY
1-pyrrolyl	70.8±3	269.2±12.6	1991BOR/JI(b)
carbazol-9-yl	91.6±2	383.3±4.2	1992ARE/VEN
$CH_3N_2^{\bullet}$	51.5±1.8	215.5±7.5	1987ACS/PET
$C_2H_5N_2^{\bullet}$	44.8±2.5	187.4±10.5	1987ACS/PET
$iC_3H_7N_2^{\bullet}$	34.9±2	146.0±8.4	本书
$nC_4H_9N_2^{\bullet}$	33.6±2	140.6±8.4	本书
$tC_4H_9N_2^{\bullet}$	23 3±2	97.5±4.2	本书
$(NO_2)HN^{\bullet}$	38.8	162.3	2001KOS/MIR(b)
$(CH_3)(NO_2)N^{\bullet}$	33.2	139.0	2001KOS/MIR(b)
$(NO_2)_2N^{\bullet}$	47.8	200.0	2001KOS/MIR(b)
$CH_3N^{\bullet}CH_2N(NO_2)CH_3$	44.3	185.4	2001KOS/MIR(b)

12.3.4 S-中心自由基

表 12.3.4 S-中心自由基的生成热

S-中心自由基	$\Delta_f H^\circ(R)$		文献
	kcal/mol	kJ/mol	
SO	1.2±0.3	5.0±1.3	1998CHA
SO_2	–70.95±0.05	-296.84±0 21	1998CHA
SO_3	94.6±0.17	–395.77±0.7	1998CHA
S_2O	13.5±8	–56.5±33.5	1998CHA
$HOS^{\bullet}$	-0.9±0.7	–3 8±2 9	1993BAL/CAS
$HC(O)S^{\bullet}$	13.5	56.5	1990TAK
$HS^{\bullet}O_2$	53	–221.8	1980BOY/GUP
$HOS^{\bullet}O_2$	92	–384.9	1984MAR
$NCS^{\bullet}$	71.7±2	300±8	1999ARM
$HS^{\bullet}$	34.2±0.2	143.0±0.8	1996WIL/HOW
$CH_3S^{\bullet}$	29.8±0.4	124 7±1 7	1994BER/ELL
$C_2H_5S^{\bullet}$	24.1	101	1999ARM

续表

S-中心自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$nC_3H_7S^\bullet$	19.1	80	1999ARM
$iC_3H_7S^\bullet$	17.9±2	74.9±8.4	1980JAN/REE
$tC_4H_9S^\bullet$	10.5±2	43.9±8.4	1980JAN/REE
$C_6H_5S^\bullet$	58.0±1.1	242.7±4.6	2002SAN/MUR
$C_6H_5CH_2S^\bullet$	58.8	246	2001ORL/TUR
$CH_3S^\bullet O$	−16.0±2.4	67±10	2001IUPAC
$CH_3S^\bullet O_2$	57.2	−239.3	1971SOL/BEN
$HSS^\bullet$	27.6±3.5	115.5±14.6	1993OHA/DEP
$CH_3SS^\bullet$	16.4±2	68.6±8.4	1986HOW/GRI
$C_2H_5SS^\bullet$	10.4±2	43.5±8.4	1986HOW/GRI
$iC_3H_7SS^\bullet$	3.3±2	13.8±8.4	1986HOW/GRI
$tC_4H_9SS^\bullet$	−4.6±2	−19.2±8.4	1986HOW/GRI
$HOC(S)S^\bullet$	26.4±1.1	110.5±4.6	1990MUR/LOV
$HC(O)S^\bullet$	13.5	56.5	1990TAK
SF	3.1±1.5	13.0±6.3	1998CHA
SF_2	−70.9±4	−296.7±16.7	1998CHA
SF_3	120.2±8	−503.0±33.5	1998CHA
SF_4	−182.4±5	−763.2±20.9	1998CHA
SF_5	−210.3±3.6	−879.9±15.1	1998CHA
$ClS^\bullet$	37.4±4	156.5±16.7	1998CHA
SN	63±25	263.6±105	1998CHA
SCl	37.4±4	156.5±16.7	1998CHA

12.3.5 Si-, Ge-, Sn-, Pb- 和 P-中心自由基

表 12.3.5 Si-, Ge-, Sn-, Pb- 和 P-中心自由基的生成热

自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
SiF	−4.8±3	−20.1±12.6	1998CHA
SiF_4	−152.5±1.5	−638±6	1998BEC/WAL
$^\bullet SiF_3$	−235.9±4	−987±20	1998BEC/WAL
SiCl	47.4±1.6	198.3±6.7	1998CHA
$SiCl_2$	40.4±0.7	−169±3	1998BEC/WAL
$^\bullet SiCl_3$	77.0±2	322±8	1998BEC/WAL
SiBr	56.2±1.1	235±46	1988CHA
$SiBr_2$	11.0±2	46±8	1998BEC/WAL
$^\bullet SiBr_3$	48.2±1.5	−201.7±6.3	1998CHA
SiI	75.0±10	313.6±41.8	1998CHA
SiI_2	22.1±2	92.5±8.4	1998BEC/WAL

续表

自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$^{\bullet}SiI_3$	8.4±15	35 3±62.8	1998CHA
SiH	90±2	376.6±8.4	1998CHA
$SiH_2(^1A_1)$	65.2±0.5	273±2	1998BEC/WAL
$SiH_2(^3B_1)$	86.2	360.7	1987BER/GRE
$^{\bullet}SiH_3$	47.9±0.6	200.4±2.5	1994BER/ELL
$MeSi^{\bullet}H_2$	33.7±1.5	141±6	1998BEC/WAL
$Me_2Si^{\bullet}H$	18.6±1.5	78±6	1998BEC/WAL
$Me_3Si^{\bullet}$	3.6±1.6	15±7	1998BEC/WAL
$^{\bullet}Si_2H_3$	~96	~402	1991RUS/BER(c)
$H_3SiSi^{\bullet}H_2$	55.9±1.5	234±6	1998BEC/WAL
$C_6H_5Si^{\bullet}H_2$	65.5	274	1998BEC/WAL
$H_3SiSi^{\bullet}H$	74.6±2	312±8	1998BEC/WAL
$MeSi^{\bullet}H$	48.3±1.5	202±6	1998BEC/WAL
$Me_2Si^{\bullet\bullet}$	32.3±2	135±8	1998BEC/WAL
SiN	75±10	313.6±41.8	1998CHA
$^{\bullet}GeH_3$	53±2	221.8±8.4	1994BER/ELL
GeF	−17.0±2.4	−71±10	1991GUR/VEY
GeF_2	−137.2±4.8	- 574±20	1991GUR/VEY
$^{\bullet}GeF_3$	−192.9±12	−807±50	1991GUR/VEY
GeCl	16.5±4.3	69±18	1991GUR/VEY
$GeCl_2$	−40.9±1.2	-171±5	1991GUR/VEY
$^{\bullet}GeCl_3$	−64.0±12	−268±50	1991GUR/VEY
GeBr	32.8±1.2	137±5	1991GUR/VEY
$GeBr_2$	−14.6±1.2	−61±5	1991GUR/VEY
$^{\bullet}GeBr_3$	−28.4±12	119±50	1991GUR/VEY
GeI	50.4+6	211±25	1991GUR/VEY
GeI_2	12.0±1	50.2±4	1991GUR/VEY
$^{\bullet}GeI_3$	10±12	42±50	1991GUR/VEY
SnF	−22 7±1.7	−95±7.2	1991GUR/VEY
SnF_2	−122.1±2.2	511±9.2	1991GUR/VEY
$^{\bullet}SnF_3$	−154.6±12	−647±50	1991GUR/VEY
SnCl	8 3±2 9	35±12	1991GUR/VEY
$SnCl_2$	48.4±1.7	202.6±7.1	1991GUR/VEY
$^{\bullet}SnCl_3$	−69.8±12	292±50	1991GUR/VEY
SnBr	18.2±2.9	76±12	1991GUR/VEY
$SnBr_2$	−28.4±0.7	−119±2.8	1991GUR/VEY
$^{\bullet}SnBr_3$	−38.0±12	−159±50	1991GUR/VEY
SnI	41.3±2.9	173±12	1991GUR/VEY
SnI_2	−1.9±1	8.1±4.2	1991GUR/VEY

续表

自由基	$\Delta_f H^\circ$(R)		文献
	kcal/mol	kJ/mol	
$^{\bullet}SnI_3$	1.9±12	−8±50	1991GUR/VEY
$^{\bullet}Sn(CH_3)_3$	31.6	132.2	1998GAL/PAU
$^{\bullet}Sn(C_6H_5)_3$	124±5	518.8±21	1992CAR
PbH	56.5±4.6	236.2±19.2	1998CHA
PbF	−19.2±2.5	−80.3±10.5	1998CHA
PbF_2	-104±2	-435.1±8.4	1998CHA
$^{\bullet}PbF_3$	117±14.3	−490±60	1991GUR/VEY
PbCl	3.6±12	15.1±50	1998CHA
$PbCl_2$	−41.6±0.3	−174.1±1.3	1998CHA
$^{\bullet}PbCl_3$	−42.5±19	−178±80	1991GUR/VEY
PbBr	16.9±10	70.9±42	1998CHA
$PbBr_2$	-25.0±1.5	−104.4±6.3	1998CHA
$^{\bullet}PbBr_3$	−24.9±19	-104±80	1991GUR/VEY
PbI	25.7±9	107.4±37.7	1998CHA
PbI_2	−0.76±1	-3.2±4.2	1998CHA
$^{\bullet}PbI_3$	5.2±19	22±80	1991GUR/VEY

参 考 文 献

1946~1969

1946STE Steacie, E W R. 1946. Atomic and free radical reactions. The kinetics of gas-phase reactions involving atoms and organic radicals. Am Chem Soc Monograph No. 22. New York: Reinhold Pub

1950SZW Szwarc M. 1950. The determination of bond dissociation by pyrolytic methods. Chem Rev, 47:75~73

1950SZW/ROB Szwarc M, Roberts J S. 1950. The O–O bond dissociation energy in tertiarybutyl-peroxide. J Chem Phys, 18:561~562

1958COT Cottrell T L. 1958. The Strength of chemical bonds, 2nd Ed. London: Butterworths Sci Pub

1958PRI/TRO Price S J W, Trotman-Dickenson A F. 1958. Metal-carbon bonds. 3. The pyrolyses of trimethyl bismuth, trimethyl antimony and dimethyl tin dichloride. Trans Faraday Soc, 54:1630~1637

1958SEM Semenov N N. 1958. Some Problems in Chemical Kinetics and Reactivity. Princeton University Press

1958SMI Smith P. 1958. Standard enthalpy and free energy of formation of diimide. J Chem Phys, 29:683~684

1959DRO/MAR Drowart J, de Maria G, Boerboom A J H, Inghram, M G. 1959. Mass spectrometric study of inter-group-IVB molecules. J Chem Phys, 30:308~313

1960ERR Errede L A. 1960. Simple equations for calculating bond dissociation energies. J Phys Chem, 64:1031~1034

1960HAR/HON Harrison A G, Honnen L R, Dauben H J, Lossing F P. 1960. Free radicals by mass spectrometry. 20. Ionization potentials of cyclopentadienyl and cycloheptatrienyl radicals. J Am Chem Soc, 82:5593~5598

1961GOW/JON Gowenlock B G, Jones P P, Majer J R. 1961. Bond dissociation energies in some molecules containing alkyl-substituted CH_3, NH_2, and OH. Trans Farad Soc, 57:23~27

1961HER Herzberg G. 1961. Bakerlian Lecture-Spectra and structures of free methyl and free methylene. Proc Roy Soc (London) A, 262(131):291

1962BRY Bryant W M D. 1962. Free energies of formation of fluorocarbons and their radicals — thermodynamics of formation and depolymerization of polytetrafluoethylene. J Polym Sci, 56:277~296

1962HOL Holmes J L. 1962. Kinetics of the reaction between nitric oxide and hydrogen iodide and the dissociation energy D(H NO). Proc Chem Soc. 75~76

1962MOR Mortimer C T. 1962. Reaction heats and bond strengths. New York: Pergamon Press

1963EBE Eberson L. 1963. Kolbe electrolytic synthesis. 4. Theoretical investigation of the mechanism by standard potential calculations. Acta Chem Scand, 17:2004~2018

1963SAN/MOS Sandoval A A, Morser H C, Kiser R W. 1963. Ionization and dissociation processes in phosphorus trichloride and diphosphorus tetrachloride. J Phys Chem, 67:124~126

1963SCH Schexnayder C J. 1963. Tabulated Values of Bond Dissociation Energies, Ionization Potentials, and Electron Affinities of Some Molecules Found in High-Temperature Chemical Reactions. NBS, Washington DC

1964EBE Eberstein I J. 1964. Princeton Univ Dept. Aerosp Tech Rept. 708, Dissertation, 238 pp. 1964, Contr. AD 49(638)126, UM AAD65-00047, Diss Abstr Intl. 25(10):5805

1964MIL/PAL Miller W J, Palmer H B. 1964. Chemiluminescence and radical reaction in diffusion flames of alkali metals with organic halides. J Chem Phys, 40:3701~3705

1964NEA Neale R S. 1964. A correlation of bond dissociation energy with ionization potential and electron affinity. J Phys Chem, 68:143~146

1965BEN Benson S W. 1965. Bond energies. J Chem Educ, 42:502~518

1965GRZ/KER Grzechowiak J, Kerr J A, Trotman-Dickenson A F. 1965. Reactions of difluoroamino radicals. 1. Hydrogen abstraction from acetone and the strength of the C–H bond in acetone. J Am Chem Soc, 87:5080~5082

1965TSC Tschuikow-Roux E. 1965. The C -C bond dissociation energy in C_2F_6. J Phys Chem, 69:1075~1077

1966AMP/COO Amphlett J C, Coomber J W, Whittle E. 1966. The C–H bond dissociation energy in fluoroform. J Phys Chem, 70:593~594

1966BOT/DIB Botter R, Dibeler V H, Walker J A, Rosenstock H M. 1966. Mass-spectrometric study of photoionization. 4. Ethylene and 1,2-dideuteroethylene. J Chem Phys, 45:1298~1301

1966BOT/DIB(b) Botter R, Dibeler V H, Walker J A, Rosenstock H M. 1966. Experimental and theoretical studies of photoionization-efficiency curves for C_2H_2 and C_2D_2. J Chem Phys, 45:1271~1278

1966EGG/BEN Egger K W, Benson S W. 1966. Iodine and nitric oxide catalyzed isomerization of olefins. 7. The stabilization energy in the pentadienyl radical and the kinetics of the positional isomerization of 1,4-pentadiene. J Am Chem Soc, 88:241~246

1966GOL/ROD Golden D M, Rodgers A S, Benson S W. 1966. The kinetics and mechanism of the reaction $I_2 + C_3H_6 = C_3H_5I + HI$ and the heat of formation of the allyl radical. J Am Chem Soc, 88:3196~3198

1966HOM/LOS Homer J B, Lossing F P. 1966. Free radicals by mass spectrometry. 35. Heat of formation of allyl radical from biallyl pyrolysis. Can J Chem, 44:2211~2216

1966KER Kerr J A. 1966. Bond dissociation energies by kinetic methods. Chem Rev, 66:465~500

1966PAC/PHE Pack J L, Phelps A V. 1966. Electron attachment and detachment. 1. Pure O_2 at low energy. J Chem Phys, 44:1870~1883

1966TSA Tsang W. 1966. Thermal decomposition of hexamethylethane, 2,2,3-trimethylbutane, and neopentane in a single-pulse shock tube. J Chem Phys, 44:4283~4295

1966VED/GUR Vedeneed V I, Gruvich L V, Kondrat'yev V N, Medvedev V A, Frankevich Ye L. 1966. Bond Energies, Ionization Potentials and Electron Affinities. Eng. Ed. London: Edward Arnold Pub

1966WAL/GOL Walsh R., Golden D M, Benson S W. 1966. The thermochemistry of the gas phase equilibrium $I_2 + C_6H_5CH_3 = C_6H_5CHI_2 + HI$ and the heat of formation of the benzyl radical. J Am Chem Soc, 88:650~656

1967COO/WHI Coomber J W, Whittle E. 1967. Bond dissociation energies from equilibrium studies. 3. $D(CF_3–Cl)$, $D(C_2F_5–Cl)$ and enthalpy of formation of trifluochloromethane. Trans Faraday Soc, 63:2656~2667

1967COO/WHI(b) Coomber J W, Whittle E. 1967. Bond dissociation energies from equilibrium studies. 2. $D(CF_3–CF_3)$ and enthalpy of formation of C_2F_6. Trans Faraday Soc, 63:1394~1401

1967COO/WHI(c) Coomber J W, Whittle E. 1967. Bond dissociation energies from equilibrium studies. 1. $D(CF_3–Br)$, $D(C_2F_5–Br)$, and $D(n\text{-}C_3F_7–Br)$. Trans Faraday Soc, 63:608~619

1967DRO/PAT Drowart J, Pattoret A, Smoes S. 1967. Mass spectrometric studies of the vapotization of refracratory compounds. Pro Brit Cerem Soc Ogneupory, 8:67~89

1967LOU/LAI Loucks L F, Laidler K J. 1967. Mercury-photosensitized decomposition of dimethyl ether. 1. Mechanism. Can J Chem, 45:2763~2766

1967PET Petry R C. 1967. Chemical properties of chlorodifluoramine. J Am Chem Soc, 89:4600~4604

1967ROD/GOL Rodgers A S, Golden D M, Benson S W. 1967. Kinetics of the reaction of iodobenzene and hydrogen iodide. Heat of formation of the phenyl radical and its implications on the reactivity of benzene. J Am Chem Soc, 89:4578~4583

1967TSA Tsang W. 1967. Thermal decomposition of 4,4-dimethyl-1-pentene in a single-pulse shock tube. J Chem Phys, 46:2817~2822

1968CZA/CAS Czarnowski J, Castellano E, Schumacher H J. 1968. Energy of the O–F bond in trifluoromethyl hypofluorite. J Chem Soc Chem Comm, No. 20:1255

1968DAV/OKA Davis D D, Okabe H. 1968. Determination of bond dissociation energies in hydrogen cyanide. Cyanogen and cyanogen halides by the photodissociation method. J Chem Phys, 49:5526~5531

1968DAY/BAS Day J P, Basolo F, Pearson R G. 1968. Kinetics and mechanism of nucleophilic substitution in nickel tetracarbonyl. J Am Chem Soc, 90:6927~6933

1968DIX/LAM Dixon R N, Lamberton H M. 1968. The A, 3Ili-X, 3R-band systems of arsylene and arsenicdeuteride. J Mol Spectros, 25:12~33

1968GAY Gay A G. 1868. Dissociation Energies and Spectra of Diatomic Molecules. 3rd ed. London: Chapman and Hall

1968GRI/BOG Grishin N N, Bogolyubov G M, Petrov A A. 1968. Compounds with P–P bonds. 6. Mass spectrometric studies of phosphines; energy of the P–P bond in diphosphines. J Gen Chem USSR, 38:2683~2886

1968HEN/DUF Henrickson C H, Duffy D, Eyman D P. 1968. Lewis acidity of alanes. Interactions of trimethylalane with amines, ethers, and phosphines. Inorg Chem, 7:1047~1051

1968JAM/SUA James D G, Suart R D. 1968. Kinetic study of the cyclohexadienyl radical. 3. Mutual interaction and thermal decomposition. Trans Faraday Soc, 64:2752~2769

1968LAC/SKI Lacher J R, Skinner H A. 1968. Bond energy additivity and bond interaction in fluo-halogenated hydrocarbons. J Chem Soc A, 1034~1038

1968WAL/PAP Walling C, Papioannou C G. 1968. Bond dissociation energies of tert-butyl hypohalites, J Phys Chem, 72:2260~2262

1968WIL/HAM Williams J M, Hamill W H. 1968. Ionization potentials of molecules and free radicals and appearance potentials by electron impact in the mass spectrometry. J Chem Phys, 49:4467~4477

1968ZMB/UY Zmbov K F, Uy O M, Margrave J L. 1968. Mass spectrometric study of the high temperature equilibrium $C_2F_4 = 2CF_2$ and the heat of formation of the CF_2 radical. J Am Chem Soc, 0:5090~5092

1969BEN/CRU Benson S W, Cruickshank F R, Golden D M, Haugen G R, O'neal, H E, Rodgers A S, Show R, Walsh R. 1969. Additivity rules for the estimation of thermochemical properties. Chem Rev, 69:279~324

1969BER/CHU Berkowitz J, Chupka W A, Walter T A. 1969. Photoionization of hydrogen cyanide: electron affinity and heat of formation of CN. J Chem Phys, 50:1497~1500

1969BOG/GRI Bogolyabov G M, Grishin N N, Petrov A A. 1969. Organic derivatives of Group V and VI elements. 8. Mass spectra of phosphines and diphosphines. J Gen Chem USSR, 39:1808~816

1969BRE/ROS Brewer L, Rosenblatt G M. 1969. Dissociation energies and free energy functions of gaseous monoxides. Adv High Tem Chem, 2:1~83

1969CRU/BEN Cruickshank F R, Benson S W. 1969. Kinetics and mechanism of the reaction of iodine with tetrahydrofuran. Carbon-hydrogen bond dissociation energy in tetrahydrofuran. J Am Chem Soc, 91:1289~1292

1969CRU/BEN(b) Cruickshank F R, Benson S W. 1969. Carbon-hydrogen bond dissociation energy in methnol. J Phys Chem, 73:733~737

1969DEV/ONE Devore J A, O'Neal H E. 1969. Heats of formation of the acetyl halides and the acetyl

radical. J Phys Chem, 73:2644~2648

1969FIN/HAM Finch A, Hameed A, Gardner P J, Paul N. 1969. Phosphorus-phosphorus bond. Some electron impact studies. J Chem Soc Chem Commun, No. 8, 391

1969FRA/HUY Franklin J A, Huybrechts G H, Cillien C. 1969. Addition of a chlorine atom to tetrachloroethylene, Trans Faraday Soc, 65:2094~2102

1969FRE/KRA Frey H M, Krantz A. 1969. Thermal isomerization of trans-1-cyclopropylbuta-1,3-dine. J Chem Soc A, 1159~1161

1969GOL/BEN Golden D M, Benson S W. 1969. Free radical and molecule thermochemistry from studies of gas-phase iodine-atom reactions. Chem Rev, 69:125~134

1969GOL/GAC Golden D M, Gac N A, Benson S W. 1969. Equilibrium constant for allyl radical recombination. Direct measurements of allyl resonance energy. J Am Chem Soc, 91:2136~2137

1969LAR/HAR Larson C W, Hardwidge E A, Rabinovitch B S. 1969. Competitive unimolecular decomposition of alkyl radicals. Neopentyl rupture. J Chem Phys, 50:2769~2770

1969MAH/FER Mahoney L R, Ferris F C, DaRooge M A. 1969. Calorimetric study of the 2,4,6-tri-butylphenoxy radical in solution. J Am Chem Soc, 91:3883~3889

1969MCA/LOS McAllister T, Lossing F P. 1969. Free radicals by mass spectrometry. 16. Ionization potential and heat of formation of the PH_2 radical. J Phys Chem, 73:2996~2998

1969MIR/LEB Miroshnichenko E A, Lebedev Yu A. 1969. N–O bond energy in 3-nitroisoxazoline-2-oxide, Khimiya Geterotsiklicheskikh Soedinenii. No. 6, 963~964

1969PAN/ZER Pankratov A V, Zercheninov A N, Chesnokov V I, Zhdanova, N.N. 1969. Standard enthalpy of formation of difluoroamine. Zh Fiz Khim, 43:394~397

1969PRI/PER Pritchard G O, Person M J. 1969. Hydrogen atom abstraction reaction of CF_2H and CFH_2 radicals, and the C–H bond dissociation energy in CF_2H_2. Int J Chem Kinet, 1:509~525

1969SOL/BEN Solly R K, Benson S W. 1969. Carbon-hydrogen bond strengths in methyl formate and the kinetics of the reaction with iodine. Int J Chem Kinet, 1:427~437

1969TSA Tsang W. 1969. Thermal decomposition of 3,4-dimethyl-1-pentene, 2,3,3-trimethyl-pentane, 3,3-dimethylpentane, and isobutylbenzene in single pulse shock tube. Int J Chem Kinet, 1:245~278

1969VIN/DAU Vincow G, Dauben H J, Hunter F R, Volland W V. 1969. Resonance energy of cycloheptatrienyl radical. J Am Chem Soc, 91:2823~2827

1970~1974

1970AMP/WHI Amphlett J C, Ahittle E. 1970. Kinetics of bromination of trifluoroacetaldehyde and the bond dissociation energy D(CF_3CO–H). Trans Faraday Soc, 66:2016~2021

1970COX/PIL Cox J D, Pilcher G. 1970. Thermochemistry of Organic and Organometallic Compounds. New York: Academic Press

1970DAR Darwent D deB. 1970. Bond Dissociation Energies in Simple Molecules, NBSDS-NBS, 31 Washington, DC

1970DUN/PRI Dunlop A N, Price S J W. 1970. Pyrolysis of dimethyl and dimethylzinc-d6 by the toluene carrier method. Can J Chem, 48:3205~3208

1970EGG/JOL Egger K W, Jola M. 1970. Kinetics of the gas-phase isomerization of 1, trans-3, trans-5-heptatriene into the cis-isomer catalyzed by nitric oxide and the stabilization energy in the pentadienyl radical. Int J Chem Kinet, 2:265~280

1970FON/HUD Foner S N, Hudson R L. 1970. Mass spectrometric studies of atom-molecule reactions using high-intensity crossed molecular beams. J Chem Phys, 53:4377~4386

1970FUR/GOL Furuyama S, Golden D M, Benson S W. 1970. Kinetics study of the gas-phase reaction

	c-C_5H_{10} + I_2 = c-C_5H_8 + 2HI. Heat of formation of cyclopentyl radical. Int J Chem Kinet, 2:83~92
1970FUR/GOL(b)	Furuyama S, Golden D M, Benson S W. 1970. Kinetic study of the gas-phase reaction c-C_5H_8 + I_2 = c-C_5H_6 + 2HI. Heat of formation and the stabilization energy of the cyclopentenyl radical. Int J Chem Kinet, 2:93~99
1970JON/WHI	Jones S H, Whittle E. 1970. Reactions of trifluoromethane radicals with cyclanes and the determination of C–H bond dissociation energies in cyclanes. Int J Chem Kinet, 2:479~492
1970KIN/GOL	King K D, Golden D M, Benson S W. 1970. Kinetics of the gas-phase thermal bromination of acetone. Heat of formation and stabilization energy of the acetonyl radical. J Am Chem Soc, 92:5541~5546
1970LEY/MAY	Leyland L M, Majer J R, Robb J C. 1970. Heat of formation of the CF_2Cl radical. Trans Faraday Soc, 66:898~900
1970LOW	Lowder J E. 1970. Spectroscopic studies of hydrogen bonding in ammonia. J Quant Spectrosc Radiat Transfer, 10:1085~1094
1970OHA/HUB	O'Hare P A G, Hubbard W N, Glemser O, Wegener J. 1970. Thiazyl tri- and mono-fluororides: enthalpy of formation and dissociation enthalpy of N=S bonds. J Chem Thermodyn, 2:71~76
1970OHA/WAH	O'Hare P A G, Wahl A C. 1970. Hartree-Fock wavefunctions and computed properties for the ground states of SF and SeF and their positive and negative ions. Comparison of the theoretical results with experiment. J Chem Phys, 53:2834~2846
1970OKA/INA	Okazaki R, Inamoto N. 1970. Nuclear maganetic resonance spectra of nitrosobenzene. Anomalous chemical shifts in ortho-substituted nitrosobenzenes. J Chem Soc B Phys Org, No. 8:1583~1586
1970ONE/BAG	O'Neal H E, Bagg J W, Richardson W H. 1970. Heat of formation the norbornyl radical and the bridgehead bond dissociation energies in norbornane. Int J Chem Kinet, 2:493~496
1970ONE/BEN	O'Neal H E, Benson S W. 1970. Kinetic data gas-phase unimolecular reactions. Natl Ref Data Serv, NSRDS-NBS 21. Washington DC
1970SOL/GOL	Solly R K, Dolden D M, Benson S W. 1970. Kinetics and thermochemistry of the gas-phase reaction of methyl ethyl ketone with iodine. 1. Resonance energy of the methylacetonyl radical. Int J Chem Kinet, 2:381~391
1970TRE	Trenwith A B. 1970. Dissociation of 1-butene,3-methyl-1-butene, and 3,3-dimethyl-1-butene and the resonance energy of the allyl, methyl allyl, and dimethyl ally radicals. Trans Faraday Soc, 66:2805~2811
1970TSA	Tsang W. 1970. Rate and mechanism of thermal decomposition of 4-methyl-1-pentyne in a single-pulse shock tube. Int J Chem Kinet, 2:23~36
1970TSA(b)	Tsang W. 1970. Comparative rate single-pulse shock tube studies on the thermal decomposition of cyclohexene, 2,2,3-trimethylbutane, isopropyl bromide, ethylcyclobutane. Int J Chem Kinet, 2:311~323
1971COR/BAF	De Corpo JJ, Bafus D A, Franklin J L. 1971. Enthalpies of formation of the mono-halomethyl radicals from mass spectrometric studies of the dihalomethane. J Chem Thermodyn, 3:125~127
1971DAN/TIP	Danen W C, Tipton T J, Saunders D G. 1971. Halogen abstraction studies. 2. Free-radical abstraction of iodine from bridgehead iodides. J Am Chem Soc, 93:5186~5189
1971FER/WHI	Ferguson K S, Whittle E. 1971. Kinetics of the vapor-phase bromination of cyclanes and butane. Carbon-hydrogen bond dissociation energies in cyclanes. Trans Faraday Soc, 67:2618~2628
1971FUR/GOL	Furugama S, Golden D M, Benson S W. 1971. Kinetics and thermochemistry of the

gas-phase reaction of cyclopentadiene and iodine. Relevance to the heat of formation of cyclopentadienyl iodide and cyclopentadienyl radical. Int J Chem Kinet. 3:237~248

1971KER/TIM Kerr J A, Timlin D M. 1971. Kinetic study of the thermal elimination of hydrogen fluoride from 1,2-difluoroethane. Determination of the bond dissociation energies D(CH_2F-CH_2F) and D(CH_2F-H). Int J Chem Kinet, 3:427~44

1971KIN/GOL King K D, Golden D M, Benson S W. 1971. Kinetics and thermochemistry of the gas-phase bromination of bromoform. C–H bond dissociation energy in bromoform and the C–Br dissociation energy in carbon tetrabromide. J Phys Chem, 75:987~989

1971LAU/OKA Laufer A H, Okabe H. 1971. Heat of formation and bond dissociation energy of diazomethane by a photodissociation method. J Am Chem Soc, 93:4137~4140

1971LOS Lossing F P. 1971. Free radicals by mass spectrometry. 43. Ionization potentials and ionic heats of formation for vinyl, allyl, and benzyl radicals. Can J Chem, 49:357~362

1971MAT/PEP Matyushin Y N, Pepekin V I, Golova S P, Godovikova T I, Khmel'nitskii L I. 1971.Enthalpy of formation of dimethylfuroxan and dimethylfurazan. Ivvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, No. 1, 181~183

1971MCM/GOL McMillen D F, Golden D M, Benson S W. 1971. Kinetics of the gas-phase reaction of cyclopropylcarbinyl iodine and hydrogen iodide. Heat of formation and stabilization energy of the cyclopropylcarbinyl radical. Int J Chem Kinet, 3:359~374

1971MIL/HAR Millward G E, Hartig R, Tschuikow-Roux E. 1971. Kinetics of the shock wave thermolysis of 1,1,2,2-tetrafluoroethane. J Phys Chem, 75:3195~3201

1971OKA Okabe H. 1971. Fluorescence and predissociation of sulfur dioxide. J Am Chem Soc, 93:7095~7096

1971SOL/BEN Solly R K, Benson S W. 1971. Kinetics of the gas-phase reaction of benzaldehyde with iodine. Heat of formation and stabilization energy of the benzoyl radical. J Am Chem Soc, 93:1592~1595

1971SOL/BEN(b) Solly R K, Benson S W. 1971. Kinetics of the gas-phase reaction of methyl benzoate with bromine and iodine. Methoxyl C–H bond strength of methyl esters. Int J Chem Kinet, 3:509~522

1971WAL Walsh R. 1971. Kinetics of the gas-phase iodine-catalyzed isomerization of methyl acetylene and the propargyl stabilization energy. Trans Faraday Soc, 67:2085~2095

1972ALF/GOL Alfassi Z B, Golden D M. 1972. Bond dissociation energy of the carbon-hydrogen bond in ethanol. Kinetic study of the reaction iodine + ethanol. J Phys Chem, 76:3314~3319

1972BAS/WHI Bassett J E, Whittle E. 1972. Reaction of pentafluoroethyl radicals with hydrogen chloride. Determination of the bond dissociation energy D(C_2F_5-H). J Chem Soc Faraday Trans 1, 68:492~498

1972CAR/GOW Carmichael P J, Gowenlock B G, Johnson C A F. 1972. Carbon-nitrogen bond dissociation energy values in C-nitroso compounds. Int J Chem Kinet, 4:339~343

1972CLY/CON Clyne M A A, Connor J. 1972. Third-order recombination reactions of difluoroamino radicals. J Chem Soc Faraday Trans 1, 68:1220~1230

1972FER/WHI Ferguson K C, Whittle E. 1972. Kinetics of the reaction between hydrogen bromide and bromopentafluoroethane. Determination of the bond dissociation energy D(C_2F_5–Br). J Chem Soc Faraday Trans 1, 68:306~314

1972FER/WHI(b) Ferguson K C, Whittle E. 1972. Kinetics of the reaction between hydrogen bromide and bromopentafluoroethane. Determination of the bond dissociation energy D(CF_3–Br). J Chem Soc Faraday Trans 1, 68:295~305

1972FER/WHI(c) Ferguson K C, Whittle E. 1972. Competitive study of the reactions of atomic bromine with bromotrifluoromethane and bromopentafluoroethane (Br + RBr == Br_2 + R). J Chem Soc Faraday Trans. 1, 68:641~646

1972FOO/TAI Foon R, Tait K B. 1972. Chlorine abstraction reactions of flurine. 2. Kinetic

determination of the bond dissociation energy D(CCl_2F–Cl). J Chem Soc Faraday Trans 1, 68:104~111

1972FOO/TAI(b) Foon R, Tait K B. 1972. Chlorine abstraction reactions of flurine. 3. Thermochemical data for chlorofluoroalkanes. J Chem Soc Faraday Trans 1, 68:1121~1130

1972GOL/SOL Golden D M, Solly R K, Gac N A, Benson S W. 1972. Very low pressure pyrolysis. 5. Benzylamine, N-methylbenzylamine, and N,N-dimethylbenzylamine and the heat of formation of the amino, methylamino, and dimethylamino radicals. J Am Chem Soc, 94:363~369

1972JON/PRI Johnson R P, Price S J W. 1972. Pyrolysis of tetramethyltin. Can J Chem, 50:50~54

1972LEY/KEN Levy J B, Kennedy R C. 1972. Bistrifluoromethyl peroxide. 1. Thermodynamics of the equilibrium with carbonyl fluoride and trifluoromethyl hypofluorite. J Am Chem Soc, 94:3302~3305

1972MCM/GOL McMillen D F, Golden D M, Benson S W. 1972. Rate of the gas-phase iodination of cyclobutane. Heat of formation of the cyclobutyl radical. Int J Chem Kinet, 4:487~495

1972PEP/MAT(a) Pepekin V I, Matyushin Y N, Feshchenko A G, Smirnov S P, Apin A Y. 1972 Dissociation energy of the N–O bond in benzofurazan 1-oxide. Dok Akadem Nauk SSSR Chem, 202:91~92

1972PEP/MAT(b) Pepekin V I, Matyushin Y N, Rozantsev G G, Shevelev S A, Apin, A Y. 1972. Enthalpies of formation of dinitrophenylmethane, trinitrophenylethane, and fluoro-dinitrophenylmethane, Ivvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, No. 12, 2703~2705

1972TSA Tsang W. 1972. Hydrocarbon decomposition. 6. Thermal decomposition of 3,4-dimethylhexane, 2,2,3-trimethylpentane, tert-butylcyclohexane, and related hydrocarbons. J Phys Chem, 76:143~156.

1972WAY/STA Wyatt J R, Stafford F E. 1972. Mass spectrometric determination of the heat of formation of ethynyl radical, C_2H, and of some related species. J Phys Chem, 76:1913~1918

1973ALF/GOL Alfassi Z B, Golden D M. 1973. Kinetics of the reaction of iodine with acrolein. Bond dissociation energy of the carbonyl carbon-hydrogen bond. J Am Chem Soc, 95:319~323

1973ALF/GOL(b) Alfassi Z B, Golden D M, Benson S W. 1973. Kinetics of the molecular iodine-catalyzed isomerization of allyl chloride to cis and trans-1-chloro-1-propene. Stabilization energy of the chloroallyl radical. Int J Chem Kinet, 5:155~167

1973ALF/GOL(c) Alfassi Z B, Golden D M. 1973. Kinetics of the gas-phase reaction of allyl alcohol with iodine. Heat of formation and stabilization energy of the hydroxyallyl radical. Int J Chem Kinet, 5:295~303

1973BAT/MIL Batt L, Milne R T. 1973. Methyl-nitroso bond dissociation energy. Int J Chem Kinet, 5:1067~1069

1973BEN Bentrude W G. 1973. Phosphorus radicals. *In:* Free Radicals. Vol. 2, New York: Wiley, 1973, 595~663

1973CAR/GOW Carmichael P J, Gowenlock B G, Johnson C A F. 1973. Carbon-nitrogen bond dissociation energies in halogenated C-nitroso compounds and in di-tert-butyl nitroxide. J Chem Soc Perkin Trans. 2, 1853~1856

1973DIB/WAL Dibeler V H, Walker J A, Rosenstock H M. 1973. Hot bands in the molecular and dissociative photoionization of acetylene and the heat of formation of the ethynyl ion. J Chem Phys, 59:2264~2268

1973EGG/COC Egger K W, Cocks A T. 1973. Homopolar and hetropolar bond dissociation energies and heats of formation of radicals nad ions in the gas phase. 1. Data on organic molecules. Helv Chim Acta, 56:1516~1536

1973EGG/COC(b) Egger K W, Cocks A T. 1973. Homopolar and heteropolar bond dissociation energies and heats of formation of radicals and ions in the gas phase. 2. Relation between structure and bond dissociation on organic molecules. Helv Chim Acta, 56:1537~1552

1973FER/OKA Ferguson K C, Okafo E N, Whittle E. 1973. Bond dissociation energies from equilibrium studies. 4. Bromine, methane equilibrium with hydrogen bromide, methyl bromide. Determination of methyl-bromide bond dissociation energy and standard heat of formation of methyl bromide. J Chem Soc Faraday Trans 1, 69:295~301

1973GOL/SPO Golden D M, Spokes G N, Benson S W. 1973. Very low-pressure pyrolysis (VLPP), a versatile kinetic method. Angew Chem, 85:602~614

1973KNO/SCH Knoll H, Scherker K, Geiseler G. 1973. Thermal decomposition of biacetyl. Int J Chem Kinet, 5:271~283

1973MAH/MEN Mahoney J R, Mendenhall G D, Ingold K U. 1973. Calorimetric and equilibrium studies on some stable nitroxide and iminoxy radicals. Approximate oxygen-hydrogen bond dissociation energies in hydroxylamines and oximes. J Am Chem Soc, 95:8610~8614

1973MCK/DUN McKean D C, Duncan J, Batt L. 1973. Carbon-hydrogen stretching frequencies, bond lengths, and dissociation energies. Spectrochim Acta, 29A:1037~1049

1973MEN/GOL Mendenhall G D, Golden D M, Benson S W. 1973. Thermochemistry of the bromination of carbon tetrachloride and the heat of formation of carbon tetrachloride. J Phys Chem, 77:2707~2709

1973OKA/DIB Okabe H, Dibeler V H. 1973. Photon impact studies of cyanoacetylene and acetonitrile in the vacuum ultraviolet. Heats of formation of ethynyl and acetonitrile. J Chem Phys, 59:2430~2435

1973ONE/BEN Benson S W, O'Neal H E. 1973. Thermochemistry of free radicals. *In:* Free Radicals. Vol. 2, New York: Wiley, 275~359

1973PER/GOL Perona M J, Golden D M. 1973. Very low-pressure pyrolysis. 8. Decomposition of di-tert-amyl peroxide. Int J Chem Kinet, 5:55~65

1973ROD/FOR Rodgers A S, Ford W G F. 1973. Analysis of the kinetics of the thermal and chemically activated elimination of hydrogen fluoride from 1,1,1-trifluoroethane. C–C bond dissociation energy and the heat of formation of 1,1,1-trifluoroethane. Int J Chem Kinet, 5:965~975

1973ROD/WU Rodgers A S, Wu E C. 1973. Kinetics of the positional isomerization of 2,3-dimethyl-2-butene. Heat of formation of the 2,3-dimethylbutenyl radical and the effect of methyl substituents on the allyl radical stabilization energy. J Am Chem Soc, 95:6913~6917

1973SHA/FRA Sharma D K S, Franklin J L. 1973. Heats of formation of free radicals by mass spectrometry. J Am Chem Soc, 95:6562~6566

1973TRE Trenwith A B. 1973. Dissociation of 3-hydroxylbut-1-ene, and the resonance energy of the hydroxyally radical. Trans Faraday Soc, 69:1737~1743

1973TSA Tsang W. 1973. Pyrolysis of 2,4-dimethylhexene-1 and the stability of isobutenyl radicals. Int J Chem Kinet, 5:929~946

1973WAT/THO Watkins K W, Thompson W W. 1973. Addition of ethyl radicals to carbon monoxide. Kinetic and thermochemical properties of the propionyl radical. Int J Chem Kinet, 5:791~803

1973WU/ROD Wu E C, Rodgers A S. 1973. Gas-phase kinetics of the reaction of 1,1,1-trifluoroethyl iodide with hydrogen iodide. C–I bond dissociation energy in 2,2,2-trifluoroethyl iodide. Int J Chem Kinet, 5:1001~1006

1974BAT/CHR Batt, L, Christie K, Milne R T, Summers A J. 1974. Heats of formation of C_1-C_4 alkyl nitrites (RONO) and their RO–NO bond dissociation energies. Int J Chem Kinet, 6:877~885

1974CAL/KAN Calle L M, Kanaan A S. 1974. Enthalpies and entropies of sublimation of

tetraphenylsilane and hexaphenyldisilane. Bond dissociation energies of the silicon-carbon and silicon-silicon bonds. Chem Thermodyn, 6:935~942

1974CHO/MEN Choo K Y, Mendenhall G D, Golden D M, Benson S W. 1974. Pyrolysis of 2-nitrosoisobutane and the bond dissociation energies of nitroso compounds. Int J Chem Kinet, 6:813~828

1974KRE/PRI Krech M J, Price S J W, Yared W F. 1974. Determination of D[pentafluoroiodobenzene] by the toluene carrier method. Int J Chem Kinet, 6:257~263

1974OKA/WHI Okafo E N, Whittle E. 1974. Bond dissociation energies from equilibrium studies. 5. The equilibrium $Br_2 + CH_2F_2 = HBr + CHBrF_2$, and $Br + CH_3F = HBr + CH_2BrF$. Determination of $D(CHF_2–Br)$ and heat of formation of radical CHF_2Br. J Chem Soc Faraday Trans 1, 70:1366~1375

1974PEP/ERL Pepekin V I, Erlikh R D, Matyushin Yu N, Lebedev Yu A. 1974. Energy of cleavage of the carbon-azide bond in triphenylazidomethane and benzyl and phenyl azides. Enthalpy of formation of the triphenylmethyl radical. Dokl. Akad Nauk SSSR, 214:865~867

1974WAT/WAR Watkins K W, Ward W W. 1974. Addition of methyl radicals to carbon monoxide. Chemically and thermally activated decomposition of acetyl radical. Int J Chem Kinet, 6:855~873

1974WU/ROD Wu E C, Rodgers A S. 1974. Thermochemistry of gas-phase equilibrium $CF_3CH_3 + I_2 = CF_3CH_2I + HI$. The carbon-hydrogen bond dissociation energy in 1,1,1-trifluoroethane and the heat of formation of the 2,2,2-trifluoroethyl radical. J Phys Chem, 78:2315~2317

1975~1979

1975CHE/ROD Chen S S, Rodgers A S, Chao J, Wilhoit R C, Zwolinski B J. 1975. Ideal gas thermodynamic properties of six fluoroethane. J Phys Chem Ref Data, 4:441~456

1975CHO/GOL Choo, K Y, Golden D M, Benson S W. 1975. Very-low-pressure pyrolysis of nitroso- and pentafluoronitrosobenzene C–NO bond dissociation energies. Int J Chem Kinet, 7:713~724

1975DAV/HOW Davidson I M T, Howard A V. 1975. Mechanism of thermolysis of hexamethyldisilane and the silicon-silicon bond dissociation energy. J Chem Soc Faraday Trans 1,71:69~77

1975GOW/JON Gowenlock B G, Jonhson C A F, Keary C M, Pfaf J. 1975. Carbon-nitrogen bond dissociation energy in nitrosyl cyanide. J Chem Soc Perkin Trans 2, 371:351

1975KIN/GOD King K D, Goddard R D. 1975. Very low pressure pyrolysis (VLPP) of alkyl cyanide. 2. n-Propyl cyanide and isobutyl cyanide. Heat of formation and stabilization energy of the cyanomethyl radical. Int J Chem Kinet, 7:837~855

1975KIN/GOD(b) King K D, Goddard R D. 1975. Very low pressure pyrolysis (VLPP) of alkyl cyanide. 1. Thermal unimolecular reactions of isopropyl cyanide. J Am Chem Soc, 97:4505~4509

1975LOS/TRA Lossing F P, Traeger J C. 1975. Stabilization in cyclopentadienyl, cyclopentenyl, and cyclopentyl cations. J Am Chem Soc, 97:1579~1580

1975MAH/DAR Mahoney L R, DaRooge M A. 1975. Kinetic behavior and thermochemical properties of phenoxy radicals. J Am Chem Soc, 97:4722~4731

1975MAT/NAS Matveev V G, Nasin G M. 1975. Izv. Akad. Nauk SSSR Ser Khim, No. 4:774~778

1975OKA/WHI Okafo E N, Whittle E. 1975. Kinetics of the thermal bromination of trifluoro-iodomethane. Determination of the bond dissociation energy $D(CF_3–I)$. Int J Chem Kinet, 7:273~285

1975OKA/WHI(b) Okafo E N, Whittle E. 1975. Competitive study of the reaction Br + Rf I = IBr + Rf

and determination of bond dissociation energies D(Rf-I) where Rf = trifluoromethyl, pentafluoroethyl, heptafluoropropyl, iso-heptafluoropropyl, and nonafluorobutyl. Int J Chem Kinet, 7:287~300

1975PAU/BAC Paul S, Back M H. 1975. A kinetic determination of the dissociation energy of the carbon-oxygen bond in anisole. Can J Chem, 53:3330~3338

1975PEP/LEV Pepekin V I, Lebedev V P, Balepin A A, Lebedev A Yu. 1975. Thermochemistry of C-nitroso compounds, Dokl. Akad. Nauk SSSR 221:1118~1121

1975PEP/MAT Pepekin V I, Matyashin Y N, Nikolaeva A D, Kirsanov A P, Platonova L V, Lebedev Y A. 1975. Dissociation energy of the nitrogen-oxygen bond in bis(nitratomethyl)furoxan. Izv. Akad. Nauk SSSR Ser. Khim, No. 8:1870~1871

1975REE/BRA Reed K J, Brauman J I. 1975. Electron affinities of alkoxy radicals and the bond dissociation energies in aliphatic alcohols. J Am Chem Soc, 97:1625~1626

1975RIC/STE Richardson J H, Stephenson L M, Brauman J I. 1975. Photodetachment of electrons from large molecular systems. Pyrrolate ion. Electron affinity of C_4H_4N. J Am Chem Soc, 97:1160~1162

1975STO/ING Stockbauer R, Inghram M G. 1975. Threshold photoelectron-photoion coincidence mass spectrometric study of ethylene and ethylene-D4. J Chem Phys, 62:4862~4870

1975VAN/RIN Vanderwielen A J, Ring M A, O'Neal H E. 1975. Kinetics of the thermal decomposition of methyldisilane and trisilane. J Am Chem Soc, 97:993~998

1976BAT/MCC Batt L, McCulloch R D. 1976. Pyrolysis of dimethyl peroxide. Int J Chem Kinet, 8:491~500

1976BAT/MCC(b) Batt L, McCulloch R D. 1976. The gas-phase pyrolysis of alkyl nitrites. 2. s-Butyl nitride. Int J Chem Kinet, 8:911~933

1976BAT/MIL Batt L, Milne R T. 1976. The gas-phase pyrolysis of alkyl nitrites. 1. t-Butyl nitride. Int J Chem Kinet, 8:59~84

1976BEN Benson S W. 1976. Thermochemical kinetics, 2nd ed. New York: Wiley

1976DES/FOR Descamps B, Forst W. 1976. Kinetics of the thermal decomposition of bis(trifluoromethyl) peroxide, J Phys Chem, 80: 933~939

1976DON/WAL Doncaster A M, Walsh R. 1976. Gas phase reaction between iodine and tetramethylsilane. 2. Kinetics and the bond dissociation energy D(Me_3SiCH_2–H). J Chem Soc Faraday Trans 1, 72:2908~2916

1976KIN/GOD King K D., Goddard R D. 1976. Very low-pressure pyrolysis of alkyl cyanides.3. tert-Butyl cyanide. Effect of the cyano group on bond dissociation energies and reactivity. J Phys Chem, 80:546~552

1976KOM/KRE Kominar R J, Krech, M J, Price S J W. 1976. Pyrolysis of iodobenzene by the toluene carrier technique and determination of D(C_6H_5–I). Can J Chem, 54:2981~2984

1976LEW Lewis D K. 1976. Di-tert-butyl peroxide decomposition behind shock waves. Can J Chem, 4:581~585

1976LOS/TRA Lossing F P, Traeger J C. 1976. Free radicals by mass-spectrometry. 46. Heats of formation of C_5H_7 and C_5H_9 radicals and cations. Int J Mass Spectrom Ion Proc, 19:9~22

1976MCC/DIB McCulloh K E, Dibeler V H. 1976. Enthalpy of formation of methyl and methylene radicals of photoionization studies of methylene and ketene. J Chem Phys, 64:4445~4450

1976PIC/ROD Pickard J M, Rodgers A S. 1976. Gas-phase kinetics of reaction of 1,1-difluoroiodoethane with hydrogen iodide— C–I bond dissociation energy in 1,1-difluoroiodoethane. Int J Chem Kinet, 8:809~815

1976TSA Tsang W. 1976. Thermal-stability of alcohols. Int J Chem Kinet, 8:173~192

1976VAN/TRO Van den Bergh H, Troe J. 1976. Kinetic and thermodynamic properties of nitrosyl

iodide and nitryl iodide intermediate complexes in iodine recombination. J Chem Phys, 64:7356~742

1976WAL/WEL Walsh R, Wells J M. 1976. Kinetics of gas-phase reaction between iodine and trichlorosilane and bond dissociation energies D($SiCl_3$-H). J Chem Soc Faraday Trans 1, 72:1212~1220

1976WU/ROD Wu E C, Rodgers A S. 1976. Kinetics of the gas phase reaction of pentafluoroethyl iodide with hydrogen iodide. Enthalpy of formation of the pentafluoroethyl radical and the pi bond dissociation energy in tetrafluoroethylene. J Am Chem Soc, 98:6112~6115

1977BAT/MIL Batt L, Milne R T. 1977. Gas-phase pyrolysis of alkyl nitrites. 3. Isopropyl nitrite. Int J Chem Kinet, 9:141~156

1977BAT/MIL(b) Batt L, Milne R T. 1977. Gas-phase pyrolysis of alkyl nitrites. 4. Ethyl nitrite. Int J Chem Kinet, 9:549~565

1977BAT/MIL(c) Batt L, Milne R T, McCulloch R D. 1977. Gas-phase pyrolysis of alkyl nitrites. 5. Methyl nitrite. Int J Chem Kinet, 9:567~587

1977COL/BEN Colussi A J, Benson S W. 1977. Very low-pressure pyrolysis of 2-phenylethylamine-enthalpy of formation of aminomethyl radical. Int J Chem Kinet, 9:307~316

1977COL/BEN(b) Colussi A J, Benson S W. 1977. Very low-pressure pyrolysis of phenyl methyl sulfide and benzyl methyl sulfide — enthalpy of formation of methylthio and phenylthio radicals. Int J Chem Kinet, 9:295~306

1977COL/BEN(c) Colussi A J, Benson S W, Hwang R J, Tiee J J. 1977. Intermolecular isotope effect in laser multiphoton dissociation of CH_2DCH_2Cl. Chem Phys Lett, 52:349~354

1977COl/ZAB Colussi A J, Zabel F, Benson S W. 1977. Very low-pressure pyrolysis of phenyl ethyl ether, phenyl allyl ether, and benzyl methyl-ether and enthalpy of formation of phenoxy radical. Int J Chem Kinet, 9:161~178

1977DAV/FEH Davidson J A, Fehsenfeld F C, Howard C J. 1977. Heats of formation of NO_3 and NO_3-association complexes with HNO_3 and HBr. Int J Chem Kinet, 9:17~29

1977DON/WAL Doncaster A M, Walsh R. 1977. Kinetic determination of bond dissociation energy D(Me_3Ge–H) and its implications for bond strengths. J Chem Soc Chem Commun, 446~447

1977DRO/SMO Drowart J, Smoes S J. 1977. Determination by the mass spectrometric Kundsen cell method and discussion of the dissociation energies of the molecules diselenium (g), sulfur selenide (g) and selenium telluride (g). Chem Soc Faraday Trans 2, 73:1755~1767

1977HEN/KEN Hendry D G, Kenley R. 1977. Generation of peroxy radicals from peroxy nitrates (RO_2NO_2). Decomposition of peroxyacyl nitrates. J Am Chem Soc, 99:3198~3199

1977IRE/GOR Ireton R, Gorden A S, Tardy D C. 1977. Thermal decomposition of perfluoro-di-tert-butyl peroxide. Int J Chem Kinet, 9: 769~775

1977KIN King K D. 1977. Very low-pressure pyrolysis (VLPP) of 3,3-dimethylbut-1-yne (tert-butyl acetylene). The heat of formation and stabilization energy of the dimethylpropargyl radical. Int J Chem Kinet, 9:907~915

1977OKA Okabe H. 1977. Photodissociation of thiophosgene. J Chem Phys, 66:2058~2062

1977PED/RYL Pedley J B, Rylance J. 1977. Sussex-N.P.L. Computer analysed thermochemical data: Organic and organometallic compounds. University of Sussex

1977PIC/ROD Pickard J M, Rodgers A S. 1977. The kinetics and thermochemistry of the reaction of 1,1-difluoroethane with iodine. The difluoromethylene-hydrogen bond dissociation energy in 1,1-difluoroethane and the heat of formation of 1,1-difluoroethyl. J Am Chem Soc, 99:691~694

1977PIC/ROD(b) Pickard J M, Rodgers A S. 1977. Kinetics and equilibrium of gas-phase reaction $CH_3CF_2Br + I_2 = CH_3CF_2I + IBr$. C–Br bond dissociation energy in 1,1-difluorobromoethane. Int J Chem Kinet, 9:759~767

1977TRE/WRI Trenwith A B, Wrigley S P.1977. Dissociation of 2-methybut-1-ene and resonance energy of 2-methyl allyl radical. J Chem Soc Faraday Soc 1, 73:817~822

1978APP/KLU Applequist D F, Klug J H. 1978. Energies of the cycloalkyl and 1-methylcycloalkyl free radicals by the decarbonylation method. J Org Chem, 43:1729~1733

1978ATR/BAL Atri G M, Baldwin P R, Evans G A, Walker R W. 1978. Decomposition of 2,2,3.3-tetra-methyl-butane in presence of oxygen. J Chem Soc Faraday Trans 1, 74:366~379

1978BAL/GOL Baldwin A C, Golden D M. 1978. Application of RRKM theory using a hindered rotational Gorin model transition state to the reaction $HO_2NO_2 + N_2 = HO_2 + NO_2 + N_2$. J Phys Chem, 82:644~647

1978BEN Benson S W. 1978. Thermochemistry and kinetics of sulfur-containing molecules and radicals. Chem Rev, 78:23~43

1978CAC/LIS Caceres T, Lissi E A, Sanhueza E. 1978. Auto-oxidation of diethyl hydroxylamine. Int J Chem Kinet, 10:1167~1182

1978COL/BEN Colussi A J, Benson S W. 1978. Very low-pressure pyrolysis of N-methyl aniline and N,N-dimethyl aniline — enthalpy of formation of anilino and N-methyl anino radicals. Int J Chem Kinet, 10:1139~1149

1978CZA/SCH Czarnowski J, Schumacher H J. 1978. Kinetics of thermal decomposition of bis-pentafluorine sulfur peroxide in presence of carbon monoxide. Int J Chem Kinet, 10:111~116

1978DAY/GOW Day J S, Gowenlock B G, Johnson C A F, McInally I D, Pfab J. 1978. Appearance potential studies of some geminal substituted C-nitroso compounds. J Chem Soc Perkin Trans 2, 1110~1112

1978DON/WAL Doncaster A M, Walsh R. 1978. Kinetics of gas-phase reaction between iodine and trifluorosilane and bond dissociation energy $D(SiF_3–H)$. Int J Chem Kinet, 10:101~110.

1978KAT/RAJ Katz M G, Rajbenbach L A. 1978. Correlation of activation – energies of radical – molecule metathesis reactions with enthapic, polar, and steric parameters. Int J Chem Kinet, 10:955~970

1978KIN King K D. 1978. Very low-pressure pyrolysis (VLPP) of but-1-yne — Heat of formation and stabilization energy of propargyl radical. Int J Chem Kinet, 10:545~555

1978KOM/KRE Kominar R J, Krech M J, Price S J W. 1978. Pyrolysis of bromobenzene by toluene carrier technique and determination of $D(C_6H_5–Br)$. Can J Chem, 56:1589~1592

1978MAR/COM Marquaire P M, Come G M. 1978. Non quasi-stationary state pyrolysis induction period of neopentane pyrolysis. React Kinet Catal Lett, 9:165~169

1978OKA/WHI Okafo E N, Whittle E.1978. Kinetics of thermal gas-phase reaction $Br_2 + C_6F_5I = BrI + C_6F_5Br$ — Attempt to determine bond dissociation energy $D(C_6F_5–I)$. Int J Chem Kinet, 10:591~598

1978ROD Rodgers A S. 1978. Thermochemistry of fluorocarbon radicals. Fluorine-containing free radicals. ACS Symp, 66:298~313

1978TSA Tsang W. 1978. Thermal stability of intermediate sized acetylenic - compounds and heats of formation of propargyl radicals. Int J Chem Kinet, 10: 687~711

1978TSA(b) Tsang W. 1978 Thermal stability of cyclohexane and 1-hexene. Int J Chem Kinet, 10:1119~1138

1978TSA(c) Tsang W. 1978. Evidence for strongly temperature-dependent, A factor in alkane decomposition and high heats of formation for alkyl radicals. Int J Chem Kinet, 10:821~837

1978TSA(d) Tsang W. 1978. Thermal stability of primary amines. Int J Chem Kinet, 10:40~66.

1978WHI/GAR White J N, Gardiner W C. 1978. Thermochemical properties of HSO radical. Chem Phys Lett, 58:470~472

1978ZAB/BEN Zabel F, Benson S W, Golden D M. 1978. Heat of formation of acetonyl radical VLPP

studies of acetonyl bromide. Isopropenylmethylether, and hexanedione-2,5 in a search for acetonyl stabilization energy. Int J Chem Kinet, 10:295~306

1979BAG/BEN Baghal-Vajooee M H, Benson S W. 1979. Kinetics and thermochemistry of the reaction Cl + cyclopropane = HCl + cyclopropyl radical. Heat of formation of the cyclopropyl radical. J Am Chem Soc, 101:2838~2840

1979BAR/SCO Bartmess J E, Scott J A, McIver R T. 1979. Scale of acidities in the gas phase from methanol to phenol. J Am Chem Soc, 101:6046~6056

1979BER Berkowitz J. 1979. Photoionization, Photodissociation, and Photoelectron Spectroscopy. New York: Academic Press, 1979. 285

1979CZA/SCH Czarnowski J, Schumacher H J. 1979. Kinetics and the mechanism of the thermal decomposition of bis-pentafluorosulfurtrioxide (SF_5OOOSF_5). Int J Chem Kinet, 11:613~619

1979DEF/HEH DeFrees D J, Hehre W J, McIver R T, McDaniel D H. 1979. Heat of formation and adiabatic electron affinity of amidogen. J Phys Chem, 83:232~237

1979DON/WAL Doncaster A M, Walsh R. 1979. Kinetics of the gas-phase reaction between iodine and trimethylgermane and the bond dissociation energy D(Me_3Ge-H). J Phys Chem, 83:578~581

1979DON/WAL(b) Doncaster A.M, Walsh R. 1979. Gas-phase study of the reaction system Me_3SiI + HBr = Me_3SiBr + HI. Equilibrium and the bond dissociation energy D(Me_3Si-I). J Phys Chem, 83:3037~3040

1979DON/WAL(c) Doncaster A M, Walsh R. 1979. Kinetics of the gas-phase reaction between iodine and trimethylsilane and the bond dissociation energy D(Me_3Si–H). J Chem Soc Faraday Trans 1, 75:1126~1131

1979EVA/WAL Evans G.A, Walker R W. 1979. Reaction of tert-butyl radical with hydrogen and with oxygen. J Chem Soc Faraday Trans 1, 75:1458~1464

1979GLA/MAI Glanzer K, Maier M, Troe J. 1979. Shock-wave study of the thermal dissociation of CF_3NO. Chem Phys Lett, 61:175~178

1979HUB/HER Huber K P, Herzberg G. 1979. Molecular Spectra and Molecular Structure. 4, Constants of Diatomic Molecules. New York: Reinhold

1979HWA/BEN Hwang R J, Benson S W. 1979. Kinetics of iodination of hydrogen sulfide by iodine and the heat of formation of the SH radical. Int J Chem Kinet, 11:579~583

1979HWA/BEN(b) Hwang RJ, Benson S W. 1979. Thermochemistry of the reaction of hydrogen sulfide with iodine and the heat of HSI — New sulfur compound. J Am Chem Soc, 101:2615~2617

1979JAC Jackson R.A. 1979. Bond dissociation energies of group IVB organometallic compounds. J Organomet Chem, 166:17~19

1979JAN/BRA Janousek B K, Brauman J I, Simons J. 1979. Experimental and theoretical determination of the electron-affinity of the ethynyl radical, HC_2 · . J Chem Phys, 71:2057~2061

1979KIN King K D. 1979. Very low-pressure pyrolysis (VLPP) of hex-1-ene — Kenitics of the retro-ene decomposition of a monoolefin. Int J Chem Kinet, 11:1071~1080

1979KIN/NGU King K D, Nguyen T T. 1979. Very low-pressure pyrolysis of 4-phenyl-1-butyne. The propargyl resonance energy. J Phys Chem, 83:1940~1943

1979PIP Piper L G. 1979. Heat of formation of NH. J Chem Phys, 70:3417~3419

1979PRI/SAP Price S J W, Sapiano H J. 1979. Determination of heat of formation of $C_{12}F_{10}$ (gas) from studies of the combustion of decafluorobiphenyl in oxygen and calculation of D(C_6F_5–C_6F_5). Can J Chem, 57:1468~1470

1979ROS/GOL Rossi M J, Golden D M. 1979. Absolute rate constants for metathesis reactions of allyl and benzyl radicals with HI (DI). Heat of formation of allyl and benzyl radicals. J Am Chem Soc, 101: 1230~1235

1979ROS/KIN Rossi W J, King K D, Golden D M. 1979. The equilibrium constant and rate constant for allyl radical recommbination in the gas phase. J Am Chem Soc, 101:1223~1230

1979TIE/AND Tiedemann P W, Anderson S L, Ceyer S T, Hirooka T, Ng C Y, Mahan B H, Lee Y T. 1979. Proton affinity of hydrogen halides determined by the molecular beam photoionization method. J Chem Phys, 71:605~609

1979VAY/BEN Vayjooee M H B, Benson S W. 1979. Kinetics and thermochemistry of the reaction Cl + cyclopropane = HCl + cyclopropyl. Heat of formation of the cyclopropyl radical. J Am Chem Soc, 101, 2838~2840

1979VAY/COL Vayjooee M H B, Colussi A J, Benson S W. 1979. Very low-pressure study of the kinetics and equilibrium – Cl + CH_4 reversible CH_3 + HCl at 298 K. Heat of formation of the CH_3 radical. Int J Chem Kinet, 11:147~154

1979WAL/TSA Walker J A, Tsang W. 1979. Thermal decomposition of hexamethylethane in a flow system. Int J Chem Kinet, 11:867~882

1980~1984

1980BAL/WAL Baldwin R R, Walker R W. 1980. Decomposition of 2,2,3-trimethylbutane in the presence of oxygen. J Chem Soc Faraday Trans 1, 76:825~837

1980BAR/STE Barton B.D, Stein S E. 1980. Pyrolysis of alkyl benzenes. Relative stability of methyl substituted benzyl radicals. J Phys Chem, 84:2141~2145

1980BOY/GUP Boyd R J, Gupta A, Langler R F, Lownie S P, Pincook J.A. 1980. Sulfonyl radicals, sulfinic acid, and related species. An ab initio molecular orbital study. Can J Chem, 58:331~338

1980DAV/WOO Davidson I M T, Wood I T. 1980. Primary reactions in the pyrolysis of allyl trimethylsilane. J Organomet Chem, 202:C65~C67

1980DEF/MCI DeFeers D J, McIver R T Jr, Hehre W J. 1980. Heats of formation of gaseous free radicals via ion cyclotron double resonance spectroscopy. J Am Chem Soc, 102:3334~3338

1980FRA/JUS Frank P, Just T. 1980. High-temperature thermal decomposition of acetylene and diacetyl relative concentrations. Comb Flame, 38:231~248

1980HOW Howard C J. 1980. Kinetic study of the equilibrium HO_2 + NO = OH + NO_2 and thermochemistry of HO_2. J Am Chem Soc, 102:6937~6941

1980JAN/REE Janousek B K, Reed K J, Brauman J I. 1980. Electron photodechment from mercaptyl anions (RS^-). Electron affinity of mercaptyl radical and the sulfur-hydrogen bond strength in mercaptans. J Am Chem Soc, 102:3125~3129

1980KIA/ZAR Kiang T, Zare R N. 1980. Stepwise bond dissociation energies in sulfur hexafluoride. J Am Chem Soc, 102:4024~4029

1980KOM/KRE Kominar R J, Krech M J, Price S J W. 1980. Determination of D($C_6F_5CH_2$ – Br) by toluene carrier method. Can J Chem, 58:1906~1908

1980MCM/TRE McMillen D F, Trevor P L, Golden D M. 1980. Highly stabilized radicals: benzylic radicals in polycylic aromatic systems. J Am Chem Soc, 102:7400~7402

1980MIL/ERE Miletic M, Eres D, Vejikovic M, Zmbov K F. 1980. Mass-spectrometric study of the ionization and fragmentation of carbon disulfide by monoenergetic electron-impact. Int J Mass Spectrom Ion Proc, 35:231~242

1980TRE Trenwith A B. 1980. Dissociation of 1,3-hexadiene and the resonance energy of the pentadienyl radical. J Chem Soc Faraday Trans 1, 76:266~271

1981AYR/BAC Ayranci G, Back M H. 1981. Kinetics of the bimolecular initiation process in the thermal reactions of ethylene. Int J Chem Kinet, 13:897~911

1981BAR/RAJ Baruch G, Rajbenbach L A, Horowitz A. 1981. Cl-atom transfer from $CFCl_3$ to the C_6H_{11} radical. An indirect estimation of the $CFCl_2$–Cl bond dissociation energy. Int J Chem Kinet, 13:473~480

1981BAR/STE Barton B D, Stein S E. 1981. Pyrolysis of ethylpyridines. Relative stability of isometric picolinyl radicals. J Chem Soc Faraday Trans 1, 77:1755~1762

1981BAT/BUR Batt L, Burrows J P, Robinson G N. 1981. On the isomerization of the methoxy radical. Relevance to atmospheric chemistry and combustion. Chem Phys Lett, 78:467~470

1981BAT/ROB Batt L, Robinson G N. 1981. Thermochemistry of nitro compounds, amines and nitroso compounds. *In:* Chemistry of the Functional Groups, Patai S, Suppl F eds. Chichester: Wiley, 1035~1083

1981CAN/MAR Canosa C E, Marshall R M, Sheppard A. 1981. The rate constant for H + iso-C_4H_8 → tert-C_4H_9 in the range of 298~563 K. Int J Chem Kinet, 13:295~301

1981CAS/MAR Castelhano A L, Marriott P R, Griller D. 1981. Heats of formation of tert-butyl and ethyl radicals. J Am Chem Soc, 103:4262~4263

1981CZA/SCH Czarnowski J, Schumacher H J. 1981. The kinetics and the mechanism of the thermal decomposition of bis(trifluoromethyl) trioxide. The influence of carbon monoxide on its decomposition. Int J Chem Kinet, 13:639~649

1981DON/WAL Doncaster A M, Walsh R. 1981. Kinetics of the gas-phase reaction between iodine and monosilane and the bond dissociation energy D(SiH_3–H). Int J Chem Kinet, 13:503~514

1981ELL/POT Ellul R, Potzinger P, Reimann B, Camilleri B. 1981. Arrhenius parameters for the system $(CH_3)_3Si + D_2 = (CH_3)_3SiD + D$. The $(CH_3)_3Si$–D bond dissociation energy. Ber Bunsenges Phys Chem, 85:407~412

1981EVA/WHI Evans B S, Whittle E. 1981. The kinetics of the reactions of C_2F_5 radicals with Br_2 and HBr. Int J Chem Kinet, 13:59~67

1981FOR/HIP Forte E, Hippler H, van den Bergh H. 1981. Ion thermodynamic properties and ultraviolet-spectrum. Int J Chem Kinet, 13:1227~1233

1981GRI/LOS Griller D, Lossing F P. 1981. On the thermochemistry of alpha-aminoalkyl radicals. J Am Chem Soc, 103:1586~1587

1981HEN/KNO Heneghan S P, Knoot P A, Benson S W. 1981. The temperature-coefficient of the rates in the system $Cl + CH_4 = CH_3 + HCl$ thermochemistry of the methyl radical. Int J Chem Kinet, 13:677~691

1981KIN King K D. 1981. Kinetics of competitive pathways in the thermal unimolecular decomposition of hex-1-yne. Int J Chem Kinet, 13:273~282

1981KIN/NGU King K D, Nguyen T T. 1981. Very low-pressure pyrolysis (VLPP) of pentynes. 2, 4-methylpent-2- yne and 4,4-dimethylpent-2-yne. Heats of fotmation and resonance stabilization energy of methyl-substituted propargyl radicals. Int J Chem Kinet, 13:255~272

1981MIL/STE Miller R E, Stein S E. 1981. Liquid-phase pyrolysis of 1,2-diphenylethane. J Phys Chem, 85:580~589

1981NGU/KIN Nguyen T T, King K D. 1981. Kinetics of decomposition and interconversion of 3-methylbut-1-yne and 3-methylbuta-1,2-diene. Resonance stabilization energies of propargylic radicals. J Phys Chem, 85:3130~3136

1981ONO/NG Ono Y, Ng C Y. 1981. The heat of formation of C_2H^+. J Chem Phys, 74:6985~6986

1981PEL/JAC Pellerite M J, Jackson R L, Brauman J I. 1981. Proton affinity of the gaseous azide ion. The N–H bond dissociation energy in hydrazoic acid. J Phys Chem, 85:1624~1626

1981ROB/STE Robaugh D A, Stein S E. 1981. Very low-pressure pyrolysis of ethylbenzene, isopropylbenzene, and tert-butylbenzene. Int J Chem Kinet, 13:445~462

1981RUI/BAY Ruiz R P, Bayes K D, Macpherson M T, Pilling M J, Direct observation of the equilibrium between allyl radicals, oxygen, and allylperoxy radical. J Phys Chem, 85:1622~1624

1981STE Stein S E. 1981. A fundamental chemical kinetics approach to coal conversion, New approaches in coal chemistry. ACS Symp Ser, 169:97~129

1981STE/ROW Steinkruger F J, Rowland F S. 1981. Bond dissociation energies of C–H bonds in several aloethylenes, as estimation from the recoil tritium abstraction reaction. J Phys Chem, 85:136~140

1981SUL/DEP Sullivan S A, DePuy C H, Damrauer R. 1981. Gas-phase reactions of cyclic silanes. J Am Chem Soc, 103:480~481

1981TSA Tsang, W. 1981. Comparative-rate single-pulse shock tube studies on the thermal stability of polyatomic molecules, in shock waves in Chemistry. Lifshitz A ed. New York: Marcel Dekker, 59~129

1981WAL Walsh R. 1981. Bond dissociation energy values in silicon-containing compounds and some of their implications. Acc Chem Res, 14:246~252

1981YAM/ZEL Yampol'skii Yu P, Zelentsov V V. 1981. Heat of formation of the ethynyl radical C_2H. React Kinet Catal Lett, 17:347~353

1982BAR/DON Barber M. Doncaster A M, Walsh R. 1981.The kinetics of the gas-phase reaction between iodine phenylsilane and the bond dissociation energy $D(C_6H_5SiH_2–H)$. Int J Chem Kinet, 14:669~677

1982BAT/ROB Batt L, Robinson G N. 1982. Thermochemistry of nitro compounds, amines and nitroso compounds, *In:* Chemistry of the Functional Groups, Patai S and Suppl F eds. Chichester: Wiley.1035~1083

1982BAT/WAL Batt L, Walsh R. 1982. A reexamination of the pyrolysis of bis(trifluoromethyl) peroxide. Int J Chem Kinet, 14:933~944

1982BEN/WEI Benson S W, Weissman M. 1982. Mechanism of the pyrolysis of C_2HCl_5, molecular and radical steps. Int J Chem Kinet, 14:1287~1304

1982CAS/GRI Castelhano A L, Griller D. 1982. Heats of formation of some simple alkyl radicals. J Am Chem Soc, 104:3655~3659

1982HAS/SCH Hase W, Schlege H B. 1982. Resolution of a paradox concerning the forward and reverse rate constants for $C_2H_5 = H + C_2H_4$. J Phys Chem, 86:3901~3904

1982KHA/NIA Khachatryan L A, Niazyan O M, Mantashyan A A, Vedeneev V I, Teital'boim M A. 1982. Experimental determination of the equilibrium constant of the reaction $CH_3 + O_2 = CH_3O_2$ during the gas-phase oxidation of methane. Int J Chem Kinet, 14:1231~1241

1982MCM/GOL McMillen D F, Golden D M. 1982. Hydrocarbon bond dissociation energies. Annu Rev Phys Chem, 33:493~532

1982MCM/LEW McMillen D F, Lewis K E, Smith G P, Golden D M. 1982. Laser-powered homogeneous pyrolysis. Thermal studies under homogeneous conditions, validation of the technique, and application to the mechanism of azo compound decomposition. J Phys Chem, 86:709~718

1982MEO Meot-Ner M. 1982. Carbon-hydrogen bond dissociation energies in alkylbenzenes. Proton affinity of the radicals and the absolute proton affinity scale. J Am Chem Soc, 104:5~10

1982MOR/PIL Morgan C A, Pilling M J, Tulloch J M, Ruiz R P, Bayes K D. 1982. Direct determination of the equilibrium constant and thermodynamic parameters for the reaction $C_3H_5 + O_2 = C_3H_5O_2$. J Chem Soc Faraday Trans 2, 78:1323~1330

1982NAP/SAN Nappa M J, Santi R, Diefenbach S P, Halpern J. 1982. Diverse mechanisms of carbon-hydrogen bond formation through binuclear reductive elimination reactions. J Am Chem Soc, 104:619~621

1982NGU/KIN Nguyen T T, King K D. 1982. Very low-pressure pyrolysis (VLPP) of pentynes. 3. Pent-2-yne, Heat of formation and resonance stabilization energy of the 3-methylpropargyl radical. Int J Chem Kinet, 14:613~621

1982TRE Trenwith A B. 1982. Dissociation of 3-methylpenta-1,4-diene and the resonance energy of the pentadienyl radical. J Chem Soc Faraday Trans 1, 78:3131~3136

1982TRE/WRI Trenwith A B, Wrigley S P. 1982. Pyrolysis of but-1-yne and the resonace energy of the propargyl and 3-methylpropargyl radicals. J Chem Soc Faraday Trans 1, 78:2337~2347

1982WAG/EVA Wagman D D, Evans W H, Park V B, Schumm R H, Halow, I, Bailey S M, Churney K L, Nuttall R L. 1982. The NBS Tables of chemical thermodynamic properties. Selected values for inorganic and C_1 and C_2 organic substance in SI Units. J Phys Chem Ref Data, 11, Suppl 2

1983BAT/LIU Batt L, Liu M TH. 1983. Pyrolysis of peroxides in the gas phase, *In*: Chemical Peroxides. Patai S ed. New York: Wiley. 685~710

1983BAT/WAL Batt L, Walsh R. 1983. A reexamination of the pyrolysis of bis(trifluoromethyl) peroxide. Addendum: concerning $D(CF_3O_2–CF_3)$ and $D(CF_3–O_2)$. Int J Chem Kinet, 15:605~607

1983BER/SIM Bernstein M, Simon J D, Peters K S. 1983. Metal-carboyl bond strengths. Applications of photo-acoustic calorimetry. Chem Phys Lett, 100:241~244

1983BUR/CAS Burkey T J, Castelhano A L, Griller D, Lossing F P. 1983. Heats of formation and ionization potentials of some alpha-aminoalkyl radicals. J Am Chem Soc, 105:4701~4703

1983EVA/WEE Evans B S, Weeks I, Whittle E. 1983. Bromination of fluoroalkanes. 5. Kinetics of forward and reverse reactions in the system $Br_2 + C_3F_7H$, $HBr + IC_3F_7Br$. J Chem Soc Faraday Trans 1, 79:1471~1482

1983FRI Fricdricj L E. 1983. The two hydrogen-oxygen bond dissociation energies of hydroquinone. J Org Chem, 48:3851~3852

1983HEN/BEN Heneghan S P, Benson S W. 1983. Kinetics and equilibrium in the system Br + tert-BuO_2H = $HBr + BuO_2$. O–H bond dissociation energy in $tBuO_2$–H. Int J Chem Kinet, 15:815~822

1983JEN/PER Jenkins T C, Perkins M J. 1983. Acyl nitroxides. 4. Estimation of O–H bond dissociation energies for N-tert-butylhydroxamic acids. J Chem Soc Perkin Trans. 2:717~720

1983MAR/PAR Martin J P, Paraskevopoulos G. 1983. Rates of OH radical reactions. 9. A kinetic study of the reactions of OH radicals with fluoroethanes. Estimates of C–H bond strengths in fluoroalkanes. Can J Chem, 61:861~865

1983NOB/WAL Noble P N, Walsh R. 1983. Kinetics of the gas-phase reaction between iodine and monogre and the bond dissociation energy $D(GeH_3–H)$. Int J Chem Kinet, 15:547~560

1983NOB/WAL(b) Noble P N, Walsh R. 1983. The kinetics of secondary reactions in the iodination of monogermane. The effect of iodine substitution on the Ge–H bond dissociation energy. Int J Chem Kinet, 15:561~568

1983OAK/JON Oakes J M, Jones M E, Bierbaum V M, Barney G. 1983. J. Photoelectron spectroscopy of anions from CCO^- and $HCCO^-$. J Phys Chem, 87:4810~4815

1983PAT/GOL Patrick R, Golden D M.1983. 3rd-order rate constants of atmospheric importance. Int J Chem Kinet, 15:1189~1227

1983PED/MAR Pedley J B, Marshall E M. 1983. Thermochemical data for gaseous monoxides. J Phys Chem Ref Data, 12:967~1031

1983PIC/ROD Pickard J M, Rodgers A S. 1983. Kinetics of the gas-phase reaction $CH_3F + I_2$ = $CH_2FI + HI$. The C–H bond dissociation energy in methyl and methylene fluorides. Int J Chem Kinet, 15:569~577

1983PRA/DEH Pratt S T, Dehmer P M. 1983. On the dissociation energy of ArO_2^+. J Chem Phys, 78:6336~6338

1983ROS/GOL Rossi M J, Golden D M. 1983. Laser-induced kinetics: Arrhenius parameters for tert-butyl + XI = iso-C_4H_9X + I (X = H or D) and the heat of formation of the tert-butyl radical. Int J Chem Kinet, 15:1283~1300

1983SER/GOR Seres L, Gorgenyi M, Farkas J. 1983. The azoethane-initiated thermal reaction of isobutene. Heat of formation of the 2-methyl-2-pentyl radical. Int J Chem Kinet, 15:1133~1145

1983SHU/BEN Shum L G S, Benson S W. 1983. Thermochemistry and kinetics of the reaction of methyl mercaptan with iodine. Int J Chem Kinet, 15:433~453

1983SHU/BEN(b) Shum L G S, Benson S W. 1983. Review of the heat of formation of the hydroperoxyl radical. J Phys Chem, 87:3479~3482

1983SPY/SAU Spyrou S M, Sauers I, Christophorou L G. 1983. Electron attachment to the perfluoroalkanes n-C_NF_{2N-2} (N=1~6) and perfluoroisobutane. J Chem Phys, 78:7200~7216

1983TRE Trenwith A B. 1983. Pyrolysis of propionitrile and the resonance stabilization energy of the cyanomethyl radical. J Chem Soc Faraday Trans 1, 79:2755~2764

1983WEI/BEN Weissman M, Benson S W. 1983. Heat of formation the $CHCl_2$ radical. Bond dissociation energies in chloromethanes and chloethanes. J Phys Chem, 87:243~244

1984AHO/WHI Ahonkhai S I, Whittle E. 1984. Kinetics of the competitive chlorinations of some perfluoroalkyl iodides. Determination of the bond dissociation energies D(CF_3–I), D(C_2F_5–I), and D(i-C_3F_7 -I). Int J Chem Kinet, 16:543~558

1984BAL/DRE Baldwin R R., Drewery G R, Walker R W. 1984. Decomposition of 2,3-dimethylbutane in the presence of oxygen. 1. Thermochemistry of the reaction 2,3-dimethylbutane = 2(isopropyl). J Chem Soc Faraday Trans 1, 80:2827~2841

1984BAL/KEE Baldwin R R, Keen A, Walker R W. 1984. Studies of the decomposition of oxirane and of its addition to slowly reacting mixtures of hydrogen and oxygen at 480°C. J Chem Soc Faraday Trans 1, 80:435~456

1984CAO/BAC Cao J R, Back M H. 1984. The heat of formation of the ethyl radical. Int J Chem Kinet, 16:961~966

1984COX/WAG Cox J D, Wagman D D, Medvedev V A. 1984. CODATA Key Values for Thermodynamics. New York: Hemisphere Pub http://codata.org/codata/databases/key1.html

1984DEM De Maria G. 1984. Vaporization studies by Knudsen cell mass spectrometry and thermodynamic stability of high-temperature gaseous species, in thermochemistry and its applications to chemical and biological systems. NATO-ASI Ser. C119, Dordrecht:Reidel. 157~181

1984DOB/ING Doba T, Ingold K U. 1984. Kinetic applications of electron paramagnetic resonance spectroscopy. 42. Some reactions of the bis(trifluoromethyl)aminoxyl radical. J Am Chem Soc, 106:3958~3963

1984GRE/COL Grela M A, Colussi A J. 1984. Pyrolysis of ethylenediamines. The stabilization energies of aminomethyl and N,N-dimethylaminomethyl radicals. J Phys Chem, 8:5995~5998

1984HOL/LOS Holmes J L, Lossing F P. 1984. Heats of formation of organic radicals from appearance energies. Int J Mass Spectrom Ion Proc, 58:113~120

1984HOL/LOS(b) Holmes J L, Lossing F P, Terlouw J K. 1984. Heat of formation and homolytic bond dissociation energies in the keto-enol tautomers of acetaldehyde and acetone. J Am Chem Soc, 108:1086~1087

1984KON/BEN Kondo O, Benson S W. 1984. Kinetics and equilibrium of the reaction between bromine and ethyl ether. The C–H bond dissociation energy in ethyl ether. Int J Chem Kinet,

16:949~960

1984KON/BEN(b) Kondo O, Benson S W. 1984. Kinetics and equilibrium in the system Br + CH_3OOH == HBr + CH_3OO. An upper limit for the heat of formation of the methylperoxy radical. J Phys Chem, 88:6675~6680

1984KRA/BUT Krajnovich D, Butler L J, Lee Y T. 1984. UV photodissociation of C_2F_5Br, C_2F_5I, and 1,2-C_2F_4BrI, Chem Phys, 81:3031~3047

1984LIA/LIB Lias S G, Liebman J F, Levin R D. 1984. Evaluated gas phase basicities and proton affinities of molecles. Heats of formation of protonated molecules. J Phys Chem Ref Data, 13:695~808

1984MAR Margitan J J. 1984. Mechanism of the atmospheric oxidation of sulfur. Catalysis by hydroxyl radicals. J Phys Chem, 88:3314~3318

1984MEA Mead R D, Stevens A E, Lineberger W C. 1984. Photodetachment in negative ion beams. *In*: Gas Phase Ion Chemistry. Bowers M T ed. New York: Academic Press, Vol. 3, 231~248

1984NON/WAL Nonhebel D C, Walton J C. 1984. Estimation of bond dissociation energies, including D($RSCH_2$–H), from barriers to internal rotation. J Chem Soc Chem Commun, 731~732

1984PAC/WIM Pacey P D, Wimalaseba J H. 1984. Kinetics and thermochemistry of the ethyl radical. The induction period in the pyrolysis of ethane. J Phys Chem, 88:5657~5660

1984PRI/NIL Pritchard G O, Nilsson W B, Kirtman B. 1984. Orbital energy and entropy correlation for disproportionation versus combination in the reaction of $CF_yH_{(3-y)}$ (y = 1,1,2,3) with ethyl radicals. The heat of formation of fluoromethylene. Int J Chem Kinet, 16:1637~1643

1984ROS/MCM Rossi M J, McMillen D F, Golden D M. 1984. Aliphatic C–H bond scission processes in diphenylmethane and 2-benzyl- and 4-benzylpyride. The heat of formation of the diphenylmethyl and alpha-phenylethyl radical in the gas phase. J Phys Chem, 88:5031~5039

1984SCH/HOU Schultz J C, Houle F A, Beauchamp J L. 1984. Photoelectron spectroscopy of isomeric C_4H_7 radicals. Implications for the thermochemistry and structures of the radicals and their corresponding carbonium ions. J Am Chem Soc, 106:7336~7347

1984SMI/ADA Smith D, Adams N G, Ferguson E E. 1984. The heat of formation of $C_3H_2^+$. Int J Mass Spectrom Ion Proc, 61:15~19

1984TRA Traeger J C. 1984. A study of the ally cation thermpochemistry by photoionization mass spectrometry. Int J Mass Spectrom Ion Proc, 58:259~271

1984TSA Tsang W. 1984. Single pulse shock tube on the thermal stability of ketones. Int J Chem Kinet, 16:1543~1556

1985~1989

1985BUR/DOB Burton G W, Doba T, Gabe E J, Hughes L, Lee F L, Prasad L, Ingold K U. 1985. Autoxidation of biological molecules. 4. Maximizing the antioxidant activity of phenols. J Am Chem Soc, 107:7053~7065

1985CHA/DAV Chase M W Jr, Davies C A, Downey J R Jr, Frurip D J, McDonald R A, Syverud A N. 1985. JANAF thermochemical tables, 3rd ed. J Phys Chem Ref Data, 14:927~1856

1985DEA Dean A M. 1985. Predictions of pressure and temperature effects upon radical addition and recombination reactions. J Phys Chem, 89:4600~4608

1985GON/LAR Gonzalez A C, Larson C W, McMillen D F, Golden D M. 1985. Mechanism of decomposition of nitroaromatics. Laser-powered homogeneous pyrolysis of substituted nitrobenzenes. J Phys Chem, 89:4809~4814

1985GRE/COL Grela M A, Colussi A J. 1985. Pyrolysis of 2-phenylethylamines. Heats of formation of aminomethyl radicals R_2NCH_2 (R = H, CH_3). Int J Chem Kinet, 17:257~264

1985KIE/WEI Kiefer J H, Wei H C, Kern R D, Wu C H. 1985. The high temperature pyrolysis of 1,3-butadine. Heat of formation and rate of dissociation of vinyl radical. Int J Chem Kinet, 17:225~253

1985SHA/SEM Sharma R B, Semo N M, Koski W S. 1985. Heat of formation of the vinyl radical. Int. J. Chem. Kinet, 17:83~833

1985SLA/RAT Slagle I R, Ratajczak E, Heaven M C, Gutman D, Wagner A F. 1985. Kinetics of polyatomic free radicals produced by laser photolysis. 4. Study of the equilibrium i-$C_3H_7 + O_2$ — i-$C_3H_7O_2$ between 592 and 692 K. J Am Chem Soc, 107:1838~1845

1985TRA Traeger J C. 1985. Heat of formation for the formyl cation by photoionization mass spectrometry. Int J Mass Spectrom Ion Proc, 66:271~282

1985TSA Tsang W. 1985. The stability of alkyl radicals. J Am Chem Soc, 107:2872~2880.

1985WOD/LEE Wodtke A M, Lee Y T. 1985. Photodissociation of acetylene at 193.3 nm. J Phys Chem, 89:4744~4751

1986BER/CUR Berkowitz J, Curtiss L A, Gibson S T, Greene J P, Hillhouse G L, Pople J A. 1986. Photoionization mass spectrometric study and ab initio calculations of ionization and bonding in phosphorus-hydrogen compounds; heats of formation, bond energies, and the 3B1-1A1 seperation in dihydrophosphorus (1+). J Chem Phys, 84:375~384

1986BIL/GRI Billmers R, Griffith L L, Stein S E. 1986. Hydrogen transfer between anthracene structures. J Phys Chem, 90:517~523

1986BOR/BAU Bordwell F G, Bausch M J. 1986. Acidity-oxidation-potential (AOP) values as estimates of relative bond dissociation energies and radical stability in dimethyl sulfoxide solution. J Am Chem Soc, 108:1979~1985

1986BOR/BAU(b) Bordwell F G, Bausch M J. 1986. Radical cation acidities in dimethyl sulfoxide solution. J Am Chem Soc, 108:2473~2474

1986BRO/LIG Brouard M, Lightfoot P D, Pilling M .J. 1986. Observation of equilibrium in the system H + C_2H_4 = C_2H_5. The determination of the heat of formation of C_2H_5. J Phys Chem, 90:445~450

1986BUR/MAJ Burkey T J. Majewski M, Griller D. 1986. Heats of formation of radicals and molecules by a photoacoustic technique. J Am Chem Soc, 108:2218~2221

1986FRE/WAL Frey H M, Walsh R, Watts I M. 1986. Kinetics of the reaction of silylene with hydrogen and a possible resolution of discrepancies over the heat of formation of silylene. J Chem Soc Chem Commun, 1189~1191

1986GIB/GRE Gibson S T, Gree J P, Berkowitz J. 1986. A photoionization study of selenyl (SeH) and hydrogen selenide (H_2Se). J Chem Phys, 86:4815~4824

1986GRI/WAY Griller D, Wayner D D M. 1986. New approaches to free radical thermochemistry. Rev Chem Intermed, 7:31~44

1986HAW/GRI Hawari J A, Griller D, Lossing F P. 1986. Thermochemistry of perthiyl radicals. J Am Chem Soc, 108:3273~3275

1986HAY/KRU Hayashibara K, Kruppa G H, Beauchamp J L.1986. Photoelectron spectroscopy of the o-, m-, and p-methylbenzyl radicals. Implications for the thermochemistry of the radicals and ions. J Am Chem Soc, 108:5441~5443

1986HOL/LOS Holmes J L, Lossing F P, Terlouw J K. 1986. Heat of formation and homolytic bond dissociation energies in the keto-enol tautomers of acetaldehyde and acetone. J Am Chem Soc, 108:1086~1087

1986HOW/GRI Howari J A, Griller D, Lossing F P. 1986.Thermochemistry of perthiyl radicals. J Am Chem Soc, 108:3273~3275

1986KIR/ACR Kirchner J J, Acree W E Jr, Pilcher G, Li S F. 1986. Enthalpies of combustion of 4-N-phenylmethylene benzenamine N-oxide derivatives, of N-phenylmethylene benzenamine, and of trans-diphenyldiazene N-oxide. The dissociation enthalpy of the N–O bonds. J Chem Thermodyn, 18:793~799

1986LIN/LIN Lin C Y, Lin M C. 1986. Thermal decomposition of methyl phenyl in shock waves: the kinetics of phenoxy radical reactions. J Phys Chem, 90:425~431

1986MAH/ISL Mahmood A J, Islam T S A, Quader M A, Chowdhury G K. 1986. Decomposition of benzoyl peroxidein vacuum. J Bangladesh Acad Sci, 10:239~242

1986MIT/HAC Mitchell S A, Hackett P A, Rayner D M, Cantin M. 1986. Reactions of gallum atoms. J Phys Chem, 90:6148~6154

1986MOR Morse M D. 1986. Clusters of transition-metal atoms. Chem Rev, 86:1049~1109

1986NOB/QUI Noble M, Quian C X W, Reisler H, Wittig C. 1986. The unimolecular reaction of 2-methyl-2-nitrosopropane on singlet and triplet surfaces: Spectroscopy, real-time rate measurements, and nitric oxide energy distributions. J Chem Phys, 85:5763~5773

1986PED/NAY Pedley J B, Naylor R D, Kirby S P. 1986. Thermochemical data of organic compounds, 2nd ed. New York: Chapman and Hall

1986ROB/STE Robangh D A, Stein S E. 1986. Stabilities of highly conjugated radicals from bond homolysis rates. J Am Chem Soc, 108:3224~3229

1986RUC/BEC Ruchardt C, Beckhaus H D. 1986. Steric and electronic substituent effects on the carbon-carbon bond. Top Curr Chem, 130:1~22.

1986SLA/RAT Slagle I R, Ratajczak E, Gutman D. 1986. Study of the thermochemistry of the $C_2H_5 + O_2 = C_2H_5O_2$ and t-$C_4H_9 + O_2 = $ t-$C_4H_9O_2$ reactions and of the trend in the alkylperoxy bond strengths. J Phys Chem, 90:402~407

1986STE/KRU Stepanov R S, Kruglyakova L A, Buke E S. 1986. Kinetics of thermal decomposition of substituted alkyl and aryl azides. Kinet Katal, 27:479~482

1986TSA Tsang W. 1986. Thermodynamic and kinetic properties of the cyclohexadienyl radical. J Phys Chem, 90:1152~1155.

1986WAL Walsh R. 1986. Thermochemical kinetics: A success story. J Phys Chem, 90:389~394.

1986WAY/DAN Wayner D D M, Danneberg J J, Griller D. 1986. Oxidation potentials of alpha-aminoalkyl radicals. Bond dissociation energies for related radical cations. Chem Phys Lett, 131:189~191

1987ACS/PET Acs G, Peter A. 1987. Data on the thermochemistry of azoalkanes. Int J Chem Kinet, 19:929~942

1987AGR/SET Agrawalla B S, Setser D W. 1987. Vibrational distributions and rate constants from reactions of oxygen-atoms with hydrogen iodide, germane, silane, hydrogen selenide, and hydrogen sulfide (HI, GeH_4, SiH_4, H_2Se, and H_2S). J Chem Phys, 86:5421~5432

1987BAT Batt L. 1987. Reactions of alkoxy and alkyl peroxy radicals. Int Rev Phys Chem, 6:53~90

1987BEN Benson S W. 1987. Bond dissociation energies. A continuing story. J Chem Soc Faraday Trans 1, 83:791~804

1987BEN/KON Benson S W, Kondo O, Marshall R M. 1987. Absolute constants for the reaction of Br atom with i-C_4H_{10}. Int J Chem Kinet, 19:829~839

1987BER/GRE Berkowitz J, Greene J P, Cho H, Ruscic B. 1987. Photoionization mass spectrometric studies of SiH_n (n=1~4). J Chem Phys, 86:1235~1248

1987CHU/FOL Chuang M C, Foltz M F, Moore C B. 1987. T1 barrier height, S1-T1 intersystem crossing rate, and S0 radical dissociation threshold for H_2CO, D_2CO and HDCO. J. Chem. Phys, 87:3855~3864

1987DOB/BEN Dobis O, Benson S W. 1987. Analysis of flow dynamics in a new, very low-pressure reactors. Application to the reaction $Cl + CH_4 = HCl + CH_3$. Int J Chem Kinet, 19:691~708

1987KAM/HAW Kaminska J M K, Hawari J A, Griller D, Chatgilialoglu C. 1987. Reduction of silicon-hydrogen bond strengths. J Am Chem Soc, 109:5267~5268

1987KEE/RUP Kee R J, Rupley F M, Miller J A. 1987. The Chemical Thermodynamic Database, Sandia Nantional Labs Reprort SAND87-8215B

1987KOC/FRE Koch W, Frenking G. 1987. Theoretical investigation of the structures and electron affinities of NCO and NCS isomers, CH_2NCH_2 and CH_2N. J Phys Chem, 91:49~53

1987LIA/AUS Lias S G, Ausloos P. 1987. Structures and heats of formation of butenylium ions in the gas phase. Int J Mass Spectrom Ion Proc, 81:165~181

1987LOV/WAN Lovejoy E R, Wang N S, Howard C J. 1987. Kinetic studies of the reactions of HSO with NO_2, NO and O_2. J Phys Chem, 91:5749~5755

1987MAN/BRO Manka M, Brown R L, Stein S E. 1987. Rate constants for hydrogen abstraction by resonance stabilized radicals in high-temperature liquids. Int J Chem Kinet, 19:943~957

1987MAR/RIN Martin J R, Ring M A, O'Neal H E. 1987. The decomposition kinetics of disilane and the heat of formation of silylene. Int J Chem Kinet, 19:715~724

1987MOR/ELL Moran S, Ellis H B Jr, DeFrees D J, McLean A D. 1987. Carbanion spectroscopy: $^-CH_2NC$. J Am Chem Soc, 109:6004~6010

1987MOR/ELL(b) Moran S, Ellis H B Jr, DeFrees D J, McLean A D, Ellison G B. 1987. Carbanion spectroscopy: CH_2CN^-. J Am Chem Soc, 109:5996~6003

1987PAG/RAT Pagsberg P, Ratajczak E, Sillesen A, Jodkowski J T. 1987. Spectrokinetic studies of the gas-phase equilibrium $F + O_2 = FO_2$ between 295 K and 359 K. Chem Phys Lett, 141:88~94

1987PRO/NAZ Prokudin V G, Nazin G M. 1987. Carbon-nitrogen bond dissociation energy in 2-nitrofuran. Izv. Akad. Nauk SSSR Ser. Khim, 678~679, 1987

1987SHI/ACH Shiromaru H, Achiba Y, Kimura K, Lee Y T. 1987. Determination of the C–H bond dissociation energies of ethylene and acetylene by observation of the threshold energies of H^+ formation by synchrotron radiation. J Phys Chem, 91:17~19

1987STE/SUR Stein S E, Suryan M M. 1987. Initial steps in lignin thermolysis: Model compound studies of substituted anisoles. Coal Sci Technol, 11 (Int Conf Coal Sci, 1987), 749~756

1987TSC/PAD Tschuikow-Roux E, Paddison S. 1987. Bond dissociation energies and radical heats of formation in CH_3Cl, CH_2Cl_2, CH_3Br, CH_2Br_2, CH_2FBr, and $CHFCl_2$. Int J Chem Kinet, 19:15~24

1987TSC/SAL Tschuikow-Roux E, Salomon D R, Paddison, S. 1987. Reaction of atomic Br with ethyl bromide. The heat of formation of the CH_3CHBr radical and the alpha-C–H bond dissociation energy. J Phys Chem, 91:3037~3040

1987TSC/SAL(b) Tschuikow-Roux, E, Salomon, D.R. 1987. Photobromination of C_2H_5Cl in the presence of C_2H_6. The heat of formation of the CH_3CHCl radical and the D(CH_3CHCl–H) bond dissociation energy. J Phys Chem, 91:699~702

1987VAR/DEN Varlamov V T, Denisov E T. 1987. Study of forward and back reactions of a peroxy radical with diphenylamine by kinetic spectrophotometry. Dokl Akad Nauk USSR, 293:126~128

1987WET/BRA Wetzel D M, Brauman J I. 1987. Electron photodetachment spectroscopy of trapped negative ions. Chem Rev, 87:607~622

1987WOD/LEE Wodtke A M, Lee Y T. 1987. High-resolution photofragmentation-translation spectroscopy. *In:* Molecular Photodissociation Dynamics. Ashfold M N, Baggott J E, eds. Royal Soc Chem London, 31~59

1987WU/KER Wu C H, Kern R D. 1987. Shock tube of allene pyrolysis. J Phys Chem, 91:6291~6296

1987WU/SIN Wu C H, Singh H J, Kern R D. 1987. Pyrolysis of acetylene behind reflected shock waves. Int J Chem Kinet, 19:975~966

1987ZAV Zavitsas A A. 1987. Quantitative relationship between bond dissociation energies, infrared stretching frequencies, force constants in polyatomic molecules. J Phys Chem, 91:5573~5577

1988BER Berkowitz J. 1988. Photoionization mass spectrometric studies of AsH_n (n=1~3). J Chem Phys, 89:7065~7076

1988BOR Bordwell F G. 1988. Equilibrium acidities in dimethyl sulfoxide solution. Acc Chem Res, 21:456~463

1988BOR/ALG Bordwell F G, Algrim D J. 1988. Acidities of anilines in dimethyl sulfoxide solution. J Am Chem Soc, 110:2964~2968

1988BOR/BAU Bordwell F G, Bausch M J, Branca J C, Harrelson J A. 1988. Acidities of benzyl phenyl sulfones and of the corresponding radical cations. Homolytic bond dissociation energies (BDEs) of alpha-carbon-hydrogen bonds in benzyl phenyl sulfones. J Phys Org Chem, 1:225~239

1988BOR/CHE Bordwell F G, Cheng J P, Harrelson J A. 1988. Homolytic bond dissociation energies in solution from equilibrium acidity and electrochemical data. J Am Chem Soc, 110:1229~1231

1988BOR/CHE(b) Bordwell F G, Cheng J P, Bausch M J, Bares J E. 1988. Acidities of radical cations derived from arylacetonitriles. J Phys Org Chem, 1:209~223

1988BOR/CHE(c) Bordwell F G, Cheng J P, Seyedrezai S E, Wilson C A. 1988. Properties of anions, radicals, and radical cations derived from 9-(dialkylamono)fluorenes. J Am Chem Soc, 110:8178~8183

1988CHA/LUS Chateauneuf J, Lusztyk J, Ingold K U. 1988. Spectroscopic and kinetic characteristics of aroyloxyl radicals. 2. Benzoyloxyl and ring-substituted aroyoxyl radicals. J Am Chem Soc, 110:2886~2893

1988CHE/JON Chen Y, Jonas D M, Hamilton C E, Green P G, Kinsey J L, Field R W. 1988. Aceetylene-isomerization and dissociation. Ber Bunsenges Phys Chem, 92:329~336

1988COL Colussi A J. 1988. Thermochemistry of free radicals. *In:* Chemical Kinetics of Samall Organic Reactions. Alfassi B ed. Boca Raton: CRC Press, Vol 1, Chapter 2, 25~43

1988COR/COL Coronel M E J, Colussi A J. 1988. Electron-spin-resonance equilibrium measurements of the O–H bond energy in alpha-tocopherol. Int J Chem Kinet, 20:749~752

1988COX/HAY Cox R A, Hayman G D. 1988. The stability and photochemistry od dimers of the ClO radical and implications for antarctic ozone depletion. Nature, 332:796~800

1988CUI/HE Cui J P, He Y Z, Tsang W. 1988. Single-pulse shock tube studies on the stability of 1-phenyl-2-butene and the strength of the vinyl-H bond in propene. Energy & Fuels, 1:614~618

1988FAH/STE Farhr A, Stein S E. 1988. Reactions of vinyl and phenyl radicals with ethylene, ethene and benzene. 22nd Int. Symp. Comustion, The Combustion Institute, Pittsburgh PA. 1023~1029

1988FUJ/HAI Fuji M, Haijima A, Ito M. 1988. Predissociation of acetylene in A1A state. Chem Phys Lett, 150:380~385

1988GRE/COL Grela M A, Colussi A.J. 1988. Decomposition of methylamono and aminomethyl radicals. The heats of formation of methyleneimine (CH_2=NH) and hydrazyl (N_2H_3) radical. Int J Chem Kinet, 20:713~718

1988GRI/KAM Griller D, Kaminska J M K, Maccoll A. 1988. Bond dissociation energies for common organic compounds. J Mol Struc (Theochem), 163:125~131

1988HER Herron J T. 1988. Thermochemistry of sulfoxides and sulfones, *In*: The Chemistry of Solphones and Sulphoxides. Patai S, Rappoport C and Stirling C J M ed. New York: Wiley, 95~106

1988HOL/LOS Holmes J L, Lossing F P. 1988. Heats of formation and bond dissociation energies in halogen-substituted methyl and ethyl radical. J Am Chem Soc, 110:7343~7345

1988HOL/LOS(b) Holmes J L, Lossing F P, Maccoll, A. 1988. Heats of formation of alkyl radicals from appearance nergies. J Am Chem Soc, 110:7339~7342

1988LI/PIL Li S, Pilcher G. 1988. Enthalpy of formation of pyridine-N-oxide: the dissociation enthalpy of the N- O bond. J Chem Thermodyn, 20:463~465

1988LIA/BAR Lias S G, Bartmess J E, Liebman J F, Holmes J L, Levin R D, Mallard W G. 1988. Gas-Phase Ion and Neutral Thermochemistry. J Phys Chem Ref Data, 17, Suppl 1

1988LYM/HOL Lyman J L, Holland, R. 1988. Oxygen fluoride chemical kinetics. J Phys Chem, 92:7232~7241

1988MCD/DAV McDaniel A H, Davidson J A, Cantrell C A, Shetter R E, Calvert J G. 1988. Enthalpies of formation of dinitrogen pentoxide and the nitrate free radical. J Phys Chem, 92:4172~4175

1988MOR/ELL Moran S, Ellison G B.1988. Photoelectron spectroscopy of sulfur ions. J Phys Chem, 92:1794~1803

1988MUL/SAA Mulder P, Saastad O W, Griller D. 1988. Oxygen-hydrogen bond dissociation energies in para-substituted phenols. J Am Chem Soc, 110:4090~4092

1988MUR/LEO Murray K K, Leopold D G, Miller T M, Lineberger W C. 1988. Photoelecon spectroscopy of the halocarbene anions HCF^-, HCBr, HCl, CF_2^-, and CCl^-. J Chem Phys, 89:5442~5453

1988PAK/CAI Pak K, Cai M F, Dzugan T P, Bondybey V E. 1988. Dissociation energy and excited-state properties of diatomic tin. Faraday Diss Chem Soc, 86:153~162

1988PAR/BEN Parmar S S, Benson S W. 1988. Kinetics of the reaction $Cl + C_2H_4 = C_2H_3 + HCl$. Heat of formation of the vinyl radical. J Phys Chem, 92: 2652~2657

1988PEN/CAO Peng B, Cao J, Wen Y, Zhong X, Zhang J, Gu H, Fang W, Wu X, Zhu, Q. 1988. Laser photofragmentation of CH_3SSCH_3 at 248 nm. Wuli Huaxue Xuebao, 4:225~228

1988ROD/JER Rodgers A S, Jerus P. 1988. Kinetics of the bromine catalyzed elimination of HCl from 1,1,1-trichloroethane. Int J Chem Kinet, 20:565~575

1988RUS/SEE Russell J J, Seetula J A, Senkan S M, Gutman D. 1988. Kinetics and thermochemistry of the methyl radical. Study of the CH_3 + HCl reaction. Int J Chem Kinet, 20:759~773

1988RUS/SEE(b) Russell J J, Seetula J A, Gutman D. 1988. Kinetics and thermochemistry of CH_3, C_2H_5, and i-C_3H_7. Study of the equilibrium R + HBr = R–H + Br. J Am Chem Soc, 110:3092~3099

1988RUS/SEE(c) Russell J J, Seetula J A, Gutman D. 1988. Kinetics and thermochemistry of the t-C_4H_9 radical. Study of the equilibrium t-C_4H_9 + HBr = i-C_4H_{10} + Br. J Am Chem Soc, 110:3084~3091

1989ACR/KIR Acree W E Jr, Kircher J J, Tucker S A, Pilcher G, da Silva M D M C R. 1989. Enthalpies of combustion of three benzyllidene t-butylamine N-oxide derivatives and of 4-nitrobenzylidene t-butylamine: the dissociation enthalpies of the N–O bonds. J. Chem. Thermodyn, 21: 443~448

1989BOR/CHE Bordwell F G, Cheng J P. 1989. Radical-cation acidities in solution and in the gas phase. J Am Chem Soc, 111:1792~1795

1989BOR/HAR Bordwell F G, Harrelson J A. 1989. Oxidation potentials of carbanions and homolytic bond dissociation energies of their conjugate acids. J Org Chem, 54:3101~3105

1989CAO/ZHA Cao JR, Zhang J M, Zhong X, Huang Y H, Fang W Q, Wu X J, Zhu Q H. 1989. Photofragmentation of vinyl iodine at 248 nm. Heat of formation of vinyl radical. Chem

Phys, 138:377~382

1989CHA/GIN Chandrasekharaiah M S, Gingerich K A. 1989. Thermodynamic properties of gaseous species, *In:* Handbook on the Chemistry and Physics of Rare Earths; Gschneidner K A Jr, Ering L eds. Amsterdam: Elsevier, Vol. 12, Chapter 86, 409~431

1989CHE/ALB Chen E C M, Albyn K, Dussack L, Wentworth W E. 1989. Determination of bond dissociation energies from dissociation thermal electron attachment. J Phys Chem, 93:6827~6832

1989CHE/JON Chen Y, Jonas D M, Kinsey J L, Field R W. 1989. High-resolution spectroscopic detection of acetylene-vinylidene isomerization by spectral cross-correlation. J Chem Phys, 91:3976~3987

1989COX/WAG Cox J D, Wagman D D, Medvededv V A. 1989. CODATA Key Values for Thermodynamics, New York: Hemisphere Pub Corp. http://www.codata.org/codata/databases/key1.html

1989ERV/HO Ervin K M, Ho J, Lineberger W C. 1989. A suty of the singlet and triplet-state of vinylidene by photoelectron-spectroscopy of $H_2C_2^-$, $D_2C_2^-$, and HDC_2^-. Vinylidene acetylene isomerization. J Chem Phys, 91:5974~5992

1989FRE/OLM Freund H, Olmstead W N. 1989. Detailed chemical kinetic modeling of butylbenzene pyrolysis. Int J Chem Kinet, 21:561~574

1989GRE/KIN Green P G, Kinsey J L, Field R W. 1989. A new determination of the dissociation energy of acetylene. J Chem Phys, 91:5160~5163

1989GRI/SIM Griller D, Simoes M J A, Muldewr P, Sim B A, Wayner D D M. 1989. Unifying the solution thermochemistry of molecules, radicals, and ions. J Am Chem Soc, 111:7872~7876

1989GRI/WAY Griller D, Wayner D D M. 1989. Radical thermochemistry and organic reactions. Pure Appl Chem, 61:717~724

1989GUR/VEY Gurvich L V, Veyts I V, Alcock C B. 1989. Thermodynamic Properties of Individual Substances, Vol 1, Part 1 and 2. New York: Hemisphere Pub Corp

1989HAY/COX Hayman G D, Cox R A. 1989. UV Absorption-spectrum and thermochemistry of Cl_2O_3 formed in the photolysis of OClO-containing mixtures at low temperature. Chem Phys Lett, 155:1~7

1989KAM/GIL Kaminska J M K, Gilbert B C, Griller D. 1989. Solvent effects on the thermochemistry of free-radical reactions. J Am Chem Soc, 111:3311~3314

1989MAC/DOO Mackie C, Doolam K R, Nelson P F. 1989. Kinetics of the thermal decomposition of ethoxybenzene (anisole). J Phys Chem, 93:664~670

1989MAR/ROS Markgraf W M, Rossi M J, Golden D M. 1989. Rate constants for the reactions t-C_4H_9 + DX = C_4H_9X + X (X = Br, I). 295 < T(K) <384: Heat of formation of the tert-butyl radical. J Am Chem Soc, 111:956~962

1989MEO Meot-Ner M. 1989. Ion chemistry of ferrocene. Thermochemistry of ionization and protonation and solvent clustering. Slow and entropy-driven proton-transfer kinetics. J Am Chem Soc, 111:2830~2834

1989MIS/POL Misyura A V, Polumbrik O M, Markovskii L N. 1989. Energy of nitrogen-hydrogen bond cleavage in 2,6-diaryl-4-phenyl-1,2,3,4-tetrahydro -sym-tetrazines and comparative activity of sym-tetrazinyls in dehydrogenationreactions of hydrazobenzene. Russ J Org Chem, 25:424~431

1989NAT/MIN Nathanson G M, Minton T K, Shane S F, Lee Y T. 1989. Ultraviolet photodissociation and thermochemistry of CH_2BrCH_2I, CF_2BrCF_2I, and CF_2ICF_2I. J Chem Phys, 90:6157~6170

1989NOR/NG Norwood K, Ng C Y. 1989. A sate-selected study of the unimolecular decomposition of $C_2H_2^+$ using photoion phtoelectron coicidence method. J Chem Phys, 91:2898~2900

1989PAR/BEN Parmar S S, Benson S W. 1989. Kinetics and thermochemistry of the reaction C_2D_6 + Cl = C_2D_5 + DCl. The heat of formation of the C_2D_5 and C_2H_5 radicals. J Am Chem Soc, 111:57~61

1989RED/RAO Reddy R R, Rao T V R, Reddy A S R. 1989. Curve fitting approach. On the dissociation energies of ClO and IO. Indian J Pure Appl Phys, 27:243~245

1989RUS/SCH Ruscic B, Schwarz M, Berkowitz J A. 1989. Photoionization study of the COOH species. J Chem Phys, 91:6780~6785

1989RUS/SEN Russell J J, Senkan S M, Seetula J A, Gutman D. 1989. Kinetics and thermochemistry of C_2H_3 and CH_2CCl radicals: Study of the C_2H_3 + HCl = C_2H_4 + Cl and CH_2CCl + HCl = C_2H_3Cl + Cl reactions. J Phys Chem, 93:5184~5188

1989SEG/LAV Segall J, Lavi R, Wen Y, Wittig C. 1989. Acetylene C–H bond dissociation energy using 193.3 nm photolysis and sub-Doppler resolution H-atom spectroscopy: 127±1.5 kcal/mol. J Phys Chem, 93:7287~7289

1989SIM/GRI Simoes J A M, Griller D. 1989. Enthalpy of formation of the benzoyl radical by photoacoustic calorimetry. Chem Phys Lett, 158:175~177

1989SUR/KAF Suryan M M, Kafafi S A, Stein S E. 1989. The thermal decomposition of hydroxy- and methoxy-substituted anisoles. J Am Chem Soc, 111:1423~1429

1989SUR/KAF(b) Suryan M M, Kafafi S A, Stein S E. 1989. Dissociation of substituted nisoles: substituent effects on bond strengths. J Am Chem Soc, 111:4594~4600

1989SUR/STE Suryan M M, Stein S E. 1989. Stability of substituted benzyl radicals; dissociation rates of amino-, hydroxy, and cyanoethylbenzenes. J Phys Chem, 93:7362~7365

1989TAC/SAL Taccone R A, Salinovich O, Staricco E H. 1989. Kinetics and thermochemical parameters of chlorine atom transfer reactions from CF_3Cl, CF_3CF_2Cl, CF_2ClCF_2Cl, and $CF_2ClCFCl_2$ in gas-phase. Int J Chem Kinet, 21:331~341

1989TIL/PAK Tilset M, Parker V D. 1989. Solution homolytic bond dissociation energies of organotrasition-metal hydrides. J Am Chem Soc, 111:6711~6717. Correction, 1990. J Am Chem Soc, 112:2843

1989TSC/CHE Tschuikow-Roux E, Chen Y. 1989. Concerning the heat of formation of the isopropyl radical. J Am Chem Soc, 111:9030~9031

1989WAL Walsh R. 1989. Thermochemistry, *In:* The Chemistry of Organosilicon Compounds, Part 1. Patai S and Rapport Z eds. New York: Wiley. Chapter 5,371~391

1989WET/SAL Wetzel D M, Salomon K E, Berger S, Brauman J I. 1989. Gas-phase acidities of organosilanes and electron affinities of organosilyl radicals. J Am Chem Soc, 111:3835~3841

1989WOD/HIN Wodtke A M, Hintsa E J, Somorjai J, Lee Y T. 1989. Photodissociation of vinyl bromide and the heat of formation of the vinyl radical. Israel J Chem, 29:383~391

1989ZHA/CON Zhao X S, Continetti R E, Yokoyama A, Hintsa E J, Lee Y T. 1989. Dissociation of cyclohexene and 1,4-cyclohexadiene in a molecular beam. J Chem Phys, 91:4118~4127

1990~1994

1990AND/FAH Anderson L C, Fahey D W. 1990. Studies with nitryl hypochlorite. Thermal dissociation rate and catalytic conversion to nitric oxide using an NO/O_3 chemiluminescence detector. J Phys Chem, 94:644~652

1990ARN/AMA Arnett E M, Amarnath K, Harvey N G, Venimadhavan S. 1990. Heterolysis and homolysis energies for some carbo-oxygen bonds. J Am Chem Soc, 112:7346~7353

1990BAL/BUN Baldwin D P, Buntine M A, Chandler D W. 1990. Photodissociation of acetylene. Determination of D(HCC–H) by photofragment imaging. J Chem Phys, 93:6578~6584

1990BAR/GRI Barttmess J E, Griffith S S. 1990. Tautomerization energies of benzoannelated toluenes.

J Am Chem Soc, 112:2931~2936

1990BAU/GOS Bausch M J, Gostowski R, Jirka G, Selmarten D, Winter G. 1990. Dimethyl sulfoxide phase NH equilibrium acidities for urazole and substituted urazoles: For urazole and 1-substituted urazoles, which proton is more acidic? J Org Chem, 55:5806~5808

1990BAU/GOS(b) Bausch M J, Gostowski R, Jirka G, Selmarten D, Winter G. 1990. Dimethyl sulfoxide phase C–H bond dissociation eneregies for phenalene and benzanthrene. J Org Chem, 55:5805~5806

1990BEC/DOG Beckhaus H D, Dogan B, Schaetzer J, Hellmann S, Ruchardt C. 1990. Thermolabile hydrocarbons. 30. Thermal stability and heat of formation of 1,1,2,2-tetraphenylethene and 1,1,1,2-tetraphenylethane. Energy of stabilization of benzhydryl and triphenylmethyl radicals. Chem Ber, 123:137~144

1990BOR/HAR Bordwell F G, Harrelson J A. 1990. Acidities and homolytic bond dissociation energies of the alpha-C–H bonds in ketones in DMSO. Can J Chem, 68:1714~1718

1990BOR/HAR(b) Bordwell F G, Harrelson J A, Lynch T Y. 1990. Homolytic bond dissociation energies for the cleavage of alpha-N–H bonds in carboxamides, sulfonamides, and their derivatives. The question of synergism in nitrogen-centered radicals. J Org Chem, 55:3337~3341

1990BOR/ZHA Bordwell F G, Zhang X M. 1990. Effects on anions and radicals of alpha-quaternary ammonium substituents. J Org Chem, 55:6078~6079

1990BRA/FRA Braun-Unkhoff M, Frank P, Just T. 1990. High-temperature reactions of benzyl radicals. Ber Bunsenges Phys Chem, 94:1417~1425

1990CHE/RAU Chen Y, Rauk A, Tschuikow-Roux E. 1990. Structure, barriers for internal rotation, vibrational frequencies, and thermodynamic function of the sec-butyl radical: An initio study. J Phys Chem, 94:6250~6254

1990COL Colussi A J. 1990. Formation and decay of O atoms in the laser flash photolysis of chlorine dioxide (OClO) at 308 nm. J Phys Chem, 94:8922~8926

1990DAV/LEE Davies J M, Haninglee M A, Pilling M J, Seakins P E. 1990. Laser flash-photolysis studies of elementary reactions of significance in combustion. Spectrochimica Acta, 46A:581~588

1990DES/TRO Destriau M, Troe J. 1990. Thermal dissociation and recombination of alkyl and haloalkyl peroxynitrates. An SACM modeling. Int J Chem Kinet, 22:915~934

1990DIA/DIO Dias A R, Diogo H P, Griller D, de Piedade M E P, Simoes J A M. 1990. Metal-carbon and metal-hydrogen bond dissociation enthalpies from classical and nonclassical calorimetric studies, *In:* Bonding Energetics in Organometallic Compounds. Marks T J. ed. ACS Symposium Ser. No. 428, Washington DC.1990, Charpter 14, 205~217

1990DOB/MAS Dobychin S L, Mashendzhinov V I, Mishin V I, Semenov V N, Shpak V S. 1990. Kinetics of thermal decomposition of perfluoroalkyl iodides and the bond energy D(R–I), R – CF_3, C_2F_5, n-C_3F_7, iso-C_3F_7, n-C_4F_9, tert-C_4F_9. Doklady Akademii Nauk SSSR, 312:1166~1168

1990ERV/GRO Ervin K M, Gronert S, Barlow S E, Gilles M K, Harrison A G, Bierbaum V M, DePuy C H, Lineberger W C, Ellison G B. 1990. Bond strengths of ethylene and acetylene. J Am Chem Soc, 112:5750~5759

1990FIS/ARM Fisher ER, Armentrout PB. 1990. Heat of formation of HO_2. A direct determination from guided ion beam studies of $O_2 + CH_4$. J Phys Chem, 94, 4396~4398

1990GUT Gutman D. 1990. The controversial heat of formation of the t-C_4H_9 radical and the tertiary C -H bond energy. Acc Chem Res, 23:375~380

1990HAL Halpern J. 1990. Thermodynamics and kinetics of transition metal-alkyl homolytic bond dissociation processes, *In:* Bonding Energetics in Orgamometallic Compounds, Marks T J. ed. ACS Symp. Ser. 428, Washington DC. Chapter 7, 100~112

1990HIP/TRO Hippler H, Troe J. 1990. Thermodynamic properties of benzyl radicals: Enthalpy of formation from toluene, benzyl iodide, and dibenzyl dissociation equilibria. J Phys Chem, 94:3803~3806

1990IRA/PET Iraqi M, Petrank A, Peres M, Lifshitz C. 1990. Proton-transfer reaction of $(C_2H_2)H^+$: The bond energy $D(C_2H–H)$. Int J Mass Spectrom Ion Proc, 100:679~691

1990KOE/SCO Koening T, Scott T W, Franz J A. 1990. Cage pair interactions and activation parameters. *In:* Bonding energetics in organometallic compounds, Marks T J ed. ACS Symposium Ser. No. 428, Washington DC. Charpter 8, 113~132

1990LEI/PIL Leitao M L P, Pilcher G, Acree W E Jr, Zvaigne A, Tucker S A, de Silva M D M C R, 1990. Enthalpies of combustion of phenazine N-oxide, phenazine, benzofuroxan, and benzofurazan. The dissociation enthalpies of the N–O bonds. J Chem Thermodyn, 22:923~928

1990LEM/BIS Lemire G W, Bishea G A, Heidecke S A, Morse M D. 1990. Spectroscopy and electronic-structure of jet-colled GaAs. J Chem Phys, 92:121~132

1990LIN/SHE Lind J, Shen X, Eriksen T E, Merenyi G. 1990. The one-electron reduction of 4-substituted phenoxyl radicals in water. J Am Chem Soc, 112:479~482

1990MAL/MCM Malhotra R, McMillen D F. 1990. A mechanistic numerical model for coal-liquefaction involving hydrogenolysis of strong bonds. Rationalization of interactive effects of solvent aromaticity and hydrogen pressure. Energy Fuel, 4:184~193

1990MCC/PFA McCoustra M R S, Pfab J. 1990. Free-jet studies of the visible spectroscopy of some perhalonitrosomethanes. Spectrochim Acta, 46A:937~955

1990MIY/TSC Miyokawa K, Tschikow-Roux E. 1990. Kinetics of alpha- and beta-hydrogen abstraction from C_2H_5Cl by Br atoms. Estimate of C–H bond dissociation energies and heats of formation of CH_3CHCl and CH_2CH_2Cl radicals. J. Phys. Chem, 94: 715~717

1990MUE/POP Mueller U, Popowski E. 1990. Photochemical determination of Si-H bond dissociation energy. Z Phys Chem (Leipzig), 271:703~713

1990MUR/LOV Murrells T P, Lovejoy E R, Ravishankara A R. 1990. Oxidation of CS_2 by reaction with OH. 1. Equilibrium constant for the reaction OH + CS_2 = CS_2OH and the kinetics of the $CS_2OH + O_2$ reaction. J Phys Chem, 94:2381~2386

1990NIC/KRE Nicovich J M, Kreutter K D, Wine P H. 1990. Kinetics and thermochemistry of ClCO formation from the Cl+ CO association reaction. J Chem Phys, 92:3539~3544

1990PER/BER Perkins M J, Berti C, Brooks D J, Grieson L, Grimes J A M, Jenkins T C, Smith S L. 1990. Acyl nitroxides: Reaction and reactivity. Pure Appl Chem, 62:195~200

1990PIL Pilcher G. 1990. Thermochemistry of phosphorus (III) compounds. *In:* The Chemistry of Organophosphorus Compounds, Hartley F R ed. New York: Wiley, vol. 1, 127~136

1990PRI/ARM Prinslow D A, Armentrout P B. 1990. Collison-induced dissociation of carbon disulfide ion (CS^{2+}). Heat of formation of the carbon sulfide (CS) radical. J Chem Phys, 94:3563~3567

1990PUT/SMI Puttemans J P, Smith G P, Golden D M. 1990. Cyclopentadinery compound thermochemistry-comment. J Phys Chem, 94:3226~3227

1990RIC/RYT Richards P D, Ryther R J, Weitz E. 1990. Diode laser probos of tert-butyl radical reaction kinetics: reaction of $C(CH_3)_3$ with HBr, DBr, and HI. J Phys Chem, 94:3663~3667

1990RUS/SCH Ruscic B, Schwarz M, Berkowitz J. 1990. Photoionization studies of GeH_n (n = 2~4). J Chem Phys, 94:1865~1875

1990RUS/SEE Russell J J, Seetula J A, Gutman D, Danis F, Caralp F, Lightfoot P D, Lesclaux R, Melius C F, Senkan S M. 1990. Kinetics and thermochemistry of the equilibrium CCl_3 + O_2. J Phys Chem, 94:3277~3283

1990SEE/GUT Seetula J A, Gutman D. 1990. Kinetics and thermochemistry of the sec-C_4H_9 + HBr =

nC_4H_{10} + Br equilibrium. J Phys Chem, 94:7529~7533

1990SEE/RUS Seetula J A, Russell J J, Gutman D. 1990. Kinetics and thermochemistry of the reactions of alkyl radicals (CH_3, C_2H_5, i-C_3H_7, s-C_4H_9 and t-C_4H_9) with HI: A reconciliation of the alkyl radical heats of formation. J Am Chem Soc, 112:1347~1353

1990SIE/AUS Sieck L. W, Ausloos P J. 1990. Kerr constants of methyl benzoate and the dimethyl esters of phthallic, isophthalic and terephthalic acids. J Phys Chem, 94:8374~8378

1990TAK Takhistov V V. 1990. Organic mass spectrometry: Thermochemical description of isomerization and fragmentation of ions and radicals in the gaseous state. Leningrad: Nauka

1990TSA/CUI Tsang W, Cui J P. 1990. Homogeneous gas-phase decyclization of tetralin and benzocyclobutene. J Am Chem Soc, 112:1665~1671

1990WAG/SLA Wagner A F, Skagle I R, Sarzynski D, Gutman D. 1990. Experimental and theoretical stuties of the ethyl + oxigen reaction kinetics. J Phys Chem, 94:1853~1868

1990WAL/TSA Walker J A, Tsang W. 1990. Single-pulse shock tube studies on the thermal decomposition of n-butyl phenyl ether, n-pentylbenzene, and phenetole and the heat of formation of phenoxy and benzyl radicals. J Phys Chem, 94:3324~3327

1990WAY/GRI Wayner D D M, Griller D. 1990. Free radical thermochemistry. *In:* Advances in Free Radicals Chemistry, Stanford: JAI Press, vol. 1, 159~192

1990ZHA/LUO 赵学庄，罗渝然，臧雅茹，万学适. 1990. 化学反应动力学原理(下). 北京: 高等教育出版社

1991ACR/TUC Acree W E Jr, Tucker S A, Zvaigzne A I, Yang M Y, Pilcher G, da Silva M D M C R. 1991. Enthalpies of combustion of 2,4,6-trimethylbenzonitrile, 2,4,6-trimethylbenzonitrile N-oxide, 2,6-dimethylbenzonitrile, 2,4,6-methoxybenzonitrile, and 2,4,6-trimethoxybenzonitrile N-oxide: the dissociation enthalpies of the N–O bonds. J Chem Thermodyn, 23:31~36

1991BAE/HIP Baer S, Hippler H, Rabu R, Siefke M, Seitzner N, Troe J. 1991. Thermodynamic and kinetic properties of the reaction $Cl + O_2 + M = ClO_2 - M$ in the range 160~300 K and 1~1000 bar. J Chem Phys, 95:6463~6470

1991BAU/FAS Bausch M J, Fasano C G, Gostowski R. 1991. Estimates of solution-phase bond dissociation energies for C D and S–S bonds in radical anions derived from aromatic sulfides. Energy Fuels, 5:419~423

1991BAU/FAS(b) Bausch M J, Fasano C G, Peterson B M. 1991. Observations of nonadditive substituent effects on the dimethyl sulfoxide solution homolytic bond strengths of anthrylmethyl C–H bonds. J Am Chem Soc, 113:8384~8388

1991BAU/FAS(c) Bausch M J, Fasano C D, Gostowski R, Selmarten D, Vaughn A. 1991. Relative homolytic strengths of C–H bonds in meldrum acid and dimethyl malonate. J Org Chem, 56:5640~5642

1991BAU/GOS Bausch M J, Gostowski R. 1991. Homolytic and heterolytic N–H bond strengths. J Org Chem, 56:6260~6262

1991BAU/GOS(b) Bausch M J, Gostowski R, Fasano C G, Selmarten D, Vaughn A, Wang L H. 1991. Comparisons of N–H, C–H ,O -H, and S–H heterolytic and homolytic bond strengths in acueous and dimethyl sulfoxide solution. J Org Chem, 56:7191~7193

1991BOR/CHE Bordwell F G, Cheng J P, Ji G Z, Satish A V, Zhang X M. 1991. Bond dissociation energies in DMSO related to the gas phase values. J Am Chem Soc, 113:9790~9795

1991BOR/CHE(b) Bordwell F G, Cheng J P. 1991. Substituent effects on the stabilities of phenoxyl radicals and the acidities of phenoxyl radical cations. J Am Chem Soc, 113:1736~1743

1991BOR/GAL Bordwell F G, Gallagher T, Zhang X M. 1991. Donor-acceptor effects on the stability of radicals derived from alpha-dialkylamino ketones. J Am Chem Soc, 113:3495~3497

1991BOR/HAR Bordwell F G, Harrelson J A. 1991. Homolytic bond dissociation energies of acidic C–

H bonds activated by one or two electron acceptors. J Org Chem, 56:4448~4450

1991BOR/JI Bordwell F G, Ji G Z, Zhang X M. 1991.Resonance stabilization of heteroallic radicals. J Org Chem, 56:254~5256

1991BOR/JI(b) Bordwell F G, Ji G Z, Zhang X M. 1991. Effects of structural charges on acidities and homolytic bond dissociation energies of the H–N bonds in amidines, carboxamides, and thiocarboxamides. J Am Chem Soc, 113:8398~8401

1991BOR/VAN Bordwell F G, Vanier N R, Zhang X M. 1991. Stereoelectronic effects on the stabilities of anions and radicals derived from 2-benzolperhydropyrimidines. J Am Chem Soc, 113:9856~9857

1991BOR/ZHA Bordwell F G, Zhang X M, Cheng J P. 1991. Comparisons of the acidities and homolytic bond dissociation energies of the acidic N–H and C–H bonds in diphenylmethanes and carbazoles. J Org Chem, 56:3216~3219

1991BRI/CAR Bridier I, Caralp F, Loirat H, Lesclaux R, Veyret B, Becker K H, Reimer A, Zabel F. 1991. Kinetic and theoretical studies of the reactions $CH_3C(O)O_2 + NO_2 + M \rightleftharpoons CH_3C(O)O_2NO_2 + M$ between 248 and 393 K between 30 and 760 torr. J Phys Chem, 95:3594~3600.

1991CLA/CUL Clatk K.B, Culshaw P N, Griller D, Lossing F P, Simoes M J A. 1991. Studies of the formation and stability of pentadienyl and 3-substituted pentadienyl radicals. J Org Chem, 56:5535~5539

1991CLA/GRI Clark K B, Griller D. 1991. The Ge–H bond dissociation energies of organogermanes. A laser induced photoacoustic study. Organometallics, 10:746~750

1991CLA/WAY Clark K B, Wayner D D M. 1991. Are relative bond energies a measure of radical stabilization energies? J Am Chem Soc, 113:9363~9365

1991CON/BAL Continetti R E, Balko B A, Lee Y T. 1991. Photodissociation of H_2S and the HS radical at 193.3 nm. Chem Phys Lett, 182:400~405

1991COR/COL Coronel M E J, Colussi A J. 1991. Determination of the homolytic dissociation energy of the O–H bond in 2,3,5,6-tetramethyl-4-methoxyphenol. An Asoc Quim Argnet, 79:181~187

1991COW/TRA Cowles D C, Travers M J, Fruch J L, Ellison G B. 1991. Photoelectron spectroscopy of CH_2N^-. J Chem Phys, 94:3517~3528

1991DOB/BEN Dobis O, Benson S W. 1991. Terperature coefficients of the rates of Cl atom reactions with C_2H_6, C_2H_5, and C_2H_4. The rates of disproportionation and recombination of ethyl radicals. J Am Chem Soc, 113:6377~6386

1991ERV/LIN Ervin K M, Lineberger W C. 1991. Photoelectron spectra of C_2^- and C_2H^-. J Phys Chem, 5:1167~1177

1991GUR/VEY Gurvich L V, Veyts I V, Alcock C B. 1991. Thermodynamic Properties of Individual Substances. 4th ed. New York: Hemisphere Pub Corp

1991HO/ERV Ho J, Ervin K M, Polak M L, Gilles M K, Lineberger W C. 1991. A study of the electronic structures of PD_2^- and PD_2 by photoelectron spectroscopy. J Chem Phys, 95:4845~4853

1991HOL/LOS Holmes J L, Lossing F P, Mayer P M. 1991. Heats of formation of oxygen-containing organic free radicals from appearance energy measurements. J Am Chem Soc, 113:9723~9728

1991HUD/JON Hudgens J W, Johnson R D, Timonen R S, Seetula J A, Gutman D. 1991. Kinetics of the reaction of $CCl_3 + Br_2$ and thermochemistry of CCl_3 radical and cation. J Phys Chem, 95:4400~4405

1991ING/FOK Ingemann S, Fokkens R H, Nibbering N M M. 1991. Gas-phase chemistry of the negative ions derived from azo- and hydrazobenzene. J Org Chem, 56:607~612

1991KOE/ZAB Koeppenkastrop D, Zabel F. 1991. Thermal decomposition of chlorofluoromethyl

peroxynitrates. Int J Chem Kinet, 23:1~15

1991KRE/NIC Kreutter K D, Nicovich J M, Wine P H. 1991. Kinetics and thermochemistry of the Br + NO_2 association reaction. J Phys Chem, 95:4020~4028

1991MAC/COL Mackie J C, Colket M B, Nelson P F, Esler M. 1991. Shock-tube pyrolysis of pyrrole and kinetic modeling. Int J Chem Kinet, 23:733~760

1991MER/LIN Merenyi G, Lind J. 1991. Chemistry of peroxidic tetrahedral intermediates of flavin. J Am Chem Soc, 113:3146~3153

1991NG Ng C Y. 1991. Molecular beam photoionization and photoelectron-photoion cioncidence studies of high temperature molecules, transient species, and clusters. *In:* Vacuum Ultraviolet Photoionization and Photodissociation of Molecules and Clusters, Ng C Y ed. Singapore:World Scientific, 169~257

1991NIC/DIJ Nicovich J N, van Dijk C A, Kreutter K D, Wine P H. 1991.Kinetics of the reactions of alkyl radicals with HBr and DBr. J Phys Chem, 95:9890~9896

1991NIC/KRE Nicovich J M, Kreutter K D, Schockelford C J, Wine P H. 1991. Thermochemistry and kinetics of the Cl + O_2 association reaction. Chem Phys Lett, 179:367~373

1991PAR/HAN Parker V D, Handoo K J, Roness F, Tilset M. 1991. Electrode potentials and the thermodynamics of isodesmic reactions. J Am Chem Soc, 113:7493~7498

1991PAU/SQU Paulino J A, Squires R R. 1991. Carbene thermochemistry from collison-induced dissociation threshold energy measurements. The heats of formation of CF_2 and CCl_2. J Am Chem Soc, 113:5573~5580

1991PIL/LUI Pilcher G, Luisa M, Leitao P, Yang M, Walsh R. 1991. Standard enthalpy of formation of hexamethyldisilane. J Chem Soc Faraday Trans, 87:841~846

1991PON/TAK Ponomarev D A, Takhistov V V, Misharev A D, Orlov V.M, Orlov, Y D. 1991. Heat of formation of hydroxy-and methoxy-substituted phenoxyl radicals. Zhurnal Organicheskoi Khimii, 27:2181~2183

1991PRI/ARM Prinslow D A, Armentrout P B. 1991. Collision-induced dissociation of carbon disulfide ion (CS_2^+). Heat of formation of the carbon sulfide (CS) radical. J Chem Phys, 94:3563~3567

1991ROT/BAU Roth W R, Bauer F, Beitat A, Ebbrecht T, Mustfeld M. 1991. The heat of formation of the allyl and methallyl radical. Chem Ber 124:1453~1460

1991RUS/APP Ruscic B, Appelman E H, Berkowitz J. 1991. Photoionization mass spectrometric study of CH_3OF. J Chem Phys, 95:7957~7961

1991RUS/BER Ruscic B, Berkowitz J. 1991. Photoionization mass spectrometric study of N_2H_2 and N_2H_3–N–H, N=N bond bond energies and proton affinity of N_2. J Chem Phys, 95:4378~4384

1991RUS/BER(b) Ruscic B, Berkowitz J. 1991. Photoionization mass spectrometric studies of the isomeric transient species CD_2OH and CD_3O. J Chem Phys, 95:4033~4039

1991RUS/BER(c) Ruscic B, Berkowitz J. 1991. Photoionization mass spectrometric study of the transient species Si_2H_n (n = 2~5). J Chem Phys, 95:2416~2432

1991SEA/PIL Seakins P W, Pilling M J. 1991. Laser flash photolysis study of the Br + i-C_4H_{10} = HBr + t-C_4H_9 reaction. Heat of formation of t-C_4H_9. J Phys Chem, 95:9874~9878

1991SEE/FEN Seetula J A, Feng Y, Gutman D, Seaking P W, Pilling M J. 1991. Kinetic and thermochemical study of SiH_3 + HBr = SiH_4 + Br and SiH_3 + HI = SiH_4 + I equilibria. J Phys Chem, 95:1658~1664

1991SEE/GUT Seetula J A, Gutman D. 1991. Kinetics of reactions of halogenation methyl radicals with hydrogen iodide. J Phys Chem, 95:3626~3630

1991SEG/WEN Segall J, Wen Y, Singer R, Wittig C. 1991. Translational energy distribution from C_2H_2 + light (193.3 nm) = C_2H + H. J Phys Chem, 95:8078~8081

1991SHI/MAN Shim I, Mandix K, Gingerich K A. 1991. Theoretical and experimental investigation of

the Ga_2 molecule. J Phys Chem, 95:5435~5442

1991SKO/DYM Skorobogatov G A, Dymov B P, Khripun V K. 1991. Determination of rate and equilibrium constant of RI ═ R + I, I + RI ═ I_2 + R for R = CF_3, C_2F_5, or C_4F_9. Kinet Katal, 32:252~259

1991SKO/DYM(b) Skorobogatov G A, Dymov B P, Tedeev R Sh. 1991. Rate and equilibrium constant for RI ═ R + I and I + RI ═ I_2 + R (R = C_3F_7, iso-C_3F_7, C_6F_{13}, $CF_3OCF_2CF_2$, $C_3F_7OCF_2CF_2$). Kinet Katal, 32:178~185

1991STE/BRO Stein S E, Brown R L. 1991. Prediction of C–H bond dissociation energies for polycylic aromatic hydrocarbons of arbitrary size. J Am Chem Soc, 113:787~793

1991TSA Tsang W. 1991.Chemical kinetic database for combustion chemistry. Part 5. Propene. J Phys Chem Ref Data, 20:221~273

1991WEN/PAU Wenthold P G, Paulino J A, Squires R R. 1991. The absolute heats of formation of o-, m-, and p-benzyne. J Am Chem Soc, 113:7414~7415

1992AND/GOR Andrieux C P, Le Gorande A, Saveant J M. 1992. Electron transfer and bond breaking. Examples of passage from a sequential to a concerted mechanism in the electrochemical reductive cleavage of arylmethyl halides. J Am Chem Soc, 114:6892~6904

1992ARN/CAL Arnaut L G, Caldwell R A. 1992. The heat of formation of the benzophenone ketyl radical by time-resolved photoacoustic calorimetry. J Photochem Photobiol A Chem, 65:15~20

1992ARN/VEN Arnett E M, Venimadhavan S, Amarnath K. 1992. Homolytic and heterolytic cleavage energies for carbon-nitrogen bonds. J Am Chem Soc, 114:5598~5602

1992BAU/DAV Bausch M J, David B, Prasad V, Wang L H, Vaughn A. 1992. Relative homolytic strengths of N–H bonds in cyclic and acyclic diacylhydrazides, imides and hydrazoic acid. J Phys Org Chem, 5:1~6

1992BAU/PAR Bauschlicher C W, Partridge H, Langhoff S R. 1992. Theoretical study of transition-metal ions bound to benzene. J Phys Chem, 96:3273~3278

1992BEA/KOP Beauchamp J L, van Koppen P A M. 1992. Fundamental gas phase studies of the mechanism and thermochemistry of organometallic reactions, NATO ASI Ser. C. 367, *In:* Energetics of Organometallic Species. Marinho J A ed. The Netherlands: Kluwer Academic Pub, 287~320

1992BEN/LEO Bengali A A, Leopold D G. 1992. Negative ion photoelectron spectroscopy of CH_2:SiH and CH_3Si. J Am Chem Soc, 114:9192~9124

1992BLU/CHE Blush J A, Chen P. 1992. Photoelectron spectrum of the vinyl radical: downward revision of the $C_2H_3^-$ ionization potential. J Phys Chem, 96:4138~4140

1992BOR/CHE Bordwell F G, Cheng J P, Satish A V, Twyman C L. 1992. Acidities and homolytic bond dissociation energies (BDEs) of benzyl-type C–H bonds in sterically congested substrates. J Org Chem, 57:5642~6546

1992BOR/JI Bordwell F G, Ji G Z. 1992. Equilibrium acidities and homolytic bond dissociation energies of the H–O bonds in oximes and amidoximes. J Org Chem, 57:3019~3025

1992BOR/SAT Borrdwell F G, Satish A V. 1992. Acidities of indenes and their radical cations. Homolytic bond dissociation energies of the benzylic C–H bonds in indenes. J Am Chem Soc, 114:10173~10176

1992BOR/ZHA Bordwell F G, Zhang X M, Alnajjar M S. 1992. Effects of adjacent acceptors and donors on the stabilities of carbon-centered radicals. J Am Chem Soc, 114:7623~7629

1992CHA/GUE Chatgilialoglu C, Guerra M, Guerrini A, Seconi G, Clatk K B, Griller D, Kaminska J M K, Simoes M J A. 1992. A study on the reducing abilities of tris(alkylthio)silanes, J Org Chem, 57:2427~2433

1992COH/BEN Cohen N, Benson S W. 1992. The thermochemistry of alkanes and cycloalkanes, *In:* The Chemistry of Alkanes and Cycloalkanes, Patai S and Rappoport Z. ed. New York:

Wiley, p.215~287

1992COL/SAN Colussi A J, Sander S P, Friedl R R. 1992. Temperature dependence and mechanism of the reaction between O and chlorine dioxide. J Phys Chem 96:4442~4445

1992CYR/CON Cyr D R, Continetti R E, Metz R B, Osborn D L, Neumark D M. 1992. Fast beam studies of cyanato free radical photodissociation. J Chem Phys, 97:4937~4947

1992DOU/MAC Doughty A, Mackie J C. 1992. KInetics of pyrolysis of a coal model compound, 2-picoline, the nitrogen heteroaromatic analogue of toluene. 2. The 2-picolyl radical and kinetic modeling. J Phys Chem, 96:10339~10348

1992GIL/ERV Giles M K, Ervin K M, Ho J, Lineberger W C. 1992. Negative ion photoelectron spectroscopy of HCF–, HCCl–, and HCI- : Photoelectron angular distributions and neutral triplet excitation energies. J Phys Chem, 96:1130~1141

1992GIL/POL Gilles M K, Polak M L, Lineberger W C. 1992. Photoelectron spectroscopy of the halogen oxide anions FO^-, ClO , IO^-, $OclO^-$, and OIO^-. J Chem Phys, 96:8012~8020

1992HOL Holmes J L. 1992. The present state and utility of ion thermochemistry. Int J Mass Spectrom Ion Proc. 118/119:381~394

1992JAC/HOS Jackson R A, Hosseini K M J. 1992. Phenol phenoxyl radical equilibria by electron-spin resonance. Are radicals derived from tocopherol and analogs exceptionally stabilized? J Chem Soc Chem Commun, 967~968

1992LIG/COX Lightfoot P D, Cox R A, Crowley J N, Destriau M, Hayman G D, Jenkin ME, Mootrgat G K, Zabel F. 1992. Organic peroxy radicals: kinetics, spectroscopy and tropospheric chemistry. Atmos Environ General topics, 26A:1805~1961

1992MAT/CRA Matimba H E K, Crabbendam A M. 1992. Ingemann S and Nibbering NMM. Gas-phase biomolecular chemistry of the bullet-CHNC and bullet-CHCN radical-anions. Int J Mass Spectrom Ion Proc, 114:85~97

1992MIC/LAZ Michael C M, Lazorou Y, Paragiannakopouos P. 1992. Infraed multiphoton dissociation of tetramethylsilane. Formation of electronically excited trimethylsilyl radical. Chem Phys Lett, 194:415~422

1992MIY/TSC Miyokawa K, Tschikow-Roux E. 1992. Reaction of atomic bromine with difluorochloromethane. The heat of formation of the $CClF_2$ radical and D($CClF_2$–H) bond dissociation energy. J Phys Chem, 96:7328~7331

1992NIC/KRE Nicvovich J M, Kreutter K D, van Dijk C A, and Wine P H. 1992. Temperature-dependent kinetic studies of the reactions Br + H_2S = SH + HBr and Br + CH_3SH = CH_3S + HBr. Heats of formation of SH and CH_3S radicals. J Phys Chem, 96:2518~2528

1992NII/GUT Niiranen J T, Gutman D, Krasnoperov L N. 1992. Kinetics and thermochemistry of the CH_3CO radical: Study of the CH_3CO + HBr = CH_3CHO + Br reaction. J Phys Chem, 96:5881~5886

1992NUZ Nuzzi M, 1992. A suty of sulfur-sulfur and carbon-sulfur bond scission in organic sulfur compounds by differential pulse polarography. Rivista dei Combustibili, 46:3~10

1992PAR Parker V.D, 1992. Homolytic bond (H-A) dissociation free energies in solution. Application of the standard potential of the (H^+/H.) couple. J Am Chem Soc, 114:7458~7462

1992RUS/BER Ruscic B, Berkowitz J. 1992. Photoionization mass spectrometric studies of the isomctric transient species CH_2SH and CH_3S. J Chem Phys, 97:1818~1823

1992SAH/RIG Sahetchian K A, Rigny R, De Maleissye J F, Batt L, Khan M A, Mathews S. 1992. The pyrolysis of organic hydroperoxides (ROOH). Int Symp Combust Proc, 24th, 637~643

1992SEA/PIL Seakins PW, Pilling M J, Niranm J T, Gutman D, Krasnoperov L N. 1992. Kinetics and thermochemistry of R + HBr = RH + Br reactions: Determinations of the heat of formation of C_2H_5, i-C_3H_7, sec-C_4H_9, and t-C_4H_9. J Phys Chem, 96:9847~9855

1992SEE/GUT Seetula J A, Gutman D. 1992. Kinetics of the CH_2OH + HBr and CH_2OH + HI reactions

and determination of the heat of formation of CH_2OH. J Phys Chem, 96:5401~5405

1992SQU Squires R R. 1992. Gas-phase carbanion chemistry. Acc Chem Res, 25:461~467

1992STA/KIN Staker W S, King K D, Nguyen T T. 1992. Kinetics of the thermal unimolecular decomposition of hex-1-nen-3-yne. Heat of formation and resonance stabilization energy of the 3-ethenylpropagryl radical. Int J Chem Kinet, 24:781~790

1992STI/NIC Stickel R E, Nicovich J M, Wang S, Zhao Z, Wine P H. 1992. Kinetic and mechanistic study of the reaction of atomic chlorine with dimethyl sulfide. J Phys Chem, 96:9875~9883

1992TSA/HER Tsang W, Herron J T. 1992. Kinetics and thermodynamics of the reaction $SF_6 = SF_5 + F$. J Chem Phys, 96:4272~4282

1992TSA/WAL Tsang W, Walker J A. 1992. Pyrolysis of 1,7-octadiene and the kinetic and thermodynamic stability of ally and 4-pentenyl radicals. J Phys Chem, 96:8378~8384

1992TUR/BAR Turnipseed A A. Barone S B, Ravishankara A R. 1992. Observation of methylthiyl radical addition to oxygen in the gas phase. J Phys Chem, 96:7502~7505

1992VEN/AMA Venimadhavan S, Amarnath K, Harvey, N G, Cheng J P, Arnett E M. 1992. Heterolysis, homolysis, and cleavage energies for th cation radicals of some carbon-sulfur bonds. J Am Chem Soc, 114:221~229

1992VIG/HEN Viggiano A A, Henchman M J, Dale F, Deakyne C A, Paulson J F. 1992. Gas-phase reactions of weak Bronsted bases I , PO_3^-, HSO_4 , FSO_3^-, and $CF_3SO_3^-$ with strong Bronsted acids H_2SO_4, FSO_3H, and CF_3SO_3H. A quantitative instrinsic superacidity scale for the sulfonic acids XSO_3H (X = HO, F, and CF_3). J Am Chem Soc, 114:4299~4306

1992WAL Walsh R. 1992. Derivation of thermodynamic quantities from kinetic measurements in gas phase silane chemistry. *In:* Energetics of Organometallic Species, Simoes J AM ed. NATO-ASI Ser. C367, Dordrecht: Kluwer, 171~187

1992WAY Wayland D D M. 1992. Electrochemistry of some organic and organometallic radicals and their application in thermochemical cycles, *In:* Energetics of Organometallic Species, Marinho J A ed. The Netherlands: Kluwer Academic, 95~108

1992YOO/RUS Yoo R K, Ruscic B, Berkowitz B. 1992. Photoionization of As2 and As4. Implications for group V clusters. J Chem Phys, 96:6696~6709

1992ZHA/BOR Zhang X M, Bordwell F G. 1992. Homolytic bond dissociation energies of the benzylic C–H bonds in radical anions and radical cations derived from fluorenes, triphenylmethanes, and related compounds. J Am Chem Soc, 114:9787~9792

1992ZHA/BOR(b) Zhang X M, Bordwell F G. 1992. Acidities and homolytic bond dissociation energies of the acidic C–H bonds in radical cations. J Org Chem, 57:4163~4168

1993ACR/TUC Acree W E Jr, Tucker S A, Pilcher G, Chowdhary A, de Silva M.D.C.R, Monte M J S. 1993. Enthalpies of combustion of 2,2′,4,4′,6,6′-hexamethylazobenzene-N,N-dioxide, 2,2′,6,6′-tetramethylazobenzene-N,N-dioxide, 2,4,6-trimethylnitrobenzene, and 2,6-dimethyl-nitrobenzene. The dissociation enethalpies of the N=N and N–O bonds. J Chem Thermodyn, 25:1253~1261

1993ACR/TUC(b) Acree W E Jr, Tucker S A, Pilcher G, Andrade M I P, de Silva M D C R. 1993. Enthalpies of combustion of p-azoxyanisole and p-azoxyphenetole. The dissociation enthalpy of the N–O bonds. Enthalpies of crystal-to-(liquid crystal) transitions. J Chem Thermodyn, 25:653~659

1993ARE Arends I W C E. 1993. Thesis, Center for Chemistry and the Environments, Gorlaeus Labs, Leiden University, The Netherlands

1993ARE/LOU Arends I W C E, Louw R, Mulder P. 1993. Kinetic study of the thermolysis of anisole in a hydrogen atmosphere. J Phys Chem, 97:7914~7925

1993ARN/FLO Arnett E M, Flowers R A, Meekhof A E, Miller L. 1993. Energies of formation for

conjugate xanthyl carbenium ions, carbanions, and radicals by hydride, proton, and electron transfer in solution and their reactions to give symmerical bixanthyls. J Am Chem Soc, 115:12603~12604

1993ARN/FLO(b) Arnett E M, Flowers R A. 1993. Bond-cleavage energies for molecules and their association radical ions. Chem Soc Rev, 22:9~15

1993BAL/CAS Balucani N, Casavecchia P, Stranges D. Volpi G G. 1993. The enthalpy of formation of the HSO radical. Chem Phys Lett, 211:469~472

1993BAU/HUB Baum G, Huber J R. 1993. Photodissociation of CF_2BrCl at 193 nm investigated by photofragment translational spectroscopy. Chem Phys Lett, 213:427~432

1993BEC/FRE Becerra R, Frey H M, Mason B P, Walsh R. 1993. Time-resolved suties of the temperature-dependence of the gas-phase reactions of methylsilylene with silane and the methysilanes. J Chem Soc Faraday Trans, 89:411~417

1993BOR/SIN Bordwell F G. Singer D L, Satish A V. 1993. Effects of structural changes on acidities and homolytic bond dissociation energies of the N–H bonds in pyridones and related heterocycles. J Am Chem Soc, 115:3543~3547

1993BOR/ZHA Bordwell F G, Zhang X M, Cheng J P. 1993. Bond dissociation energies of the N–H bonds in anilines and in the corresponding radical anions. Equilibrium acidities of aniline radical cations. J Org Chem, 58:6410~6418

1993BOR/ZHA(b) Bordwell F G, Zhang X M, Cheng J P. 1993. Coupling of acidities and oxidation potentials to estimate homolytic bond dissociation energies and radical stabilization energies. J Org Chem, 58:6067~6071

1993BOR/ZHA(c) Bordwell F G, Zhang X M. 1993. From equilibrium acidities to radical stabilization energies. Acc Chem Res, 26:510~517

1993BUR/MAU Burkholder JB, Mauldin R L, Yokelson R J, Solomon S, Ravishankara AR. 1993. Kinetic, thermochemical, and spectroscopic study of chlorine oxide (Cl_2O_3). J Phys Chem, 97:7597~7605

1993CAR/LAY Carson A S, Laye P G, Pedley, J B, Welsby A M. 1993. The enthalpies of formation of iodomethane, diiodomethane, triiodomethane, and tetraiodomethane by rotating combustion calorimetry. J Chem Thermody, 25:261~269

1993CHE/ZHA Cheng J P, Zhao Y. 1993. Homolytic bond-cleavage energies of the acidic N–H bonds in dimethyl-sulfoxide solution and properties of the corresponding radicals and radical cations. Tetrahedron, 49:5267~5276

1993CLA/WAY Clark K B, Wayner D D M, Demidji H D, Koch T H. 1993. Bond dissociation energies of 3,5,5- and 4,5,5-trimethyl-2-oxomorpholines by photoacoustic calorimetry. An assessment of the additivity of substituent effects. J Am Chem Soc, 115:2447~2453

1993COH/BEN Cohen N, Benson S W. 1993. Estimate of heats of formation of organic compounds by additivity methods. Chem Rev, 93:2419~2438

1993CON/CYR Continetti R E, Cyr D R, Osborn D L, Leahy D L, Neumark D M. 1993. Photodissociation dynamics of the N_3 radical. J Chem Phys, 99:2616~2631

1993CYR/LEA Cyr D R, Leahy D J, Osborn D L, Continetti R E, Neumark D M. 1993. Fast beam photodissociation of the CH_2NO_2 radical. J Chem Phys, 99:8751~8764

1993DAV/KIM Davis H F, Kim B, Johnston H S, Lee Y T. 1993. Dissociation energy and photochemistry of NO_3. J Chem Phys, 97:2172~2180

1993DEC/GAL Decouzon M, Gal J F, Gayraud J, Maria P C, Vaglio G A, Vople P. 1993. Fourier transform-ion cyclotron-resonance study of the gas-phase acidities of germane and methylgermane. Bond dissociation energy of germane. J Am Soc Mass Spectrom, 4:54~57

1993DIO/PIE Diogo H P, da Piedade M E M, Fernandes A C, Simoes J A M, da Silva M A V R, Monte M J S. 1993. The enthalpy of sublimation of diphenylacetylene from Knudsen

effusion studies. Thermochimica Acta, 228:15~22

1993DOB/OTT Dobe S, Otting M, Temps F, Wagner H G, Ziemer H. 1993. Fast flow kinetic studies of the reaction $CH_2OH + HCl = CH_3OH + Cl$. The heat of formation of hydroxymethyl. Ber Bunsenges Phys Chem, 97:877~884

1993EAS/ALL East A L L, Allen W D. 1993. The heat of formation of NCO. J Chem Phys, 99:4638~4650

1993ELM/MIN Elmaimouni L, Minetti R, Sawerysin J P, Devolder P. 1993. Kinetics and thermochemistry of the reaction of benzyl radical with O_2 — investigations by discharge flow/laser induced fluorescence between 393 K and 433 K. Int.J Chem Kinet, 25:399~413

1993FEN/NOZ Fenter F F, Noziere B, Caralp F, Lesclaux R. 1993. Study of the kinetics and equilibrium of the benzyl-radical association reactions with molecular oxygen. Int J Chem.Kinet, 26:171~189

1993FIS/KIC Fisher E R, Kickel B L, Armentrout P B. 1993. Collison-induced dissociation and charge-transfer reactions of SiF_x (x=1~4). Thermochemistry of SiF_x and SiF_x^+. J Phys Chem, 97:10204~10210

1993FLE/ECK Flesch R E, Eckart R, Hottmann K, Baumgartel H. 1993. Photoabsorption and photoionization of chlorine dioxide. J Phys Chem, 97:837~844

1993FOK/GRE Fokin A V, Grebennikov V N, Manelis G B, Nazin G M. 1993. Thermal decomposition of gem-bis(difluoroamines). Dokl Akad Nauk, 332:735~736

1993HEN Heneveld R J P. 1993. CCERS-92-04, Center for Chemistry and the Environments. Gorlaeus Labs, Leiden University. The Netherlands

1993HOL/LOS Holmes J L, Lossing F P, Mayer P M. 1993. The effects of methyl substitution on the structure and thermochemistry of the cyanomethyl radical and cation. Chem Phys Lett, 212:134~140

1993JEN Jenkins H D B. 1993. Thermochemistry of the azide anion. Assignment of heat of formation N_3^- using viscosity B-coefficient data. J Phys Chem, 97:7876~7879

1993LAZ/PAP Lazarou Y G, Papagiannakopoulos P. 1993. Kinetic study of the reactions of atomic chlorine with N-methylmethylenimine and 1,3,5-triethylhexahydro-1,3,5-triazine. J Phys Chem, 97:4468~4472

1993LEE/GRE Lee M A H, Gree J B, Pilling M J, Robertson S H. 1993. Direct observation of equilibrium in the system $H + C_2H_4 = C_2H_5$: Standard enthalpy of formation of the ethyl radical. J Phys Chem, 97:860~870

1993LIN/JON Lind J, Jonsson M, Eriksen T E, Merenyi G, Eberson L. 1993. One-electron reduction potential and ring opening of the succinimidyl radical in water. J Phys Chem, 97:1610~1614

1993OCC/DAA Occhiakini D, Daasbjerg K, Lund H. 1993. Estimation of reduction and standard potentials of acyl radicals. Acta Chem Scand, 47:1100~1106

1993OHA/DEP O'Hair R A J, DePuy C H, Bierbaum V M. 1993. Gas-phase chemistry and thermochemistry of the hydroxysulfide anion, HOS^-. J Phys Chem, 97:7955~7961

1993PEP/MAT Pepkin V I, Matyushin Y N, Khisamutdinov G K, Slovetskii V I, Fainziberg A A. 1993. Thermochemical propetics of alpha-azidopolynitroalkanes and the dissociation energy of $C–N_3$ bonds in organic azides. Khim Fiz, 12:1399~1403

1993RUS/BER Ruscic B, Berkowitz J. 1993. Heat of formation of CH_2OH and $D(H–CH_2OH)$. J Phys Chem, 97:11451~11455

1993RUS/BER(b) Ruscic B, Berkowitz J. 1993. Photoionization mass spectrometry of CH_2S and HCS. J Chem Phys, 98:2568~2579

1993RUS/BER(c) Ruscic B, Berkowitz J. 1993. Determination of consecutive bond energies by photoionization of SbH_n(n = 1~3) .J Chem Phys, 99:5840~5848

1993SCH/RAN Schmude R W Jr, Ran Q, Gingerich K A. 1993. Atomization enthalpy and enthalpy of formation of gaseous Si4 from mass spectrometric equilibrium measurements. J Chem Phys, 99:7998~8004

1993SEA/ROB Seaking P W, Robertson S H, Pilling M J, Slage I R, Gmurczyk G W, Bencsura A, Gutma D, Tsang W. 1993. Kinetics of the unimolecular decomposition of isopropyl: Weak collision effects in helium, argon, and nitrogen. J Phys Chem, 97:4450~4458

1993SHA/KEB Sharpe P, Kebarle P. 1993. Electron affinities, enthalpy, and entropy of electron attachent of sevral η^4-(olefin)Fe(CO)$_3$ complexes and electron-transfer kinetics. J Am Chem Soc, 115:782~789

1993TIM/SEE Timonen R S, Seetula J A, Gutman D. 1993. Kinetics of the reactions of unsaturated hydrocarbon free radicals (vinyl, propargyl, and ally) with molecular bromine. J Phys Chem, 97:8217~8221

1993TRA/HOL Traeger J C, Holmes J L. 1993. Heat of formation of hydroxymethyl. J Phys Chem, 97:3453~3455

1993WAL/HUR Wallington T J, Hurley M D, Schneider W F, Schested J, Nielsen O J. 1993. Atmospheric chemistry of CF_3O radical: Reaction with H_2O. J Phys Chem, 97:7606~7611

1993WAY/PAR Wayner D D M, Parker V D. 1993. Bond energies in solution from electrode potentials and thermochemical cycles. A simplified and general approach. Acc Chem Res, 26:287~294

1993WEI/WEL Weitz E, Wells J R, Ryther R J, House P. 1993. Bond energies and reaction kinetics of coordinatively unsaturated metal carbonyls. *In:* Laser Chemistry of Organometallics. Chaiken J ed. ACS Sym. 530, Washington DC. Chap. 12. 147~163

1993ZHA Zhang X M. 1993. Homolytic bond dissociation energies of the carbon halogen bonds in the benzyl halide radical-anion intermediates formed in radical nucleophilic-substitution reactions. J Chem Soc Perkin Trans 2, 2275~2279

1993ZHA/BOR Zhang X M, Bordwell F G. Vanderpuy M, Fried H E. 1993. Equilibrium acidities and homolytic bond dissociation energies of the acidic C–H bonds in N-substituted trimethylammonium and pyridinium cations. J Org Chem, 58:3060~3066

1993ZHA/BOR(b) Zhang X M., Bordwell F G. Bares J E, Cheng J P, Petric B C. 1993. Homolytic bond dissociation energies of the acidic C–H bonds in alpha-substituted and 10-substituted 9-methylanthracenes and their related radical anions. J Org Chem, 58:3051~3059

1993ZHA/JAC Zhang R, Jackson R L. 1993. Buffer-gas quenching as a dynamic probe of organometallic photodissociation process. *In:* Laser Chemistry of Organometallics. Chaiken J ed. ACS Sym. 530. Washington DC. Chapter 10. 122~134

1994ACR/TUC Acree W E Jr, Tucker S A, Pilcher G, Toole G. 1994. Enthalpies of combustion of 4-dimethylaminonitrosobenzene and 4-dimethylaminonitrobenzene. J Chem Thermodyn, 26:85~90

1994BAR Bartmess J E. 1994. Thermodynamics of the electron and the proton. J Phys Chem, 98:6420~6424

1994BER/ELL Berkowitz J, Ellison G B, Gutman D. 1994. Three methods to measure RH bond energies. J Phys Chem, 98:2744~2765

1994BLA/NOR Blank D A, North S W, Lee Y T. 1994. The Ultraviolet photoionization dynamics of pyrrole. Chem. Phys. 187:35~47

1994BOR/SAT Bordwell F G. Satish A V. 1994. Is resonance important in determining the acidities of weak acids or the homolytic bond dissociation enthalpies (BDEs) of their acidic H–A bonds? J Am Chem Soc, 116:8885~8889

1994BOR/ZHA Bordwell F G, Zhang X M. 1994. Polarizability effects of alkyl groups in RCH_2, R, RS, RSO_2, RO, and R_2N moieties in families of weak acids on the stabilities of adjacent

anions and radicals in DMSO solution. J Am Chem Soc, 116:973~976

1994BOR/ZHA(b) Bordwell F G, Zhang X M, Satish A V, Cheng J P. 1994. Assessment of the importance of changes in group-state energies on the bond dissociation enthalpies of O–H bonds in phenols and the S–H bonds in thiophenols. J Am Chem Soc, 116:6605~6610

1994BOW Bowers M T. 1994. Cluster ions: carbon, met-carts, and sigma-bond activation. Acc Chem Res, 27:324~332

1994BUL/WAL Bullock W J, Walsh R, King K D. 1994. Very-low-pressure pyrolysis of hexamethyldisilane. Kinetic determination of the bond dissociation enthalpy DH(Me_3Si–$SiMe_3$) and implications for the enthalpy of formation of the trimethylsilyl radical. J Phys Chem, 98:2595~2601

1994BUS/KEM Bushnell J E, Kemper P R, Borers M T. 1994. Na^+-H_2 clusters — binding energies from theory and experiment. J Am Chem Soc, 116:2044~2049

1994CAR/LAY Carson A S, Laye P G, Pedley J B, Welsby A M. 1994. The enthalpies of formation of iodoethane, 1,2-diiodoethane, 1,3-diodopropane, and 1,4-diiodobutane. J Chem Thermodyn, 26:1103~1109

1994CHA/GRI Chatgilialoglu C, Griller D, Kaminska J M K, Lossing F P. 1994. Sulfur-chlorine bond dissociation enthalpies in methane-sulfonyl and benzene-sulfonyl chlorides. J Chem Soc Perkin Trans 2, 357~360

1994CHA/MAR Chandrasekharaiah M S, Margrave J L. 1994. Enthalpies of formation of solid silicon dichalcogenides. J Phys Chem Ref Data, 23:499~507

1994COO/PAT Cooks R G, Patrick J S, Kotiaho T, McLuckey S A. 1994. Thermochemical determinations by the kinetic method. Mass Spectrom Rev, 13:287~339

1994COR/COL Coronel M E J, Colussi A J. 1994. Entropic and enthalpic effects of 4-methoxy substitution in phenoxyl radicals. J Chem Soc Perkin Trans 2, 785~787

1994DEL/LOU de Lijser H J P, Louw R, Mulder P. 1994. Thermal gas-phase hydrodehalogenation of $CBrClF_2$. J Chem Soc Perkin Trans 2, 139~145

1994DOU/MAC Doughty A, Mackie J. 1994. Kinetics of thermal decomposition of the diazines. Shock tube pyrolysis of pyrimidine. J Chem Soc Faraday Trans, 90:541~548

1994FRE/KAB Frenkel M, Kabo G J, Marsh K N, Roganov G N, Wilhoit R C. 1994. Thermodynamics of Organic Compounds in the Gas State, Vol 1 and 2. Thermodynamics Research Center, College Station, Texas

1994GIN/FIN Gingerich K A, Finkbeiner H C, Schmude R W Jr. 1994. Enthalpies of formation of small linear carbon clusters. J Am Chem Phys, 116:3884~3888

1994JEF/NIC Jefferson A, Nicovich J M, Wine P H. 1994. Temperature-dependence kinetics studies of the reactions Br + CH_3SCH_3 = CH_3SCH_2 + HBr. Heat of formation of the CH_3SCH_2 radical. J Phys Chem, 98:7128~7135

1994JON/LIN Jonsson M, Lind J, Eriksen T E, Merenyi G. 1994. Redox and acidity properties of 4-substituted aniline radical cations in water. J Am Chem Soc, 116:1423~1427

1994KAL/GUT Kalinovski I J, Gutman D. 1994. Kinetics and thermochemistry of the reaction $Si(CH_3)_3$ + HBr = $Si(CH_3)_3H$ + Br: Determination of the $(CH_3)_3Si$–H bond energy. J Phys Chem, 98:9551~9557

1994KNY/DUB Knyazev V D, Dubinsky I A, Slagle I R, Gutman D. 1994. Experimental and theoretical study of the sec-C_4H_9 = CH_3 + C_3H_6 reaction. J Phys Chem, 98:11099~11108

1994KUO/ZHA Kuo S C, Zhang Z, Klemm R B. 1994. Photoionization of hydroxymethyl (CD_2OH and CD_2OD) and methoxy (CD_3O) radicals: Photoion efficiency spectra, ionization energies, and thermochemistry. J Phys Chem, 98:4026~4033

1994LIA/LIE Lias S G, Liebman J F, Levin R D, Kafafi S A. 1994. NIST Standard Reference Database 19A, Version 2-01, Washiton DC

1994LUC/PED Lucarini M, Pedulli G F, Cipollone M. 1994. Bond dissociation enthalpy of alpha-

tocopherol and other phenols. J Org Chem, 59:5063~5070

1994MOR/ASH Mordaunt D H, Ashfold M N R. 1994. Near-ultraviolet photolysis of C_2H_2. A precise determination of D(HCC–H). J Chem Phys, 101:2630~2631

1994NAT/KOC Natterer J, Koch W, Schroder D, Goldberg N, Schwarz H. 1994. Combined experimental and theoretical study of the C -H bond strength and the gas-phase acidity of triacetylene, C_6H_2, and the electron-affinity of the C_6H-center-dot-radical. Chem Phys Lett, 229:429~434

1994NEU/KRA Neusser H J, Krause H. 1994. Binding energy and structure of van der Waals complexes of benzene. Chem Rev, 94:1829~1843

1994NIC/FRI Nickolaisen S, Friedl R R, Sander S P. 1994. Kinetics and mechanism of the ClO + ClO reaction: Pressure and temperature dependence of the bimolecular and termolecular channels and thermal decomposition of chlorine peroxide. J Phys Chem, 98:155~169

1994NIST NIST Standards Reference Database 25. 1994. Structures and Properties Database and Estimated Program, Version 2-01.

1994NOL Nolan S P. 1994. Bonding energetics of organometallic compounds, *In:* Encyclopedia of Inorganic Chemistry, King RB ed. New York: Wiley, 1994. 307~318

1994PAD/CHE Paddison S J, Chen Y, Tschuikow-Roux E. 1994. An ab initio study of the structures, barriers for internal-rotation, vibrational frequencies, and thermodynamic functions of hydrochlorofluorocarbon CH_3CF_2Cl, and the corresponding radical CH_2CF_2Cl. Can J Chem, 72:561~567

1994PED Pedley J B. 1994. Thermochemical Data and Structure of Organic Compounds, Thermodynamics Research Center, Texas A & M University, Colege Station, Texas.

1994PET Peters K S. 1994. Time-resolved photoacoustic calorimetry — from carbenes to proteins. Angew Chem. Int Ed Engl, 33:294~302

1994RAK/VER Rakus K, Vervkin S P, Schatzer J, Beckhaus H D, Ruchard C. 1994. Thermolabile hydrocarbons. 33. Thermochemistry and thermal decomposition of 9,9′-bifluorenyl and 9,9′-dimethyl-9,9′-bifluorenyl. The stabilization energy of 9-fluorenyl radicals. Chem Ber, 127:1095~1103

1994RAN/SCH Ran Q, Schmude R W Jr, Miller M, Gingerich K A. 1994. Mass spectrometric investigation of the thermodynamic properties of the Si_5 molecule. Chem Phys Lett, 230:337~342

1994RUS/BER Ruscic B, Berkowitz J. 1994. The heats of formation of some $C_2H_5O^+$ isomers, relevant bond energies in ethanol and PA(CH_3CHO). J Chem Phys, 101:10936~10946

1994RUS/BER(b) Ruscic B, Berkowitz J. 1994. The H–NCS bond energy, heats of formation of HNCS, NCS, and IP(NCS) from photoionization mass spectrometric studies of HNCS, NCS and $(NCS)_2$. J Chem Phys, 101:7975~7989

1994RUS/BER(c) Ruscic B, Berkowitz J. 1994. The H–NCO bond energy and heat of formation HCO from photoionization mass spectrometric studies of HNCO and NCO. J Chem Phys, 101:4498~4508

1994SCH/ARE Schraa G J, Arends I W C E, Mulder P. 1994. Thermal decomposition of 2,3-dihydro-1,4-benzodioxin and 1,2-dimethoxybenzene. J Chem Soc Perkin trans 2, 189~197

1994SCH/WAL Schneider W F, Wallington T J. 1994. Thermochemistry of COF_2 and related compounds. J Phys Chem, 98:7448~7451

1994SEE/KAL Seetula J A, Kalinovski I J, Slagle I R, Gutman D. 1994. Kinetics of the reaction of CH_2OH radical with oxygen atoms. Chem Phys Lett, 224:533~538

1994TUM/DEN Tumanov V E, Denisov E T. 1994. Analysis of the activation energy for $R_f + R_iH = R_fH + R_i$ reactions in terms of the transition state model. Kinet Katal, 35:821~828

1994TZE/LEE Tzeng W B, Lee Y R, Lin S M. 1994. Photodissociation of CH_2BrCl at 248 and 193 nm investigated translational spectroscopy. Chem Phys Lett, 227:467~471

1994WEN/SQU Wenthold R G, Squires R R. 1994. Biradical thermochemistry from collision-induced dissociation threshold energy measurements. Absolute heats of formation of ortho-, meta-, and para-benzyne. J Am Chem Soc, 116:6401~6412

1994WEN/SQU(b) Wenthold R G, Squires R R. 1994. Gas-phase properties and reactivity of the acetate radical anion. Determination of the C–H bond strengths in acetic acid and acetate ion. J Am Chem Soc, 116:11890~11897

1994YU/RAU Yu D, Rauk A, Armstrong D A. 1994. Radicals and ions of formic and acetic-acids. An ab initio study of the structures and gas and solution-phase thermochemistry. J Chem Soc Perkin trans 2, 2207~2215

1994ZHA/BOR Zhang X M, Bordwell F G. 1994. Element effects on the homolytic bond dissociation enthalpies of the acidic H–A bonds in HA^- radical cations and their neutral presursors. J Am Chem Soc, 116:4251~4254

1994ZHA/BOR(b) Zhang X M, Bordwell F G. 1994. Effects of pi-coordinated transition-metal groups on fluorene acidities and homolytic bond dissociation enthalpies. Organometallics, 13:2920~2921

1994ZHA/BOR(c) Zhang X M, Bordwell F G. 1994. Bond dissociation energies of the acidic H–A bonds in HA^+ radical cations and in HA radical anions in DMSO solution. J Am Chem Soc, 116:904~908

1994ZHA/BOR(d) Zhang X M, Bordwell F G. 1994. Equilibrium acidities and homolytic bond dissociation energies of the acidic C–H bonds in p-substituted triphenylphosphonium cations. J Am Chem Soc, 116:968~972

1994ZHA/BOR(e) Zhang X M, Bordwell F G. 1994. Acidities and homolytic bond dissociation enthalpies (BDEs) of the acidic H–A bonds in acyclic and cyclic alkoxycarbonyl compounds (esters and carbamates). J Org Chem, 59:6456~6458

1994ZHA/HUA Zhao Y Y, Huan Z W, Cheng J P.1994. Cleavage energies of N–H bonds in parasubstituted acetophenone semicarbazones and corresponding radical ions. Acta Chim Sinaca, 52:980~984

1995~1999

1995ACR/BOT Acree W E Jr, Bott S G, Tucker S A, de Silva M D M C R, Matos M A R, Pilcher G. 1995. Enthalpies of combustion of 2,2′,6,6′-tetraethylazobenzene N,N-dioxide, 2,4,6-tris(1,1-dimethylethyl) nitrosobenzene, and 2,4,6-tris-1,1-dimethylethyl)nitrobenzene. J Chem Thermodyn, 27:1433~1440

1995ACR/TUC Acree W E Jr, Tucker S A, de Silva M D M C R, Matos M A R, Goncalves J M, da Silva M A V R, Pilcher G. 1995. Enthalpies of combustion of 4-nitropyridine N-oxide and pyridine-3-carboxylic acid N-oxide: The dissociation enthalpies of the N–O bonds in pyridine N-oxide derivatives. J Chem Thermody, 27:391~398

1995ALN/ZHA Alnajjar M S, Zhang X M, Franz J A, Bordwell F G. 1995. Stereoelectronic effects of divalent sulfur functions on radical stabilities. J Org Chem, 60:4976~4977

1995ARE/MUL Arends I W C E, Mulder P, Clark K B, Wayner D D M. 1995. Rate constants for termination and TEMPO trapping of some resonance stabilized hydroaromatic radicals in the liquid phase. J Phys Chem, 99: 8182~8189

1995ARM Armentrout P B. 1995. Building organometallic complexes from the bare metal: Thermochemistry and electronic structure along the way. Acc Chem Res, 28:430~436

1995BOR/SAT Bordwell F G, Satish A V, Zhang S H, Zhang X M. 1995. Using thermodynamic cycles to study reactivity intermediates. Pure Appl Chem, 67:735~740

1995BOR/ZHA Bordwell F G, Zhang S, Zhang X M, Liu W Z. Homolytic bond dissociation enthalpies of the acidic H–A bonds caused by proximate substituents in sets of methyl ketones,

carboxylic esters, and carboxamides related to changes in ground state energies. J Am Chem Soc, 117:7092~7096

1995BOR/ZHA(b) Bordwell F G, Zhang S. 1995. Structural effects on stabilities of imminoxy radicals. J Am Chem Soc, 117:4858~4861

1995BOR/ZHA(c) Bordwell F G, Zhao Y. 1995. Effects of nitro groups on acidities and homolytic bond dissociation enthalpies of the acidic C–H bonds in carbon acids and their radical anions. J Org Chem, 60:6348~6352

1995BOR/ZHA(d) Bordwell F G, Zhang X M. 1995. Acidities and homolytic bond dissociation enthalpies of 4-substituted-2,6-di-tert-butylphenols. J Phys Org Chem, 8:529~535

1995BOY/NOZ Boyd A A, Nozierc B, Lesclaux R. 1995. Kinetics and thermochemistry of the reversible combination reactions of the ally and benzyl radicals with NO. J Phys Chem, 99:10815~10823

1995BRI/SAL Brinkman E A, Salomon K, Tumas W, Braunan J I. 1995. Electron affinity and gas-phase acidities of organogermanium and organotin compounds. J Am Chem Soc, 117:4905~4910

1995BUC/JOH Buckley T J, Johnson R D, Huie R E, Zhang Z, Kuo S C, Klemm B. 1995. Ionization energies, appearance energies, and thermochemistry of CF_2O and FCO. J Phys Chem, 99:4879~4885

1995CAC/PET Cacace F, de Petris G, Pepi F, Angelelli F. 1995. Gas-phase nitronium affinities, Proc. Natl. Acad. Sci. USA, 92:8635~8639

1995CHA Chatgilialoglu C. 1995. Structural and chemical properties of silyl radicals. Chem. Rev, 95:1229~1251

1995CHE/LIU Cheng J P, Liu B, Li Z, Huan Z. 1995. Heterolytic and homolytic bond dissociation energies of the N–H bonds in Ylides precursors and properties of the corresponding nitrogen-centered radicals. China Sci Bull, 40:1338~1341

1995CHE/ZHA Cheng J P, Zhao Y, Huan Z. 1995. The studies of thermodynamic stability of the C- and N-centered radicals, Sci China Ser B Chem, 25:804~809

1995DAV/BIE Davico G E, Bierbaum V M, DePuy C H, Ellison G B, Squires R R. 1995. The C–H bond energy of benzene, J Am Chem Soc, 117:2590~2599

1995DEN Denisov E T. 1995. Evaluating the dissociation energy of the O–H bond of phenols from kinetics measurements. Zh. Fiz. Khim, 69:623~631

1995DEN(b) Denisov E T. 1995. Analysis of the reasons for the high activity of aromatic amines in reactions with peroxy radicals in terms of the parabolic model. Kinet Catal, 36:345~350

1995DEN/IL Deng Y, Illies A J, James M A, McKee M L, Peschke M. 1995. A definitive investigation of the gas-phase two-center. Three electron bonds in $[H_2SSH_2]^+$, $[Me_2SSMe_2]^+$, and $[Et_2SSSEt_2]^+$: Theory and experiment. J Am Chem Soc, 117:420~428

1995GAR/MAY Gardner K A, Mayer J M. 1995. Understanding C–H bond oxidation: H and H- transfer in the oxidation of toluene by permanganate. Science, 269:1849~1851.

1995HE He Y. 1995. Single-pulse shock-tube on the decomposition of C_3F_6. *In:* Shock Waves, Proc Int Symp, 20th, 1995, Sturtevant B, Shepherd J E, Hornung, H G eds. Singapore: World Scientific, 953~958

1995HO/DUN Ho Y P. Dunbar R C, Lifshitz C. 1995. C–H bond strength of naphthalene ion. A reevaluation using new time-resolved photodissociation results. J Am Chem Soc, 117:6504~6508

1995HSU/DEM Hsu K J, DeMore W B. 1995. Temperature-dependent rate constants and substituent effects for the reactions of hydroxyl radicals with partially fluorinated ethers. J Phys Chem, 99:11141~11146

1995JON/LIN Jonsson M, Lind J, Merenyi M, Eriksen T E. 1995. N–H bond dissociation energies,

reduction potentials and Pka of multisubstituted anilines and aniline radical cations. J Chem Soc Perkin Trans 2, 61~65

1995KNY/BEN Knyazev V D, Benesura A, Dubinsky I A, Gutman D, Melius C F, Senkan S M. 1995. Kinetics and thermochemistry of the reaction of 1-chloroethyl radical with molecular oxygen. J Phys Chem, 99:230~238

1995KRA/NII Krasnoperov L N, Niiranen J T, Gutma D, Melius C F, Allendorf M D. 1995. Kinetics and thermochemistry of $Si(CH_3)_3$ + NO reaction: Direct determination of Si–N bond energy. J Phys Chem, 99:14347~14358

1995LEB/CHI Lebedev V P, Chironov V V, Kizin A N, Falyakhov I F, Saifullin I S, Klyushnikov O R, Orlov Y D, Lebedev Y A. 1995. Dissociation energy of the N–O bond in pyridine 1-oxide derivatives. Izvestiya Akademii Nauk Seriya Khimicheskaya. No. 4, 660~662

1995LEY/MAS Ley L, Masanet J, Caralp F, Lesclaux R. 1995. Kinetics of the association reactions of NO with the series of chlorofluoromethyl radicals CF_xCl_{3-x}. J Phys Chem, 99:1953~1960

1995LI/HOW Li I, Howell B A, Matyjaszewski K, Smithg P B, Priddy D B. 1995. Kinetics of decomposition of 2,2,6,6-tetramethyl-1-(1-phenylethoxy)piperidine and its implications of nitroxyl-mediated sryrene polymerization. Macromolecules, 28:6692~6693

1995LUN/DAA Lund H, Daasbjerg K, Occhialini D, Pedersen S U. 1995. Potentials and reactions of some electrogenerated radicals. Russ J Electrochem, 31:865~872

1995MIL/MIL Miller A E S, Miller T M, Viggiano A A, Morris R A, Vandoren J M, Arnold J M, Paulson J. 1995. Negative ion chemistry of SF_4. J Chem Phys, 102:8865~8873

1995MUR/BEA Murthy S, Beauchamp J L. 1995. Fourier transfor ion cyclotron resonance spectrometric studies of Lewis acid-base chemistry in monochlorosilane. J Phys Chem, 99:9118~9121

1995OHA O'Hare P A G. 1995. Thermochemistry of germanium + tellurium. II. Molar enthalpies of dissociation of bonds in GeTe, $GeTe_2$, and Ge_2Te_3. J Chem Thermodyn, 27:921~926

1995ROB/POL Robinson M S, Polak M L, Bierbaum V M, DePuy C H, Lineberger W C. 1995. Experimental studies of allene, methylacetylene, and the propargyl radical. Bond dissociation energies, gas-phase acidities, and ion-molecule chemistry. J Am Chem Soc, 117:6766~6778

1995ROT/HUN Roth W R, Hunold F. 1995. Heat of formation and stabilization energy of the pentamethycyclopentadienyl radical. Liebigs Ann Chem, No. 6, 1119~1122

1995SCH/RAN Schmude R W Jr, Ran Q, Gingerich K A, Kingcade J E Jr. 1995. Atomization enthalpy and enthalpy of formation of gaseous Si2 and Si3 from mass spectrometric equilibrium measurements. J Chem Phys, 102:2574~2579

1995SHE/QI Sheng L, Qi F, Tao L, Zhang Y, Yu S, Wong C K, Li W K. 1995. Experimental and theoretical studies of the photoionization and dissociative photoionizations of vinyl chloride. Int J Mass Spectrom Ion Proc, 148:179~189

1995TAK/PAS Takhistov V V, Pashina T A, Orlov V M, Rodin A A, Barabanov VG. 1995. Experimental and theoretical determination of heats of formation of molecules, cationa, anions and free radicals with fluoroalkyl and other fluorinated groups. Zh. Org. Khim, 31:1786~1792

1995TZE/ZAR Tzerpos N I, Zarkadis A K, Kreher R P, Reoas L, Lehnig M. 1995. Diphenylpyridylmethyl radicals. I. Synthesis, dimerization and endor spectroscopy of diphenyl(2-pyridyl, 3-pyridyl or 4-pyridyl)methyl radicals. Bond dissociation enthalpies of their dimers. J Chem Soc Perkin Trans 2, No. 4, 755~761

1995VER/GEO Veregin R P N, Georges M K, Hamer G K, Kazmaier P M. 1995. Mechanism of living free-radical polymerizations with narrow polydispersity. Electron spin resonance and kinetic studies. Macromolecules, 28:4391~4398

1995WAY/LUS Wayner D D M, Lusztyk E, Page D, Ingold K U, Mulder P, Laarhoven L J J, Aldrich H

S. 1995. Effects of solvation on the enthalpies of reaction of tert-butoxyl radicals with phenol and on the calculated O–H bond strength in phenol. J Am Chem Soc, 117:8737~8744

1995WIN/CUI Tsang W, Cui J P. 1995. Single-pulse shock tube studies on the reactions of hydrogen atoms with acetone and methyl ether. Proceed. Int. Symp. Shock Waves. 19th Marseille. Berlin: Springer, Germany. 125~130

1995ZAB Zabel F. 1995. Unimolecular decomposition of peroxynitrates. Z Phys Chem, 188:119~142

1995ZHA/BOR Zhao Y, and Bordwell, F G. 1995. Bond dissociation free energies of the H–A bonds in HA^{2-} anions. J Org Chem, 60:3932~3933

1995ZHA/DUL Zhang J, Dulligan M, Wittig C. 1995. HNCO + light = H + NCO. Center-of-mass translational energy distribution, reaction dynamics, and D(H-NCO). J Phys Chem, 99:7446~7452

1996ACR/BOT Acree W E Jr, Bott S G, Tucker S A, de Silva M D M C R, Matos M.A, Pilcher G. 1996. Enthalpies of combustion of 5-methoxybenzofurazan, 5-methoxybenzofurazan-1-oxide, 5-methylbenzofurazan-1-oxide, 5-chlorobenzofurazan-1-oxide, and 4-nitro-benzofurazan-1-oxide: The dissociation enthalpies of the N--O bonds. J Chem Thermodyn, 28:673~683

1996AND/RIV Andrade P B M, Riverson J M. 1996. Relative gas-phase acidities of fluoro- and chlorobenzene. J Mass Spectrom, 31:767~770

1996ARM/SUN Armstrong D A, Sun Q, Schuler R H. 1996. Reduction potentials and kinetics of electron transfer reactions of phenylthiyl radicals: Comparisons with phenoxyl radicals. J Phys Chem, 100:9892~9899

1996ASH/APP Asher R L, Appelman E H, Ruscic B. 1996. On the heat of formation of carbonyl fluoride, CF_2O. J Chem Phys, 105:9781~9795

1996BEN/COH Benson S W, Cohen N. 1996. Current status of group additivity. *In:* Computational Thermochemistry, ACS Symp. Ser. 677, 20~46

1996BOR/ING Born M, Ingemann S, Nibbering N M M. 1996. Experimental determination of the enthalpies of formation of formyl cyanide and thioformyl cyanide in the gas phase. J Phys Chem, 100:17662~17669

1996BOR/LIU Bordwell F G, Liu W Z. 1996. Solvent effects on homolytic bond dissociation energies of hydroxylic acids. J Am Chem Soc, 118:10819~10823

1996BOR/LIU(b) Bordwell F G, Liu W Z. 1996. Equilibrium acidities and homolytic bond dissociation energies of N–H and/or O–H bonds in N-phenylhydroxylamine and its derivatives. J Am Chem Soc, 118:8777~8781

1996BRO/BER Brown S S, Berghout H L, Crim F F. 1996. The HNCO heat of formation and the N–H and C–N bond enthalpies from initial state selected photodissociation. J Chem Phys, 105:8103~8110

1996CAM/AUT Camaioni D M, Autrey S T, Salinas T B, Franz J A. 1996. Calculation of the effects of branching and conjugation on intrinsic barriers for H atom transfer reactions involving hydrocarbons. J Am Chem Soc, 118:2013~2022

1996CHA Chase M W Jr. 1996. NIST-JANAF thermochemical tables for the bromine oxides. J Phys Chem Ref Data, 25:1069~1111

1996CHA(b) Chase M W Jr. 1996. NIST-JANAF thermochemical tables for the iodine oxides. J Phys Chem Ref Data, 25:1297~1340

1996CHA(c) Chase M W Jr. 1996. NIST-JANAF thermochemical tables for the oxygen fluorides. J Phys Chem Ref Data, 25:551~603

1996COH Cohen N. 1996. Revised group additivity values for enthalpies of formation (at 298 K) of carbon-hydrogen and carbon-hydrogen-oxygen compounds. J Phys Chem Ref Data,

25:1411~1481

1996COM/CAR Compton R N, Carman H S Jr, Desfrancois C, Abdoul-Carmine H, Schermann J P, Hendricks J H, Lyapustina S A, Bowen K H. 1996. On the binding of electrons to nitromethane: Dipole and valence bound anioins. J Chem Phys 105:3472~3478

1996DEN Denisov E T. 1996. Evaluation of the dissociation energies of the S–H bonds in thiophenols and thioalcohols on the basis of kinetic measurements. Zh. Fiz. Khim, 70:260~263

1996DIX Dixon R N. 1996. The heats of formation of HNO and DNO. J Chem Phys, 104:6905~6906

1996DOB/BER Dobe S, Berces T, Turanyi T, Marta F, Grussdorf J, Temps F, Wagner H Gg. 1996. Direct kinetic studies of the reactions Br + CH_3OH and CH_2OH + HBr: The heats of formation of CH_2OH. J Phys Chem, 100:19864~19873

1996DUB/MAT Dubikhin V V, Matveev V G, Nazin G M. 1996. Thermal decomposition of 2,4,6-trinitrotoluene in hydrocarbon solvents. Izvestiya Akademii Nauk, Seriya Khimicheskaya, No. 8, 1977~1980

1996ELL/DAV Ellison G B, Davico G E, Bierbaum V M, DePuy C H. 1996. Thermochemistry of the benzyl and allyl radicals and ions. Int J Mass Spectrom Ion Proc, 156:109~131

1996FUL/HAM Fulle D, Hamann H F, Hippler H, Troe J. 1996. High-pressure range of addition reactions of HO. 2. Temperature and pressure dependence of the reaction HO + CO =– HOCO → H + CO_2. J Chem Phys, 105:983~1000

1996FUL/HIP Fulle D, Hippler H. 1996. The high-pressure range of the reaction CH_2 with N_2. J Chem Phys, 105:5423~5430

1996GUR/VEY Gurvich L V, Veyts I V, Alcock C B. 1996. Thermodynamic Properties of Individual Substances. Vol. 3. New York: Begell House

1996HAN/HUA Han B H, Huan Z W, Mi J L, Wang H X, Cheng J P. 1996. Studies on enthalpies of C–O bond cleavage in radical ions. 2. Bond energies of radical anions. Chem J Chinese Univ, 17:1387~1393

1996HEC/HIP Heckmann E, Hippler H, Troe J. 1996. High-temperature reactions and thermodynamic properties of phenyl radicals. 26th Sym. Int. Combust. Combustion Institute. Pittsburgh, PA. 543~550

1996HUE/DUN Huey L G, Dunlea E J, Howard C J. 1996. Gas-phase acidity of CF_3OH. J Phys Chem, 100:6504~6508

1996HUN/SHE Hung W C, Shen M Y, Lee Y P, Wang N S. Cheng B M. 1996. Photoionization spectra and ionization thresholds of CH_3SO, CH_3SOH, and $CH_3SS(O)CH_3$. J Chem Phys, 105:7402~7411

1996JAM/ILL James M A, Illies A J. 1996. Studies of two-center three-electron S therefore S bonds in [n-Pr_2S therefore Sn-Pr_2]$^+$ and [i-Pr2S therefore Si-Pr_2]$^+$: Thermochemistry of adduct formation and MS/MS metastable and collision-induced dissociation spectra of the adducts. J Phys Chem, 100:15794~15799

1996JOH/HUD Johnson R D, Hudgens J W. 1996. Structural and thermochemical properties of hydroxymethyl (CH_2OH) radicals and cations derived from observations of electronic spectra and from ab inotion calculations. J Phys Chem, 100:19874~19890

1996JON Jonsson M. 1996. Thermochemical properties of peroxides and peroxyl radicals. J Phys Chem, 100:6814~6818

1996JUN/SEI Jungkamp T P W, Seinfeld J H. 1996. The enthalpy of formation of trioxy radicals ROOO (R=H, CH_3, C_2H_5). An ab initio study. Chem Phys Lett, 257:15~22

1996KAI/WAL Kaiser E W, Wallington T J. 1996. Kinetics of the reactions of chlorine atoms with C_2H_4 and C_2H_2: A determination of heat of formation for C_2H_3. J Phys Chem, 100:4111~4119

1996LEE/DEP Lee H L, DePuy C H, Bierbaum V M. 1996. Reactivity and thermochemistry of

quadricyclane in the gas phase. J Am Chem Soc, 118:5068~5073

1996LEE/LI Leeck D T, Li R, Chyall L J, Kenttamma H I. 1996. Homolytic Se–H bond energy and ionization energy of benzeneselenol and the acidity of the corresponding radical cation. J Phys Chem, 100:6608~6611

1996LI/RAN Li Q, Ran Q, Xhen C, Yu S, Ma X, Sheng L, Zhang Y, Li W K. 1996. Experimental and theoretical study of the photoionization and dissociative photoionizations of carbon tetrachloride. Int J Mass Spectrom Ino Proc, 153:29~36

1996LI/RAN(b) Li Q X, Ran Q, Chen C X, Sheng L S, Yu S Q, Zhang Y W, Ma X X. 1996. Photoionization studies of dibromomethane using synchrotron radiation. Chem J Chinese Univ, 17:264~268

1996LI/RAN(c) Li Q, Ran Q, Shen L, Chen C, Guo H, Zhang Y, Yu S, Ma X. 1996. Photoionization studies of CCl_4 using synchrotron radiation: The measurements of ionic formation enthalpies and bond energies. Chinese J Chem Phys, 9:12~17

1996LI/RAN(d) Li Q, Ran Q, Shen L, Chen C, Gao H, Zhang Y, Yu S, Ma X. 1996. Kinetic studies of CH_2Cl_2 photoionization using synchrotron radiation. Acta Physico-Chimica Sinica, 12:136~140

1996LIU/BOR Liu W Z, Bordwell F G. 1996. Gas-phase and solution-phase homolytic bond dissociation energies of H–N bonds in the conjugate acids of nitrogen bases. J Org Chem, 61:4778~4783

1996LOV/HAN Lovejoy E R, Hanson D R, Huey L G. 1996. Kinetics and products of the gas-phase reaction of SO_3 with water. J Phys Chem, 100:19911~19916

1996LUC/PED Lucarini M, Pedrielli P, Pedulli G F, Cabiddu S, Fattuoni C. 1996. Bond dissociation energies of O–H bonds in substituted phenol from equilibration studies. J Org Chem, 61:9259~9263

1996MEB/DIA Mebel A M, Diau E W, Lin M C, Morokuma K. 1996. Ab initio and RRKM calculations for multichannel rate constants of the $C_2H_3 + O_2$ reaction. J Am Chem Soc, 118:9759~9771

1996MIY/OZA Miyokawa K, Ozaki S, Yano T. 1996. Kinetics of the photobromination of fluoroethane. Estimate of the C–H bond dissociation energies and the heats of formation of the CH_3CHF and CH_2CH_2F radicals. Bull Chem Soc Jpn, 69:869~873

1996MOR/ASH Mordaunt D H, Ashfold M N R, Dixon R N. 1996. Photodissociation dynamics of (A) over-tilde state amimonia molecules. 1. State dependent μ-v correlations in the $NH_2(ND_2)$ products. J Chem Phys, 104:6460~6471

1996NIC/WAN Nicovich J N, Wang S, McKee ML, Wine P H. 1996. Kinetics and thermochemistry of the $Cl + C_2Cl_4$ association reaction. J Phys Chem, 100:680~688

1996ORL/TYN Orlando J J, Tyndall G S. 1996. Rate coefficients for the thermal decomposition of $BrONO_2$ and the heat of formation of $BrON_2$. J Phys Chem, 100:19398~19405

1996SEE Seetula J A. 1996. Kinetics and thermochemistry of the R + HBr = RH + Br (R = CH_2Cl, $CHCl_2$, CH_3CHCl, or CH_3CCl_2) equilibrium. J Chem Soc Faraday Trans, 92:3069~3078

1996SKO/DYM Skorobgatov G A, Dymov B P, Nedozrelova I V. 1996. Equilibrium constants and rate constants for the reactions RBr = R + BrI, Br + RBr = Br_2 + R (R = CH_2Cl, C_2Cl, $CHCl_2$, CCl_3, $CBrF_2$) at 300~700 K. Russ J Gen Chem, 66:1824~1833

1996SKO/DYM(b) Skorobgatov G A, Dymov B P, Nedozrelova I V. 1996. Equilibrium constants and rate constants for the reactions RI = R + I, I + RI = I_2 + R (R = CH_2Cl, CH_2I) at 300~700 K. Russ J Gen Chem, 66:1834~1840

1996STA/ZAR Stanciuc G, Zarna N, Spataru N, Constantinescu T, Caragheorgheopol A, Caldararu H. 1996. Factors affecting stability and equilibria of free radicals. XXII. Bond dissociation energy of N-alkoxypolynitroanilines. Revue Roum Chim, 41:755~761

1996TER/KAB Terentis A C, Kable S H. 1996. Near threshold dynamics and dissociation energy of the reaction H_2CO = HCO + H. Chem Phys Lett, 258:626~632

1996TSA Tsang W. 1996. Heats of formation of organic free radicals by kinetic methods. *In:* Energetics of Organic Free Radicals, Simoes J A M, Greenberg A, Liebman J F eds. New York: Blackie Academic & Professional, 22~58

1996TUM/DEN Tumanov V E, Denisov E T. 1996. Estimation of the dissociation energy of C–H bonds in oxygen-containing compounds using a transition state model resulting from the intersection of two Morse potential curves. Z. Fizicheskoi Khimii, 70:801~806

1996WAY/LUS Wayner D D M, Lusztyk E, Ingold K U. 1996. Application of photoacoustic calorimetry to the measurement of the O–H bond strength in vitamin E (alpha- and delta-) and related phenolic antioxidants. J Org Chem, 61:6430~6433

1996WEN/HU Wenthold P W, Hu J, Squires R R. 1996. o, m-, and p-Benzyne negative ions in the gas-phase: Synthesis, authentication, and thermochemistry. Photoelectron spectroscopy of the ally and 2-methylally anions. J Am Chem Soc, 118:11865~11871

1996WEN/POL Wenthoild P W, Polak M L, Lineberger W C. 1996. Photoelectron spectroscopy of the allyl and 2-methylally anioins. J Phys Chem, 100:6920~6926

1996WIL/HOW Wilson S H S, Howe J D, Ashfold M N R. 1996. On the near ultraviolet photodissociation of hydrogen sulfide. Mol Phys, 88:841~858

1996ZAR/WES Zarcharah M R, Westmoreland P R, Burgess D R, Tsang W, Melius C F. 1996. BAC-MP4 predictions of thermochemical data for C1 and C2 stable and radical. J Phys Chem, 100:8737~8747

1996ZEN/PER Zengin V, Persson B J, Strong K M, Continetti R E. 1996. Study of the low-lying electronic states of CCO by photoelectron spectroscopy of CCO^- and ab intio calculations. J Chem Phys, 105:9740~9747

1996ZHA/BOR Zhang X M, Bordwell F G. 1996. beta-Sily effects on the stabilities of carbanions and carbon-centered radicals derived from ethyl thionacetates, diethyl malonates, and ethyl acetoacetates. J Org Chem, 61:51~54

1996ZHA/FRY Zhang X M, Fry A J, Bordwell F G. 1996. Equilibrium acidities and homolytic bond dissociation enthalpies of the acidic C–H bonds in p-(para-substituted benzyl)triphenylphosphonium cations and related cations. J Org Chem, 61:4101~4106

1996ZHA/SHE Zhang Y, Sheng L, Qi F, Gao H, Yu S. 1996. Photoionization studies of some small molecules. J Electron Spectros Relat Phenomena, 79:483~485

1996ZYR/DRO Zyrianov M, Droz-Georget T, Sanov A, Reisler H. 1996. Competitive photodissociation channels in jet-cooled HNCO: Thermochemistry and near-threshold predissociation. J Chem Phys, 105:8111~8116

1997ARN/FLO Arnett E M, Flowers R A, Ludwig R T, Meekhof A E, Walek S A. 1997 Triarymethanes and 9-arylxathenes as prototye amphihydric compounds for relating the stabilities of cations, anions and radicals by C–H bond cleavage and electron transfer. J Phys Org Chem, 10:499~513

1997ASH/APP Asher R L, Appelman E H, Tilson J L, Litorja M, Berkowitz J, Ruscic B. 1997. A photoionization study of trifluomethanol (CF_3OH), trifluoroethyl hypofluorine (CF_3OF), and trifluoromethyl hypochlorite (CF_3OCl). J Chem Phys, 106:9111~9121

1997ASH/RUS Asher R L, Ruscic B. 1997. On the heats of formation of trifluoromethyl radical CF_3 and its cation CF_3^+. J Chem Phys, 106:210~221

1997BAB/VIS Baba M S, Viswanathan R, Gingerich K A. 1997. High temperature mass spectrometric studies of molecules containing silicon, boron and nitrogen. *In:* Proceeding — Electrochemical Society, High temperature materials chemistry, 6. 689~694

1997BEC/CAR Becerra R, Carpenter I W, Walsh R. 1997. Time-resolved studies of the kinetics of the reactions of CHO with HI and HBr: Thermochemistry of the CHO radical and the C–H

bond strengths in CH_2O and CHO. J Phys Chem A, 101:4185~4190

1997BEN/COH Benson S W, Cohen N. 1997. The thermochemistry of peroxides and polyoxides, and their free radicals, *In:* Peroxyl Radicals. Alfassi Z B ed. New York: Wiley, 49~68

1997BOR/ZHA Bordwell F G. Zhang X M, Eventova I, Rappoport Z. 1997. Acidities of stable simple enols and bond dissociation enthalpies of their H–O bonds in DMSO. J Org Chem, 62:5371~5373

1997CAC/PET Cacace F, de Petris G, Pepi F. 1997. Gas-phase NO^+ affinities. Proc Natl Sci USA, 94:3507~3512

1997CHE/LIU Cheng J P, Liu B, Lu Y, Mi J L, Huan Z W. 1997. Homolytic and heterolytic C–H bond dissociation energies of alpha V(or VI)- group cation-substituted toluenes and acetophenones. Gaodeng Xuexiao Huaxue Xuebao, 18:1080~1085

1997CHE/WAN Cheng J P, Wang D, Mi J, Yin Z. 1997. Effect of adjacent electron pair on the thermodynamic stabilities of some netrogen-centered radicals and anions. Chinese J. Bull. 42:1538~154

1997CIO/LIU Cioslowski J, Liu G, Moncrieff D. 1997. Thermochemistry of homolytic C–C, C–H, and C–Cl bond dissociations in polychloroethanes: Benchmark electronic structure calculations. J Am Chem Soc, 119:11452~11457

1997CLI/WEN Clifford E P, Wenthold P G, Lineberger W C, Petersson G A, Ellison G B. 1997. Photoelectron spectroscopy of the NCN- and HNCN- ions. J Phys Chem A, 101:4338~4345

1997CRE/MAY Crevier T J, Mayer J M. 1997. C–O bond homolysis in a tungsten alkoxide: The mechanism of alcohol deoxygenation by $WCl(PMe_3)_4$ and $WH_2Cl_2(PMe_3)_4$. J Am Chem Soc, 119:8485~8491

1997DOB/BEN Dobis O, Benson S W. 1997. Temperature coefficients of rate of ethyl radical reactions with HBr and Br and Br in the 228~368 K temperature range at millitorr pressures. J Phys Chem A, 101:6030~6042

1997DOR/PUG Dorrestijn E, Pugin R, Nogales M V C, Mulder P. 1997. Thermal decomposition of chromam. Reactivity of o-quinone methide. J Org Chem, 62:4804~4810

1997ELL/DAV Ellison G B, Davico G E, Bierbaum V M, DePuy C H. 1997. Thermochemistry of the benzyl and allyl radicals and ions. Int J Mass Spectrom Ion Proc, 156:109~131

1997FUL/HAM Fulle D, Hamann H F, Hippler H, Jansch C P. 1997. The high-pressure range of the addition of OH to C_2H_2 and C_2H_4. Ber Bunsenges Phys Chem, 101:1433~1442

1997HAR/EMR Hare M, Emrick T, Eaton P E, Kass S. 1997. Cubyl anion formation and an experimental determination of the acidity and C–H bond dissociation energy of cubane. J Am Chem Soc, 119:237~238

1997JAN/ZHO Janaway G A, Zhong M, Gatev G G, Chabinyc M L, Brauman J L. 1997. $[FHNO]^-$: An intermediate in a spin-forbidden proton transfer reaction. J Am Chem Soc, 119:11697~11698

1997JPL DeMore WB, Sander S P, Golden D M, Hampson R F, Kurylo M J, Howard C J, Ravishankara A R, Kolb C E, Molina M J. 1997. Chemical Kinetics and Photochemical Data for Use in Stratospheric Modelling, JPL Publication 97-4, http://jpldataeval.jpl.nasa.gov

1997KIE/ZHA Kiefer J H, Zhang Q, Kern R D, Yao J, Jursic B. 1997. Pyrolysis of aromatic azines. Pyrazine, pyrimidine, and pyridine. J Phys Chem A, 101:7061~7073

1997KNY/BEN Knyazev V D, Bencsura A, Slagle I R. 1997. Unimolecular decomposition of the FCO radical. J Phys Chem A, 101:849~852

1997KRA/KAL Krasnoperov L N, Kalinovski I J, Niiranen J T, Gutman D. 1997. Kinetics and thermochemistry of SiH_3 + NO and SiD_3 + NO reactions: Pressure falloff and SiH_3–NO bond energy. J Phys Chem A, 101:4929~4938

1997LAA/BOR Laarhoven L J J, Born J G P, Arends I W C E, Mulder P. 1997. Substituent effects on

the benzylic bond dissociation enthalpy in benzyl bromides (C–Br) and tert-butylbenzenes (C–CH_3): A gas phase thermolysis and liquid phase photoacoustic study. J Chem Soc, Perkin Trans 2, 2307~2312

1997LAA/MUL Laarhoven L J J, Mulder P. 1997. alpha-C–H bond strengths in tetralin and THF. Application of competition experiments in photoacoustic calorimetry. J Phys Chem B, 101:73~77

1997LIN/LIF Ling Y, Lifshitz C. 1997. C–H bond energy of the triphenylene radical cation. A photoionization mass spectrometry study. J Mass Spectrom, 32:1219~1225

1997LIT/RUS Litorja M, Ruscic B. 1997. Evidence of rotational autoionization in the threshold region of the photoionization spectrum of CH_3. J Chem Phys, 107:9852~9856

1997LIU/HUA Liu B, Huan Z W, Cheng J P. 1997. Thermodynamic stability of ylides and their corresponding radicals. Acta Chim Sinica, 55:123~128

1997LOV Lovejor E R. 1997. Kinetics and thermodynamics of the gas phase reaction $SO_3 + NH_3 + N_2 = H_3NSO_3 + N_2$. J Phys Chem A, 101:4950~4953

1997MAC/WAY MacFaul P A, Wayner D D M, Ingold K U. 1997. Measurement of N–H bond strengths in aromatic amines by photoacoustic calorimetry. J Org Chem, 62:3413~3414

1997MIT/TOS Mitrushenkov A, Tosi P, Bassi D. 1997. Dissociation energies and heats of formation of NH and NH^+. J Chem Phys, 106:10265~10272

1997OSB/MOR Osborn D L, Mordaunt D H, Choi H, Bise R T, Neumark D M. 1997. Photodissociation spectroscopy and dynamics of the HCCO free radical. J Chem Phys, 106:10087~10098

1997PAR/DYA Park J, Dyakov I V, Mebel A .M, Lin M C. 1997. Experimental and theoretical studies of the unimolecular decomposition of nitrosobenzene: High-pressure rate constants and the C–N bond strength. J Phys Chem A, 101:6043~6047

1997PON/TAK Ponomarev D, Takhistov V. 1997. Some regularities in the relative thermodynamic stability of free radicals. J Mol Struct, 435:259~274

1997POU/NAS Poutsma J C, Nash J J, Paulino J A, Squires R R. 1997. Absolute heats of formation of phenylcarbene and vinylcarbene. J Am Chem Soc, 119:4686~4697

1997POU/PAU Poutsma J C, Paulino J A, Squires R R. 1997. Absolute heats of formation of CHCl, CHF, and CClF. A gas-phase experimental and G2 theroretical study. J Phys Chem A, 101:5327~5336

1997ROM/JAN Romer B, Janaway G A, Brauman J I. 1997. Cyclopentadieny, indenyl, and fluorenyl anions: Gas-phase and solvation energy contributions to electron detachment energies. J Am Chem Soc, 119:2249~2254

1997RUC/GER Ruchardt C, Gerst M, Ebenhoch J. 1997. Uncatalyzed transfer hydrogenation and transfer hydrogenenolysis: Two novel types of hydrogen-transfer reactions. Angew Chem Int Ed Engl, 36:1407~1430

1997SCH/DOR van Scheppingen , W, Dorrestijn E, Arends I, Mulder P. 1997. C–O bond strength in diphenyl ether and phenyl vinyl ether: An experimental and computation study. J Phys Chem A, 101:5404~5411

1997SCH/VER Schaffer F, Verevkin S P, Rieger H J, Beckhaus H D, Ruchardt C. 1997. Geminal substituent effects. 15. Enthalpies of formation of a series of fluorinated hydrocarbons and strain-free group increments to assess ploar and anomeric stabilization and strain. Liebigs Ann/Recueil, 1333~1344

1997SEE/SLA Seetula J A, Slagle I R. 1997. Kinetics and thermochemistry of the R + HBr = RH + Br (R = n-C_3H_7, iso-C_3H_7, n-C_4H_9, iso-C_4H_9, sec-C_4H_9 or tert-C_4H_9) equilibrium. J Chem Soc Faraday Trans, 93:1709~1719

1997SHE/QI Sheng L, Qi F, Gao H, Zhang Y, Yu S, Li W K. 1997. Experimental and theoretical study of the photoionization and dissociative photoionizations of dichlorodifluoromethane. Int J Mass Spectrom Ion Proc, 161:151~159

1997TOM/HOP Tomaszkiewicz I, Hope G A, O'Hare P A G. 1997. A fluorine bomb calorimetric determination of the standard molar enthalpy of formation of silicon disulfide SiS_2 (cr) at the temperature 298.15 K. Enthalpies of dissociation of Si–S bonds. J Chem Thermodyn, 29:1031~1045

1997VER Verevkin S P. 1997. Thermochemistry of nitro compounds. Experimental standard enthalpies of formation and improved group-additivity values. Thermochimica Acta, 307:17~25

1997VER(b) Verevkin S P. 1997. Thermochemistry of amines: experimental standard molar enthalpies of formation of some aliphatic and aromatic amines. J Chem Thermodyn, 29:891~899

1997WAY/CLA Wayner D D M, Clark K B, Rauk Yu D, Armstrong D A. 1997. C–H bond dissociation energies of alkyl amines: Radical structures and stabilization energies. J Am Chem Soc, 119:8925~8932

1997WEL/BEC Welle F M, Beckhaus H D, Ruchardt C. 1997. Thermochemical stability of alpha-amino-alpha-carbonylmethyl radicals and their resonance as measured by ESR. J Org Chem, 62:552~558

1997WEN/KIM Wenthold P G, Kim J B, Jonas K L, Lineberger W C. 1997. An experimental and computational study of the electron affinity of boron oxide. J Phys Chem A, 101:4472~4474

1997WRI/CAR Wright J S, Carpenter D J, McKay D J, Ingold K U. 1997. Theroretical calculation of substituent effects on the O–H bond strength of phenolic antioxidants related to vitamin E. J Am Chem Soc, 119:4245~4252

1997ZHA/BOR Zhao Y, Bordwell F D, Cheng J P, Wang D. 1997. Equilibrium acidities and homolytic bond dissociation energies (BDEs) of the acidic H–N bonds in hydrazines and hydrazides. J Am Chem Soc, 119:9125~9129

1997ZHA/CHE Zhao H Q, Cheung Y S, Liao C L, Liao C X, Ng C Y, Li W K. 1997. A laser photofragmentation time-of-flight mass spectrometric study of acetophenone at 193 and 248 nm. J Chem Phys, 107:7230~7241

1997ZHA/CHE(b) Zhao H Q, Cheung Y S, Heck D P, Ng C Y, Tetzlaff T, Jenks W S. 1997. A 193-nm-laser photofragmentation time-of-flight mass spectrometric study of dimethylsulfoxide. J Chem Phys, 106:86~93

1997ZHA/LIN Zhao R, Lind J, Merenyi G, Eriksen T E. 1997. Significance of the intramolecular transformation of glutathione thiyl radicals to alpha-aminoalkyl radicals. Thermochemical and biological implications. J Chem Soc Perkin Trans 2, 569~574

1997ZHU/ZHA Zhu Q, Zhang X M, Fry A J. 1997. Bond dissociation energies of antioxidants. Polymer Degrad Stability, 57:43~50

1998ANN/FRA Anne A, Fraoua S, Grass V, Moiroux J, Saveant J M. 1998. The role of homolytic bond dissociation energy in the deprotonation of cation radicals. Examples in the NADH analogues series. J Am Chem Soc, 120:2951~2958

1998AUB/HOL Aubry C, Holmes J C, Walton J C. 1998. 1- and 2- adamanty radicals and cations in the gas phase: Thermochemistry and mass spectrometry. J Phys Chem A, 102:1389~1393

1998BEC/BOG Becerra R, Boganov S E, Egorov M P, Faustov, V I, Nefedov O M, Walsh R. 1998. The protope Ge–H insertion reaction of germylene with germane. Absolute rate constants, temperature dependence, RRKM modeling and the potential energy surface. J Am Chem Soc, 120:12657~12665

1998BEC/WAL Becerra R, Walsh R. 1998. Thermochemistry. *In:* The Chemistry of Organic Silicon Compounds, vol. 2. Rappoport Z. and Apeloig Y ed. New York: Wiley, 1998. Chapter 4, 153~180

1998BER/CAR Berho F, Caralp F, Rayez M T, Lesclaux R. 1998. Kinetics and thermochemistry of the

reversible combination reaction of the phenoxy radical with NO. J Phys Chem A, 102:1~8

1998BOR/LIU Bordwell F G, Liu W Z. 1998. Effects of sulfenyl, sulfinyl and sulfonyl groups on acidities and homolytic bond dissociation energies of adjacent C–H and N–H bonds. J Phys Org Chem, 11:397~406

1998BOR/ZHA Bordwell F G, Zhao Y, Cheng J P. 1998. Equilibrium acidities and homolytic bond dissociation enthalpies of m- and p-substituted benzaldoximes and phenyl methyl ketoximes. J Phys Org Chem, 11:10~14

1998BRO/BEC Brocks J. Beckhaus H D, Athelstane LJ B, Ruchardt C. 1998. Estimation of bond dissociation energies and radical stabilization energies by ESR spectroscopy. J Org Chem, 63:1935~1943

1998CHA Chase M W Jr. 1998. NIST-JANAF Thermochemical Table. 4th ed. J Phys Chem Ref Data, Monograph 9

1998CHE/LIU Cheng J P, Liu B, Zhang X M. 1998. Radical substituent effects of alpha-sulfonium groups. J Org Chem, 63:7574~7575

1998CHE/LIU(b) Cheng J P, Liu B, Zhao Y, Zgang X M. 1998. Equilibrium acidities and homolytic bond dissociation enthalpies of the acidic C–H bonds in As-substituted triphenylarsonium and related catrions. J Org Chem, 63:7072~7077

1998CHE/LU Cheng J P, Lu Y, Liu B, Zhao Y, Wang D, Sun Y, Mi J. 1998. Effects of double substitution on the thermodynamic stabilities of nitrogen radicals. Science in China Ser. B, 41:215~224

1998CHE/WAN Cheng J P, Wang K, Yin Z, Lu Y. 1998. NO affinity. The driving force of nitric oxide (NO) transfer in biomimetic N-nitrosoacetanilide and N-nitrososulfoanilide systerms. Tetrahedron Lett, 39:7925~7928

1998CHE/XIA Cheng J P, Xian M, Wang K, Zhu X. 1998. Heterolytic and homolytic Y–NO bond energy scales of nitroso-containing compounds: Chemical origin of NO release and NO capture. J Am Chem Soc, 120:10266~10267

1998CLI/WEN Clifford E P, Wenthold P G, Gareyev R, Lineberger W C, DePuy C H, Bierbaum V M, Ellison G B. 1998. Photoelectron spectroscopy, gas phase acidity, and thermochemistry of tert-butyl hydroperoxide: Mechanisms for the rearrangement of peroxyl radicals. J Chem Phys, 109:10293~10310

1998CLI/WEN(b) Clifford E P, Wenthold P G, Lineberger W C, Petersson G A, Broadus K M, Kass S R, Kato S, DePuy C H, Bierbaum V M, Ellison G B. 1998. Properties of diazocarbene [CNN] and the diazomethyl radical [HCNN] via ion chemistry and spectroscopy. J Phys Chem, 102:7100~7112

1998CLI/WEN(c) Clifford E P, Wenthold P G, Lineberger W C, Ellison G B, Wang C X, Grabowski J J, Vila F, Jordan K D. 1998. Properties of tetramethyleneethane (TME) as revealed by ion chemistry and photoelectron spectroscopy. J Chem Soc Perkin Trans 2, 5:1015~1022

1998COL/GRE Colussi A J, Grela M A. 1998. Thermochemical kinetics of bromine nitrate, bromine nitrite, halogen hydroperoxides, dichlorine pentoxide, peroxycarboxylic acids, and diacyl peroxides. Int J Chem Kinet, 30:41~45

1998COU/MON Courty A, Mons M, Dimicoli I, Piuzzi F, Brenner V, Millie P. 1998. Ionization, energies, and geometry of the phenol-A complexes (S = H_2O, CH_3OH, and CH_3OCH_3). J Phys Chem A, 102:4890~4898

1998DEN Denisov E T. 1998. The reactivity of silanes in free radical reactions: Analysis in terms of the parabolic model of the transition state. Russ Chem Bull, 47:1274~1279

1998DET/ERV DeTuri V F, Ervin K M. 1998. Proton transfer between Cll- and C_6H_5OH. O–H bond energy of phenol. Int J Mass Spectrom Ion Proc, 175:123~132

1998DOS/SIM dos Santos R M B, Simoes J A M. 1998. Energies of the O–H bond in phenol and

substituted phenols: A critical evaluation of literature data. J Phys Chem Ref Data, 27:707~739

1998HAD/RAB Hadad C M, Rablen P, Wiberg K B. 1998. C–O and C–S bonds: Stability, bond dissociation energies, and resonance stabilization. J Org Chem, 63:8668~8681

1998HUN/LIA Hunter E P L, Lias S G. 1998. Evaluated gas phase basicities and proton affinities of molecules: An update. J Phys Chem Ref Data, 27:413~656

1998JON/WAY Jonsson M, Wayner D D M, Armstrong D A, Yu A, Eauk A. 1998. On the thermodynamics of peptide oxidation: Anhydrides of glycine and alanine. J Chem Soc Perkin Trans 2, 1967~1972

1998KNY/BEN Knyazev V D, Benesura A, Slagle I R. 1998. Kinetics and thermochemistry of the reactions of CH_3CCl_2 and $(CH_3)_2CCl$ radicals with molecular oxygen. J Phys Chem A, 102:1760~1769

1998KNY/SLA Knyazev V D, Slagle I R. 1998. Thermochemistry and kinetics of the reaction of 1-methylally radicals with molecular oxygen. J Phys Chem A, 102:8932~8940

1998KNY/SLA(b) Knyazev V D, Slagle I R. 1998. Thermochemistry of the $R–O_2$ bond in alkyl and chloroalkyl peroxy radicals. J Phys Chem A, 102:1770~1778

1998KOT/MAR Kothe T, Marque S, Martschke R, Popov M, Fischer H. 1998. Radical reaction kinetics during homolysis of N-alkoxyamines: Verification of the persistent radical effect. J Chem Soc Perkin Trans 2, 1553~1559

1998LEB/CHI Lebedev V P, Chironov V V, Vorob'eva V P, Matyushin Yu N. 1998. Energy of the dissociation of the bond N–NO in methylnitrosohydrazine. Khim Fiz, 17:54~57

1998LI/LUO Li G, Luo L, Chen H, Fu S, Zhang S. 1998. Determination of enthalpy and volume changes in photolysis of coenzyme B_{12} using phtoacoustic calorimetry. Wuli Huaxue Xuebao, 14:615~619

1998LIN/MER Lind J, Merenyi G. 1998. Imidyl radicals. *In:* N-Centered. Alfassi ZB ed. New York: Wiley, 563~575

1998LIT/RUS Litorja M, Ruscis B. 1998. A photoionization study of the hydroperoxyl radical, HO_2, and hydrogen peroxide, H_2O_2. *In:* Electron Spectrosc Relat Phenom. 97:131~146

1998MAY Mayer J M. 1998. Hydrogen atom abstraction by metal-oxo complexes: Understanding the analogy with organic radical reactions. Acc Chem Res, 31:441~450

1998MIR/VOR Miroshnichenko E A, Vorob'eva V P, Matyushin Y N. 1998. Energy of the dissociation of the bond N–NO in methylnitrosohydrazine. Khimicheskaya Fizika, 17:29~31

1998NIST NIST Chemistry Webbook. Mallard W G, ed. 1998 to 2004. http://webbook.nist.gov

1998PAD/TSC Paddsison S J, Tschuikow-Roux E. 1998. Structures, vibrational frequencies, thermodynamic properties, and bond dissociation energies of the bromomethanes and bromomethyl radicals: An ab intio study. J Phys Chem A, 102:6191~6199

1998ROM/GAT Romer B, Gatev G G, Zhong M, Brauman J I. 1998. alpha-Stabilization by silyl and phosphino substitution, J Am Chem Soc, 120:2919~2924

1998RUS/MIC Ruscic B, Michael J V, Redfern P C, Curtiss L A, Raghavachari K.1998. Simultaneous adjustment of experimentally based enthalpies of formation of CF_3X, X = nil, H, Cl, Br, I, CF_3, CN and a probe of G3 theory. J Phys Chem A, 102:10889~10899

1998SCH/GIN Schmude R W, Gingerich K A. 1998. Thermodynamic investigation of small germanium-tin clusters with a mass spectrometer. J Chem Phys, 109:3069~3071

1998SCH/WES Schroeter K, Wesendrup R, Schwarz H. 1998. Substituent effects on the bond dissociation energies of cationc arene-trasition-metal complexes. Eur J Org Chem, 1:565~571

1998SEE Seetula J A. 1998. Kinetics and thermochemistry of the R + HBr = RH + Br (R = C_2H_5 or beta-C_2H_4Cl) equilibrium. An ab inyio studt of the bond energies in partly chlorinated ethanes and propanes. J Chem Soc Faraday Trans, 94:891~898

1998SIL/MAT da Silva M D M C R, Matos M A R, Vaz M C, Santos M N B F, Pilcher G, Acree W E Jr, Powell J R. 1998. Enthalpies of combustion of the pyridine N-oxide derivatives: 4-methyl-, 3-cyano-, 3-hydroxy-, 2-carboxy-, 4-carboxy-, and 3-methyl-4-nitro, and of the pyridine derivatives: 2-carboxy-, and 4-carboxy-. The dissociation enthalpies of the N–O bonds. J Chem Thermdyn, 30:869~878

1998SKE/BEL Skene W G, Belt S T, Conolly T J, Hahn P, Scaiano J C. 1998. Decomposition kinetics, Arrhenius parameters, and bond dissociation energies for alkoxyamines of relevance in "living" free radical polymerization. Macromolecules, 31:9103~9105

1998SKO/DYM Skorobogatov G A, Dymov B P, Sterba R, Tschuikow-Roux E. 1998. Molecular, thermodynamic, and kinetic parameters of $CClF_2CClHFl$ and $CClF_2CHF$ radicals in the gas phase. Russ J Gen Chem, 68:1104~1111

1998SMI Smith D W. 1998. Comment on "Heats of formation of alkyl fluorides". J Phys Chem A, 102:7086~7087

1998SRI/ARU Srivatsava A, Arunan E, Manke G, Setser D W, Sumathi R. 1998. Unimolecular reaction dynamics of CH_3COCl and FCH_2COCl: An infrared chemiluminescence and ab initio study. J Phys Chem A, 102:6412~6420

1998WEN/SQU Wenthold P G, Squires R R. 1998. Gas-phase acidities of o-, m- and p-dehydrobenzoic acid acid radicals. Determination of the substituted constants for a phenyl radical site. J Mass Spectrom Ion Proc, 175:215~224

1998YAN/JIA Yang J, Jian H, Zheng G, Xu G. 1998. Study on the O–H bond dossociation energies in chlorophenols by pulsed laser photoacoustic calorimetry. Fenxi Ceshi Tuebao, 17(5):1~4

1998ZHA/LIN Zhao R, Lind J, Merenyi G, Eriksen T E. 1998. One-electron redox potential of thiobenzoic acid. Kinetic characteristics of benzoylthiyl radical beta-fragmentation. J Am Chem Soc, 120:2811~2816

1999ABB/NOT Abboud J L M, Notario R. 1999. FT-ICR. Basic principles and some representative applications. *In:* Energetics of Stable Molecular and Reactive Intermediates, NATO Sci. Ser. C:535:281~302

1999AHM/PET Ahmed M, Peterka D S, Suits A G. 1999. The photodissociation of the vinyl radical (C_2H_3) at 243 nm studies by velocity map imaging. J Chem Phys, 110:4248~4253

1999AND Anderson W R. 1999. Heats of formation of HNO and some related species. Combust. Flame, 117:394~403

1999ARM Armstrong D A. 1999. Thermochemistry of sulfur-centered radicals. *In:* S-Centered Radicals. Alfassi ZB ed. New York: Wiley, Chapter 2, 27~61

1999ARM(b) Armstrong D A. 1999. Thermochemistry of N-centered radicals. *In:* N-Centered Radicals, Alfassi ZB ed. New York: Wiley, Chapter 23, 685~710

1999ATK/BAU Atkinson R, Baulch D L, Cox R A, Hampson R F Jr, Kerr J A, Rossi M J, Troe J. 1999. Evaluated kinetic and photochemical data for atmospheric chemistry, organic species: Supplement 7. J Phys Chem Ref Data, 28:191~393

1999BIS/CHO Bise R T, Choi H, Neumark D M. 1999. Photodissociation dynamics of the singlet and triplet states of the NCN radical. J Chem Phys, 111:4923~4932

1999BIS/CHO(b) Bise R T, Choi H, Perdson H B, Mordaunt D H, Neumark D M. 1999. Photodissociation spectroscopy and dynamics of the methylthio radical (CH_3S). J Chem Phys, 110:805~816

1999BIZ/CAB Bizarro M M, Cabral B C C, dos Santos R M, Simoes J A M. 1999. Substituent effects on the O· H bond dissociation enthalpies in phenolic compounds: agreements and controversies. Pure Appl Chem, 71:1249~1256

1999BRA/MAC Bravo R, Machado F B C. 1999. Dissociation energy of the grouns state of PCl. Chem Phys Lett, 307:511~517

1999BRO/KAS Broadus K M, Kass S R. 1999. Benzocyclobutenone enolate: an anion with an antiaromatic resonance structure. J Chem Soc Perkin Trans 2, 2389~2396

1999BUR Burcat A. 1999. Thermodynamic properties of ideal gas of nitro and nitrate energetic compounds. J Phys Chem Ref Data, 28:63~130

1999CHE/WEL Chen E C M, Welk N, Chen E S, Wentworth W E. 1999. Electron affinity, gas-phase acidity, bond dissociation energy, and negative ion states of nitromethane. J Phys Chem A, 103:9072~9079

1999CIR/KOR Ciriano M V, Korth H G, van Scheppingen W B, Mulder P. 1999. Thermal stability of 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) and related N-alkoxyamines. J Am Chem Soc, 121:6375~6381

1999COH Cohen N. 1999. Thermochemistry of organic free radicals. *In:* General Aspects of the Chemistry of Radicals. Alfassi ZB ed. New York: Wiley, 317~345

1999DET/ERV DeTuri V F, Ervin K M. 1999. Competitive threshold collision-induced dissociation: gas-phase acidities and bond dissociation energies for a series of alcohols. J Phys Chem, 103:6911~6920

1999DOM/DIN Dombrowski G W, Dinnocenzo J P, Farid S, Goodman J L, Gould I R. 1999. alpha-C–H bond dissociation energies of some tertiary amines. J Org Chem, 64:427~431

1999DOR/HEM Dorrestijn E, Hemmink S, Hulstman G, Monnier L, van Scheppingen W, Mulder P. 1999. The reduction of alpha-X-acetophenones (X=PhO, Br, Cl) in hydrogen-donating solvents at elevated temperatures. Eur J Org Chem, 3:607~616

1999FLO/DAV Flores H, Davalos J Z, Abboud J L M, Castano O, Gomperts R, Jimenez P, Notario R, Roux M V. 1999. The standard enthalpy of formation of the 1-adamantyl cation in the gas phase. An experimental and ab initio re-assessment. J Phys Chem A, 103:7555~7557

1999HEE/KOR de Heer M I, Korth H G, Mulder P. 1999. Poly methoxy phenols in solution: O–H bond dissociation enthalpies, structures, and hydrogen bonding. J Org Chem, 64:6969~6975

1999HUN/GRA Hung R R, Grabowski J J. 1999. Listening to reactive intermediates: Application of photoacoustic calorimetry to vitamin B_{12} compounds. J Am Chem Soc, 121:1359~1364

1999JUR Jursic B S. 1999. High level ab initio and density functional theory study of bond dissociation energy and enthalpy of formation for hypochloric and hypobromic acids. J Mol Struc (Theochem.), 467:173~179

1999KIM/WEN Kim J B, Wenthold P G, Lineberger W C. 1999. Ultraviolet photoelectron spectroscopy of o-, m-, and p-halobenzyl anions. J Phys Chem A, 103:10833~10841

1999LAA/MUL Laarhoven L J J, Mulder P, Wayner D D M. 1999. Determination of bond dissociation enthalpies in solution by photoacoustic calorimetry. Acc Chem Res, 32:342~349

1999LUC/PED Lucarini M, Pedrielli P, Pedulli G F, Valgimigli L, Gigmes D, Tordo P. 1999. Bond dissociation energies of the N–H bond and rate constants for the reaction with alkyl, alkoxyl, and peroxyl radicals of phenothiazines and related compounds. J Am Chem Soc, 121:11546~11553

1999LUO Luo Y R. 1999. Why is human visual system sensitive only to light of wavelengths from approximately 760 to 380 nm? An answer from thermochemistry and chemical kinetics. Biophys Chem, 83:179~184

1999LUO/CLE Luong A K, Clements T G, Continetti R E. 1999. Three body dissociation dynamics of excited states of $O_3(D_2O)$. J Phys Chem A, 103:10237~10243

1999MCM McMahon T B. 1999. High-pressure mass spectrometry. Instrumentation, techniques and applications. *In:* Energetics of Stable Molecules and Reactive Intermediates. da Piedade MEM ed. Dordrecht: Kluwer Acad Pub, 259~280

1999MEL/VIS Meloni G, Viswanathan R, Gingerich K A. 1999. Experimental and theoretical investigations of the structure and the stability of the BNSi molecule. J Chem Phys,

111:9325~9329

1999MIY/TSC Miyokawa K, Tschuikow-Roux E. 1999. Kinetics of the phtobromination of dichloro- and dibromoethane. Estimate of the C–H bond dissociation energies and the heats of formation of the CH_3CCl_2 and CH_3CBr_2 radicals. Bull Chem Soc Jpn, 72:1~5

1999RUS/LIT Ruscic B, Litorja M, Asher R. 1999. Ionization energy of methylene revisited: Improved values for the enthalpy of formation of CH_2 and the bond dissociation energy of CH_2 via simultaneous solution of the local thermochemical network. J Phys Chem A, 103:8625~8633

1999SAN/LAG dos Sabtos, R M B, Lagoa A L C., Simoes J A M. 1999. Photoacoustic Calorimetry. An examination of a non-classical thermochemistry tool. J Chem Thermodyn, 31:1483~1510

1999SCH/DAV Schwartz R L, Davico G E, Ramond T M, Lineberger W C. 1999. Singlet-triplet splittings in CX_2 (X = F, Cl, Br, I) dihalocarbenes via negative ion photoelectron spectroscopy. J Phys Chem A, 103:8213~8221

1999SEE Seetula J A. 1999. Kinetics and thermochemistry of the $C_3H_5 + HBr = C_3H_6 + Br$ equilibrium. Phys Chem Chem Phys, 1:4727~4731

1999SEN/IKE Sendt K, Ikeda E, Bacskay G B, Mackie J C. 1999. Ab initio quantum chemical and experimental (shock tube) studies of the pyrolysis kinetics of acetonitrile. J Phys Chem A, 103:1054~1072

1999SIL/MAT de Silva MDMCR, Matos M A R, Ferrao M L C C H, Amaral L M P F, Miranda M S, Acree W E Jr, Pilcher G. 1999. Enthalpies of combustion of 2-iodosobenzoic acid and 4-nitrosophenol: The dissociation ethalpy of the I–O bond. J Chem Thermodyn, 31:1551~1559

1999SIM/SIL Simoes J A M, da Silva M A V R. 1999. Experimental methods to derive bond energy data. A schematic overview. *In:* Energetics of Stable Molecules and Reactive Intermediates, NATO Sci . Ser C, 535:1~28

1999TIL Tilset M. 1999. Energetics of transition metal-X bonding probed by electrochemical techniques. *In:* Energetics of Stable Molecules and Reactive Intermediates. da Piedade M E M ed. Dordrecht:Kluwer Acad. Pub, 153~176

1999TSA Tsang W. 1999. Shock tube on the stability of polyatomic molecules and the determination of bond energies. *In.* Energetics of Stable Molecules and reactive Intermediates, NATO Sci Ser C, 535: 323~352

1999VER Verevkin S P. 1999. Strain effects in phenyl-substituted methanes. Geminal interaction between phenyl and the electron-releasing substituent in benzylamines and benzyl alcohols. J Chem Eng Data, 44:1245~1245

1999VER(b) Verevkin S P. 1999. Strain effects in phenyl substituted methanes. Geminal interactions between henyl and alkoxycarbonyl substituent. Thermochimica Acta, 332:27~32

1999VER(c) Verevkin S P. 1999. Thermochemical investigation on alpha-methyl-styrene and parent phenyl substituted alkenes. Thermochimica Acta, 326:17~25

1999VER(d) Verevkin S P. 1999. Thermochemical properties of diphenylalkanes. J Chem Eng Data, 44:175~179

1999WU/SHE Wu G, Sheng L, Gao H, Zhang Y. 1999. Studies on p-aminoazobenzene using photoionization mass spectrum with synchrotron radiation (SR). Wuli Huaxue Xuebao, 15:860~864

1999ZHA/LIN Zhao R, Lind J L, Merenyi G, Eriksen T E. 1999. One-electron reduction potential and the beta-fragmentation of acetylthiyl radical, comparisons with benzoylthiyl radical and the oxygen counterparts. J Phys Chem A, 103:71~74

1999ZHA/XU Zhang J, Xu K, Amaral G. 1999. Ultraviolet photodissociation dynamics of HN_3: the H + N_3 channel. Chem Phys Lett, 299:285~290

1999ZHO/SHE Zhou W, Sheng L, Wu G, Gao H, Qi F, Zhang Y. 1999. Experimental and theoretical study of photoionization and photodissociation of bromoethane. Wuli Huaxue Xuebao, 15:948~951

2000~2004

2000ART/NIZ Artau A, Nizzi E, Hill B T, Sunderlin L S, Wenthold P G. 2000. Bond dissociation energy in trifluoride ion. J Am Chem Soc, 122:10667~10670

2000ATK/BAU Atkinson R, Baulch D L, Cox R A, Hampson R F Jr, Kerr J A, Rossi M J, Troe J. 2000. Evaluated kinetic and photochemical data for atmospheric chemistry. Supplement 8. Halogen species — IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry. J Phys Chem Ref Data, 29:167~266

2000BIS/HOO Bise R T, Hoops A A, Alexandra A, Choi H, Neumark D M. 2000. Photoisomerization and photodissociation dynamics of the NCN, CNN, and HNCN free radicals. ACS Sym. 770, Imaging in Chemical Dynamics. 296~311

2000BOR/ING Born M, Ingemann S, Nibbering N M N. 2000. Thermochemical properties of halogen-substituted methanes, methyl radicals, and carbenes in the gas phase. Int J Mass Spectrom, 194:103~113

2000BRO/KAS Broadus K M, Kass S R, Osswald T, Prinzbach H. 2000. Dodecahedryl anion formation and an experimetal determination of the acidity and C–H bond dissociation energy of dodecahedrane. J Am Chem Soc, 122:10964~10968

2000BRO/KAS(b) Brodus K M, Kass S R. 2000. Benzocyclobutadienyl anion: Formation and energies of an antiaromatic molecule. J Org Chem, 65:6566~6571

2000BRU/CHU Brusa M A, Churio M S, Grela M A, Bertolotti S G, Previtali C M. 2000. Reaction volume and reaction enthalpy upon aqueous peroxodisulfate dissociation: S_2O_8 = $2SO_4$. Phys Chem Chem Phys, 2:2383~2387

2000CHE/BOZ Chen C J, Bozzelli J W. 2000. Kinetic analysis for HO_2 addition to ethylene, propene, and sobutene, and thermochemical parameters of alkyl hydroperoxides and hydroperoxide alkyl radicals. J Phys Chem A, 104:4997~5012

2000CHE/LIU Cheng J P, Liu B, Zhao Y, Wen Z, Sun Y. 2000. Homolytic cleavage energies of R–H bonds centered on carbon atoms of high electrohegativity: First observations of O-type variation on C–H BDEs and the implication for the governing factors leading to the distict O/S patterns of radical substituent effects. J Am Chem Soc, 122:9987~9992

2000CHE/LU Cheng J P, Lu Y, Zhu X Q, Sun Y, Bi F, He J. 2000. Heterolytic and homolytic N–H bond dissociation energies of 4-substituted hantzsch 2,6-dimethyl-1,4-dihydropyridines and the effect of one-electron transfer on the N–H bond activation. J Org Chem, 65:3853~3857

2000COO/LAN Cook P A, Langford S R, Ashfold M N R, Dixon R N. 2000. Angular resolved studies of the Lyman-alpha photodissociation of HCN and DCN: New dynamical insights. J Chem Phys, 113:994~1004

2000CUI/HE Cui J, He Y, Fan B, Wang S. 2000. Stability of perfluoropropylene at high temperature. Huaxue Wuli Xuebao, 13: 649~653

2000DEN/DEN Denisov E T, Denisova T G. 2000. Handbook of Antioxidants, Boca Raton: CRC Press

2000DEN/KHU Denisov E T, Khursan S L. 2000. Strength of C–H bonds in amines and amides and their reactivity toward peroxyl radicals. *In:* Modern Tendencies in Kinetics and Calalysis. Russ. J Phys Chem, 74, Suppl. 3, S491~S497, 2000

2000DIS/BOE Distelrath V, Boesl U. 2000. Mass selective gas phase study of ClO, OClO, ClOO and ClAr by anion-ZEKE-photoelectron spectroscopy. Faraday Discuss, 115:161~174

2000ESP Espinosa-Garcia J. 2000. Theoretical C–H bond dissociation enthalpies for CH_3OCl and

CH_3OBr. Chem Phys Lett, 316:563~568

2000FAR/BUR Farrell G L, Burkey T J. 2000. High-pressure photoacoustic calorimetry of chromium hexacarbonyl: volume of heptane displacement from chromium pentacarbonyl heptane. J Photochem Photobiol A Chem, 137:135~139

2000GIL/TAL Gilles M K, Talukdar R.K, Ravishankara A R. 2000. Rate coefficients for the OH + CF_3I reaction between 271 and 370 K. J Phys Chem A, 104:8945~8950

2000GLA/MAK Glasovac Z, Maksic M E. 2000. Benzocyclobutene: The impact of fusing a stained ring into benzene. J Org Chem, 65:1818~1824

2000GUT/GAL Guthrie J P, Gallant R T. 2000. Thermodynamics of methanesulfonic acid revisited. Can J Chem, 78:1295~1298

2000HAM/WEN Hammad L A, Wenthold P W. 2000. Synthesis, charecterrization, and reactivity of the m-xylylene anion in gas phase. The enthalpy of formation of m-xylylene. J Am Chem Soc, 122:11203~11211

2000HAR/HWA Harich S A, Hwang D W H, Yang X, Lin J M, Yang X, Dixon R N. 2000. Photodissociation of H_2O at 121.6 nm: A state-state dynamical picture. J Chem Phys, 113:10073~10090

2000KIR/KOR Kiraly Z, Kortvelyesi T, Sercs L. 2000. Thermal reaction of 2-methyl-2-butene in the presence of azomethene: Ethalpy of formation of radicals $(CH_3)_2CCH(CH_3)_2$ and tert-C_4H_9. Phys Chem Chem Phys, 3:349~354

2000KOS/MIR Kostikova L M, Miroshnichemko E A, Matyushin Y N. 2000. The energies of bond dissociation and efficient interaction energies in nitroamines. Inter Ann Conf. of ICT, 31st. p. 50/1~50/11, Karlsruhe, Germany

2000KRA/CIR Kranenburg M, Ciriano M V, Cherkasov A, Mulder P. 2000. Carbon-oxygen bond dissociation enthalpies in peroxyl radicals. J Phys Chem A, 104:915~921

2000LAF/SZA Lafleur R D, Szatary B, Baer T. 2000. A photoelectron-photoion coincidence study of the ICH_2CN ion dissociation: Thermochemistry of CH_2CN, $^+CH_2CN$, and ICH_2CN. J Phys Chem A, 104:1450~1455

2000LU/ZHU Lu J M, Zhu X Q, Li Q, He J Q, Xian M, Cheng J P. 2000. Determination of heterolytic and homolytic S – NO bond dissociation energies in acetonitrile. Chem J Chinese Univ, 21:570~572

2000MAT/LEB Matyushin Y N, Lebedev V P, Miroshnichenko E A, Kostikova L M, Inozemcev Y O. 2000. Energy of interaction NO_2-groups in nitro derivatives methane and ethane. Inter Ann Conf of ICT, 31st, p. 51/1~51/8. Karlsruhe, Germany

2000MEL/PIM Melkhanova S V, Pimenova S M, Kolesov V P, Pimerzin A A, Sarkisova V S. 2000. The standard molar enthalpies of formation of some alkyladamantanes. J Chem Thermodyn, 32:1311~1317

2000MEL/SCH Meloni G, Schmude R W, Kingcade J E, Gingerich K A. 2000. Thermodynamic stability of Sn_4, Sn_5, Sn_6, and Sn_7 clusters by Knudsen cell mass spectrometry. J Chem Phys, 113:1852~1856

2000MIR/VOR Miroshnichenko E A, Vorob'eva V P, Matyushin Y N. 2000. Bond dissociation energies for nitro derivatives of methane. Khimicheskaya Fizika, 19(6):40~43

2000MIR/VOR(b) Miroshnichenko E A, Vorob'eva V P, Matyushin Y N. 2000. Bond dissociation energies in polynitroalkanes. Khimicheskaya Fizika, 19(11):78~82

2000PED/COR Pedeconi F F, Coronel E J. 2000. EPR equilibrium study on 4-alkyl substituted phenoxyl radicals. An Asoc Quim Argent, 88: 53~58

2000RAM/DAV Ramond T M, Davico G E, Schwartz R L, Lineberger W C. 2000. Vibronic structure of alkoxy via photoelectron spectroscopy. J Chem Phys, 112:1158~1169

2000REE/KAS Reed D R, Kass S R. 2000. Experimental determination of the alpha and beta C–H bond dissociation energies in naphthalene. J Mass Spectrom, 35:534~539

2000REI/PRA Reints W, Pratt D A. Korth H G, Mulder P. 2000. O–O bond dissociation enthalpy in di(trifluoromethyl) peroxide (CF_3OOCF_3) as determined by very low pressure. Density functional theory computations on O–O and O–H bonds in (fluorinated) derivatives. J Phys Chem A, 104:10713~10720

2000REM/ERV Rempala K, Ervin K M. 2000. Collisional activation of the endoergic hydrogen atom transfer reaction S + H_2 == SH + H. J Chem Phys, 112:4579~4590

2000RUS/LIT Ruscic B, Litorja M. 2000. Photoionization of HOCO revisited: A new upper limit to the diabatic ionization energy and lower limit to the energy of formation. Chem Phys Lett, 316:45~50

2000SEE Seetula J A. 2000. Ab initio study of the transition states for determining the enthalpies of formation of alkyl and halogenated alkyl free radicals. Phys Chem Chem Phys, 2:3807~3812

2000SHI/ERV Shi Y, Ervin K M. 2000. Gas-phase acidity and C–H bond energy of diacetylene. Chem. Phys Lett, 318:149~154

2000SHI/HU Shiell R C, Hu X K, Hu Q J, Hepburn J W. 2000. A determination of the bond dissociation energy D(H – SH):Threshold ion-pair production spectroscopy (TIPPS) of a triatomic molecule. J Phys Chem A, 104:4339~4342

2000SMI/GOL Smith G P, Golden D M, Frenklach M, Moriarty N W, Eiteneer B, Doldenberg M, Bowman C T, Hanson R K, Song S, Gardiner C J, Lissianski V V, Qin Z. 2000. Thermodynamic data. GRI-Mech, http://www.me.berkeley.edu/gri_mech

2000TRA Traeger J C. 2000. Neutral and cationic heats of formation for ketene, methyketene, and imethylketene. Int J Mass Spectrom, 194:261~267

2000VER Verevkin S P. 2000. Strain effects in phenyl substituted methanes. Germinal interactions between phenyl and electron-withdrawing cyano substituent in benzylcyanides. J Chem Thermodyn, 32:207~215

2000WAL/MCC Walton J C, McCarroll A J, Chen Q, Carboni B, Nziengui R. 2000. The influence of boryl substituents on the formation and reactivity of adjacent and vicinal free radical centers. J Am Chem Soc, 122:5455~5463

2000WEN Wenthold P G. 2000. Experimental enthalpy of formation of isonitrile from collision-induced dissociation threshold energy measurements. J Phys Chem A, 104:5612~5616

2000WU/SHE Wu G, Sheng L, Zhang Y, Gao H, Chen Z. 2000. Photoionization and photodissociative ionization of azoxybenzene by vacuum ultraviolet synchrotron radiation (SR). Wuli Huaxue Xuebao, 16:948~951

2000XIA/ZHU Xian M, Zhu X Q, Lu J, Wen Z, Cheng J P. 2000. The first O–NO bond energy scale in solution: Heterolytic and homolytic cleavage enthalpies of O-nitrosyl carboxylate compounds. Organic Lett, 2:265~268

2000YAM/BOZ Yamada T, Bozzelli J W, Lay T H. 2000. Comparisons of CBS-q and G2 calculations on thermodynamic properties, transition states, and kinetics of dimethyl-ether plus O_2 reaction system. Int J Chem Kinet, 37:435~452

2000ZHA/LIN Zhao R, Lind J, Merenyi G, Jonsson M, Reiksen T E. 2000. Reduction potentials and kinetics of beta-fragmentation reactions of 4-substituted benzoylthiyl radicals. J Phys Chem A, 104:8524~8526

2000ZHE/EVA Zheng Z R, Evans D H, Nelsen S F. 2000. Studies of the anodic oxidation of 1,4-iazabicyclo[2.2.2] octane. Reactions of the radical cation. J Org Chem, 65:793~1798

2000ZHU/HE Zhu X Q, He J Q, Li Q, Xian M, Lu J, Cheng J P. 2000. N–NO bond dissociation energies of N-nitroso diphenylamine derivatives (or analogues) and their radical anions: Implications for the effect of reductive electron transfer on N–NO bond activation and for the mechanisms of NO transfer to nitranions. J Org Chem, 65:6729~6735

2001BAR/MAN Bartberger M D, Mannion J D, Powell S C, Stamler J S, Houk K N, Toone E J. 2001. S–

N dissociation energies of S-nitrosothiols: On origins of nitrosothiol decomposition rates. J Am Chem Soc, 123:8868~8869

2001BEC/CAN Becerra R, Cannady J R, Walsh R. 2001. Silylene does react with carbon monoxide: Some gas-phase kinetic and theoretical studies. J Phys Chem A, 105:1897~1903

2001BIS/HOO Bise R T, Hoops A A, Neumark D M. 2001. Photodissociation and photoisomerization pathways of the HNCN free radical. J Chem Phys, 114:9000~9011

2001BLA/RAM Blanksby S J, Ramond T M, Davico G E, Nimlos M R, Kato S, Bierbaum M, Lineberger W C, Ellison G B, Okaumura M. 2001. Negative-ion photoelectron spectroscopy, gas-phase acidity, and thermochemistry of the peroxyl radical CH_3OO and CH_2CH_2OO. J Am Chem Soc, 123:9585~9596

2001BOU/CHA Bouchoux G, Chamot R J, Leblanc D, Mourgues P, Sablier M. 2001. Proton affinity and heat of formation of vinyloxy [CH_2CHO] and acetonyl [CH_2COCH_3] radical. Chem Phys Chem, 2:235~241

2001BOZ/JUN Bozzelli J W, Jung D. 2001. Theoretical investigation on stability of the C center H_2OCl radical. J Phys Chem A, 105:3941~3946

2001CHE/ZHA Chen W, Zhang Y, Sheng L, Gao H, Zhang L. 2001. Study of p-hydroxyazobenzene by photoionization mass spectrum with synchrotron radiation. Huaxue Yanjiu Yu Yingyong, 13:524~526

2001CHI/KEN Chim R Y L, Kennedy R A, Tuckett R P, Zhou W, Jarvis G K, Collins D J, Hatherly P A. 2001. Fragmentation of energy-selected SF5CF3+ probed by threshold photoelectron photoion coincidence spectroscopy: bond dissociation energy of SF_5–CF_3 and its atmospheric implications. J Phys Chem A, 105:8403~8412

2001DAS Das T N. 2001. Absorption spectrum, pKa. and reduction potential of phenoxyl radical from 4,4'-biphenol in aqueous medium. J Phys Chem A, 105:5954~5959

2001DOR/NOV Dorofeeva O, Novikov V P, Neumann D B. 2001. NIST-JANAF thermochemical tables. 1. Ten organic molecules related to atmospheric chemistry. J Phys Chem Ref Data, 30:475~513

2001ERV Ervin K M. 2001. Experimental techniques in gas-phase ion thermochemistry. Chem Rev, 101:391~444

2001ERV/RAM Ervin K M, Ramond T M, Davoco G E, Schwartz R L, Casey S M, Lineberger W C. 2001. Naphthyl radical: Negative ion photoelectron spectroscopy, Franck-Condon simulation, and thermochemistry. J Phys Chem A, 105:10822~10831

2001FIN Finkelshtein E I. 2001. Radical stabilization energy as a measure of the spectral properties and reactivity trends in homologous groups. J Phys Org Chem, 14:543~550

2001GIB Gibson J K. 2001. Reactions of actinide ion with ethylene oxide. J Mass Spectrom, 36:284~293

2001GRO Gronert S. 2001. Mass spectrometric studies of organic ion/molecule reactions. Chem Rev, 101:329~360

2001HAM/WEN Hammad L A, Wenthold P G. 2001. Triradical thermochemistry from collision-induced dissociation threshold energy measurements. The heat of formation of 1,3,5-trimethylenebenzene. J Am Chem Soc, 123:12311~12317

2001IMR/DOB Imrik K, Dobe S, Berces T. 2001. Direct kinetic parameters for the reaction of Br atoms with neopentane. Int J Chem Kinet, 33:49~55

2001IUPAC IUPAC Subcommittee for Gas Kinetic Data Evaluation. 2001. http://www.iupac-kinetic.ch.cam.ac.uk

2001JOE Joens J A. 2001. The dissociation energy of OH and the enthalpy of formation of OH, ClOH, and BrOH from thermochemical cycles. J Phys Chem A, 105:11041~11044

2001KLE/THO Klemm R B, Thorn R P, Stief L J, Buckley T J, Johnson R D. 2001. Heat of formation of OBrO: Experimental photoionization study. J Phys Chem A, 105:1638~1642

2001KOP/WIL Kopitzky R, Willner H, Hermann A, Oberhammer H. 2001. Bis(trifluoroacety) peroxide, $CF_3C(O)OO(C(O)CF_3$. Inorg Chem, 40:2693~2698

2001KOS/MIR Kostikova L M, Miroshnichenko E A, Inozemtcev J O, Matyushin Y N. 2001. Efficient energies of interaction of functional groups and energies of dissociation bonds in alkylnitrates. Inter Ann Conf of ICT, 32nd, 104/1~104/9, Karlsruhe, Germany

2001LAG/DIO Lagoa A L C, Diogo H P, Dias M P, de Piedade M E M, Amaral L M P F, da Silva M A V R, Simoes, J A M, Guedes R C, Cabral B J C, Schwarz K, Epple M. 2001. Energetics of C–Cl, C–Br, and C–I bonds in haloacetic acids: Enthalpies of formation of XCH_2COOH (X = Cl, Br, I) compounds and the carboxymethyl radical. Chem Eur J, 7:483~489

2001LAR/SQU Lardin H A, Squires R R, Wenthold P G. 2001. Determination of the electron affinities of alpha-and beta-naphthyl radicals using the kinetic method with full entropy analysis. The C–H bond dissociation energies of naphthalene. J Mass Spectrom, 36:607~615

2001LAZ/PRO Lazarou Y G, Promitis A V, Paradimitriou V C, Paragiannakopoulos P. 2001. Theoretical calculation of bond dissociation energies and enthalpies of formation for halogenated molecules. J Phys Chem A, 105:6729~6742

2001LI/ALK Li R, Alconcel L N S, Continetti R E. 2001. Dissociative photodetachment of SO_2–SO_2^-: Evidence for the S–O bond dimer. Chem Phys Lett, 336:81~87

2001LU/WIT Lu J M, Wittbrodt J M, Wang K, Wen Z, Schlegel H B, Wang P G, Cheng J P. 2001. NO affinities of S-nitrosothiols: A direct experimental and computational investigation of RS–NO bond dissociation energies. J Am Chem Soc, 123:2903~2904

2001LUC/PED Lucarini M, Pedulli G F, Valgimigli L, Amorati R, Minisci F. 2001. Thermochemical and kinetic studies of a bisphenol antioxidant. J Org Chem, 66:5456~5462

2001LYM/NOD Lyman J L, Noda T. 2001. Thermochemical properties of SiF_6 and SiF_4 in gas and condensed phase. J Phys Chem Ref Data, 30:165~186

2001MAL/JON Malmstrom J, Jonsson M, Cotgreave I A, Hammarstrom L, Sjodin M, Engman L. 2001. The antioxidant profile of 2,3-dihydrobenzo[b]furan-5-ol and its 1-thio, 1-seleno, and 1-telluro analogues. J Am Chem Soc, 123:3434~3440

2001MAT/LEB Matyushin Y N, Lebedev V P, Miroshnichenko E A, Kostikova L M, Inosemzev Y O. 2001. The energy properties of the nitro- and nitrate derivatives adamatanes. Inter Ann Conf of ICT, 32nd, 102/1~102/12, Karlsruhe, Germany

2001MEL/GIN Meloni G, Gingerich K A. 2001. Thermodynamic investigation of the Si and Si_8 clusters by Knudsen cell mass spectrometry. J Chem Phys, 115:5470~5476

2001MER/CAS Mercader A, Castro E A. 2001. Improved correlations between 19-F-NMR chemical shifts and physical chemistry properties in fluorohalohydrocarbons. Revue Roum Chim, 46:1285~1292

2001MIR/KOS Miroshichenko E A, Kostikova L M, Inozemtcev J O, Matyushin Y N. 2001. Enthalpy characteristics of the polynitroamines. Inter Ann Conf of ICT, 32nd 103/1~103/8. Karlsruhe, Germany

2001MOR/RIV Morgon N H, Riveros J M. 2001. Electron affinity of $X_nGe(OMe)_{3-n}$ radicals (X=H, F; n = 0~2) and the Ge–H bond dissociation energy. Int J Mass Spectrom, 210/211:173~180

2001ORL Orlov Y D. 2001. Determination of new values of enthalpies of formation of nitrogen-containing organic radicals. Int Ann Conf of ICT, 32nd 92/1~92/7. Karlsruhe, Germany

2001ORL/LAV Orlov Yu D, Lavrov V O, Lebedev Yu A. 2001. Determination of enthalpies of formation of organic free radicals based on bond dissociation energies. 4. Alkyl-substituted derivatives of phenyl benzyl. Russ Chem Bull, 50:963~969

2001ORL/TUR Orlov Yu D, Turovtsev V V, Lebededev Yu A. 2001. The determination of enthalpies of formation of organic free radicals from bond dissociation energies. 5. Organosulfur

radicals. Russ Chem Bull, 50:1570~1571

2001PRA/DIL Pratt D A, DiLabio G A, Brigati G, Pedulli G F, Valgimigli L. 2001. 5-Pyrimidinols: Novel chain-breaking antioxidants more effective than phenols. J Am Chem Soc, 123:4625~4626

2001PRA/HEE Pratt D A, de Heer M I, Mulder P, Ingold K U. 2001. Oxygen-carbon bond dissociation enthalpies of benzyl phenyl ethers and anisoles. An example of temperature dependent substituent effects. J Am Chem Soc, 123:5518~5526

2001ROY/UNK Roy K, Unkhoff M B, Frank P, Just T. 2001. Kinetics of the cyclopentadiene decay and the recombination of cyclopentadienyl radicals with H-atoms: Enthalpy of formation of the cyclopentadienyl radical. Int J Chem Kinet, 33:821~833

2001SAN/MUR dos Santos R M B, Muralha V S F, Correie C F, Simoes J A M. 2001. Solvation enthalpies of free radicals: O–O bond strength in di-tert-butylperoxide. J Am Chem Soc, 123:12670~12674.

2001SEN/HAN Senosiain J P, Han J H, Musgrave C B, Golden D M. 2001. Use of quatum methods for a consistent approach to combustion modelling. Hydrocarbon bond dissociation energies. Faraday Discuss, 119:173~189

2001SIL/GON Silva M A V R, Goncalves J M, Ferreira S C C, Silva L C M, Sottomayor M J, Pilcher G, Acree W E Jr, Roy L E. 2001. Experimetal thermochemical study of the enthalpies of formation and sublimation of isonocotinamide, picolinamide, nicotinamide, isonicotinamide N-oxide, and nicotinamide N-oxide. The dissociation enthalpies of the N–O bonds. J Chem Thermodyn, 33:1263~1275

2001SIL/MAT Silva M A V R, Matos M A R, Miranda M S, Sousa M H F A, dos Santos R M B, Bizarror M M, and Simoes J A M. 2001. Standard enthalpies of formation of 2,6-di-tert-butyl-4-methylphenol and 3,5-di-tert-butylphenol and their phenoxy radicals. Struc Chem, 12:171~181

2001SUN/BOZ Sun H, Bozzelli J W. 2001. Structures, intramolecular rotation barriers, and thermochemical properties of radicals derived from H atom loss in mono, di, and trichloromethanol and parent. J Phys Chem A, 105:4504~4516

2001SUN/BOZ(b) Sun H, Bozzell J W. 2001. Structures, intramolecular rotation barriers, and thermochemical properties: ethanol, alpha-monoethanols, dichlorocthanols, and corresponding radicals derived from H atom loss. J Phys Chem A, 105:9543~9552

2001TUM/DEN Tumanov V E, Denisov E T. 2001. Evaluation of C–H bond dissociation energies in hydrocarbons and the enthalpies of the relevant radicals from kinetic data. Petrol Chem, 41: 93~102

2001TYN/COX Tyndall G S, Cox R A, Granier C, Lesclaux R, Moortgat G K, Pilling M J, Ravishankara A R, Wallington T J. 2001. Atmospheric chemistry of small organic peroxy radicals. J Geophys Res, 106(D11):12157~12182

2001VER/HEI Verevkin S P, Heintz A. 2001. Chemical equilibrium study in the reacting system of the (1-alkoxyethyl)benzene synthesis from alkanols and styrene. J Chem Eng Data, 46:984~990

2001ZIL/INO Zils R, Inomata S, Imamura T, Miyoshi A, Washida N. 2001. Determination of the equilibrium constant and thermodynamic parameters for the reaction of pentadienyl radicals with O_2. J Phys Chem, 105:1277~1282

2002ALN/ZHA Alnajjar M S, Zhang X M, Gleicher G J, Truksa S V, Franz J A. 2002. Equilibrium acidities and homolytic bond dissociation energies of acidic C–H bonds in alpha-arylacetophenones and related compounds. J Org Chem, 67:9016~9022

2002AMO/FER Amorati R, Ferroni F, Lucarini M, Pedulli G F, Valgimili L. 2002. A quantitative approach to recycling of alpha-tocopherol by coantioxidants. J Org Chem, 67:9295~9303

2002ARU/VIJ Arunan E, Vijayalashmi S P, Valera R, Setser D W. 2002. Infrared chemiluminescene: Evidence for adduct formation in the H + CH_2X reaction and studies of N + CH_2X (X = C, F, I, H) reaction. Phys Chem Chem Phys, 4:51~59

2002BEC/BOG Becerra R, Boganov S E, Egorov M P, Faustov V I, Krylova I V, Nefedov O M, Walsh R. 2002. First gas-phase detection of dimethylstannylene and time-resolved study of some of its reactions. J Am Chem Soc, 124:7555~7562

2002BOZ/SHE Bozzelli J W, Sheng C. 2002. Thermochemistry, reaction paths, and kinetics on the hydroperoxy-ethyl radical reaction with O_2: New chain branchig reactions in hydrocarbon oxidation. J Phys Chem A, 106:1113~1121

2002BRI/LUC Brigati G, Lucarini M, Mugnaini V, Pedulli G F. 2002. Determination of the substituent effect on the O–H bond dissociation enthalpies of phenolic antioxidants by the EPR radical equilibrium technique. J Org Chem, 67:4828~4832

2002CHE/CHE Chen E C M, Chen E S. 2002. The calculation of electron affinities and bond dissociation energies of pesticides and explosives analyzed in negative ion mobility spectrometry. Int J Ion Mobility Spectro, 5(3):11~14

2002CRC CRC Handbook of Chemistry and Physics. 2002. Lide D E ed. 82th ed. Florida. Boca Raton:CRC Press. http://www.hbcpnetbase.com/hbcp

2002DEN/KIE Denis P A, Kieninger M, Ventura O N, Cachau R E, Diercksen G H F. 2002. Complete basis set and density functional determination of the enthalpy of formation of the controversial HO_3 radical: A discrepancy between theory and experiment. Chem Phys Lett, 365:440~449

2002DIX/FEL Dixon D A, Feller D, Zhan C G, Francisco J S. 2002. Decomposition pathways of peroxynitrous acid: Gas-phase and solution energies. J Phys Chem A, 106:3191~3196

2002DRO/DEN Drozdova T I, Denisov E T. 2002. Reactivity of the Ge–H, Si–H, P–H and Se–H bonds in radical abstraction reactions. Kinet Catal, 43:10~18

2002EVR/DET Ervin K M, DeTuri V F. 2002. Anchoring the gas-phase acidity scale. J Phys Chem A, 106:9947~9956

2002GAL/MAK Galsovac Z, Maksic M E, Dacres J E, Kass S R. 2002. Gas phase formation of 1-phenylcyclobuten-3-yl and 1-phenylallyl anions and a determination of the allylic C–H acidities and bond dissociation energies of 1-phenylcyclobutene and (E)-1-phenylpropene. J Chem Soc Perkin Trans 2, 410~415

2002HER/HAN Herbon J T, Hanson R K, Golden D M, Bowman C T. 2002. A Shock tube study of the enthalpy of formation of OH. Proc Combus Institute, 29(Pt.1), 1201~1208

2002HIP/NAS Hippler H, Nasterlack S, Strieber F. 2002. Reaction of OH + NO_2 + M: Kinetic evidence of isomer formation. Phys Chem Chem Phys, 4:2959~2964

2002JON/LIN Jonsson M, Lind M, Merenyi G. 2002. Redox and acidity properties of 2,2′- and 4,4′-biphenol and the corresponding phenoxyl radicals. J Phys Chem A, 106:4758~4762

2002KAR/JAN Karty J M, Janaway G A, Brauman J I. 2002. Conformation-dependent reaction thermochemistry: Study of lactones and lactone enolates in the gas phase. J Am Chem Soc, 124:5213~5221

2002KAS/BRO Kass S R, Broadus K M. 2002. Reactive intermediates via Fourier transform mass spectrometry. J Phys Org Chem, 15:461~468

2002KIR/TSC Kiracofe J C R, Tschumper G S, Schaefer III H F. 2002. Atomic and molecular electron affinities: Photoelectron experimental and theoretical computations. Chem Rev, 102:231~282

2002KOS/MIR Kostikova L M, Miroshnichenko E A, Matyushin Y N, Vorobev A B, Inozemtcev J O. 2002. Enthalpy characteristics of mononitro derivatives heterocylic compounds. Int Ann Conf of ICT, 33rd, 86/1~86/8, Karlsruhe, Germany

2002KRO/TUM Kromkin E A, Tumanov V E, Denisov E T. 2002. Evaluation of C–H bond dissociation

energies in alkylaromatic hydrocarbons and the enthalpies of corresponding radicals from kinetic data. Neftekhimiya, 42:1~11

2002LAG/DIO Lagoa A L C, Diogo H P, Piedade M E M, Amaral L M P E, Guedes R C, Cabral B J C, Kulikov D V, Verevkin S P, Siedler M, Epple M. 2002. Energetics of the C–Cl in $CH_3CH(Cl)COOH$. Enthalpy of formation of (S)-2-chloropropionic acid and of the 1-carboxythyl radical. J Phys Chem A, 106:9855~9861

2002LAL/ALL Lalevee J, Allonas X, Fouassier J P. 2002. N–H and alpha-C--H bond dissociation enthalpies of aliphatic amines. J Am Chem Soc, 124:9613~9621

2002LAR/NAS Lardin H A, Nash J, Wenthold P G. 2002. Is the 1,3,5-tridehydrobenzene triradical a cyclopropenyl radical anologue? J Am Chem Soc, 124:12612~12618

2002LEE/CHE Lee J W, Chen C J, Bozzelli J W. 2002. Thermochemical and kinetic analysis of the acetyl radical (CH_3CO) + O_2 reaction system. J Phys Chem A, 106:7155~7170

2002LI/BAE Li Y, Baer T. 2002. Threshold photoelectron-photoion coincidence spectroscopy. Dissociation of the 1-chloroadamantane ions and the heat of formation of the 1-adamantyl cation. J Phys Chem A, 106:272~278

2002LI/CON Li R, Continetti R E. 2002. Studies of the excited state dynamics of N_2O_2 by dissociative photodetachment of $N_2O_2^-$. J Phys Chem A, 106:1183~1189

2002LUC/MUG Lucarini M, Mugnaini V, Pedulli G F. 2002. Bond dissociation enthalpies of polyphenols: The importance of cooperative effects. J Org Chem, 67:928~931

2002MAN Manion J A. 2002. Evaluated enthalpies of formation of the stable closed shell C_1 and C_2 chlorinated hydrocarbons. J Phys Chem Ref Data, 31:123~172

2002MAT/KON Matyushin Y N, Konkova T S. 2002. Combined study of thermochemical properties of nitrourea and its salts. Int Ann Conf of ICT, 33rd, 87/1~87/10, Karlsruhe, Germany

2002MAT/LEB Matyushin Y N, Lebedev V P, Miroshnichenko E A, Vorobeva V P, Chironov V V, Kostikova L M, Inozemtcev, J.O. 2002. Energetic characteristics of nitriles. Int Ann Conf of ICT, 33rd, 84/1~84/8, Karlsruhe, Germany

2002MAT/LEB(b) Matyushin Y N, Lebedev V P, Chironov V V, Pepekin V I. 2002. N–O bond energy in benzofuroxans. Khimicheskaya Fizika, 21(7):58~61

2002MER/LIN Mercnyi G, Lind J, Goldstein S. 2002. Thermochemical properties of alpha-hydroxy-alkoxyl radicals in aqueous solution. J Phys Chem A, 106:11127~11129

2002MIC/KOR Michel M, Korolkov M V, Weitzel K M. 2002. A new route to dissociation energy of ionic and neutral HCl via lineshape analysis of single rotational transitions. Phys Chem Chem Phys, 4:4083~4086

2002MIN/PUN Minisci F, Punta C, Recupero F, Fontana F, Pedulli G F. 2002. A new, highly selective synthesis of aromatic aldehydes by aerobic free-radical oxidation of benzylic alcohols, catalyzed by n-hydroxyphthalimide under mild conditions. Polar and enthalpic effects. Chem Commun, 7:688~689

2002MIN/PUN(b) Minisci F, Punta C, Recupero F, Fontana F, Pedulli G F. 2002. Aerobic oxidation of N-alkylamides catalyzed by N-hydroxyphthalimide under mild conditions. Polar and enthalpic effects. J Org Chem, 67:2671~2676

2002MIR/LEB Miroshnichenko E A, Lebedev V P, Matyushin Y N. 2002. Energy properties of adamantane derivatives. Dokl Phys Chem, 382:40~42

2002MON/DIM Mons M, Dimicoli I, Tardivel B, Piuzzi F, Brenner V, Millie P. 2002. Energetics of a model NH-pi interaction: The gas phase benzene-NH_3 complex. Phys Chem Chem Phys, 4:571~576

2002NIM/DAV Nimlos M R, Davico G, Geise C M, Wenthold P G, Lineberger W C, Blankeby S J, Hadad C M, Petersson G A, Ellison G B. 2002. Photoelectron spectroscopy of $HCCN^-$ and $HCNC^-$ reveals the quasilinear triplet carbenes, HCCN and HCNC. J Chem Phys, 117:4323~4339

2002NIST/COM Computational Chemistry Comparison and Benchmark Database, May 20002, http://srdata.nist.gov/cccbdb

2002PAR/CHA Park J, Chakraborty D, Jamindar S, Xia W S, Lin M C, Bedford C. 2002. Thermal decomposition of 2,2-bis(difluoroamino) propane studies by FTIR spectrometry and quantum chemical calculations: The primary dissociation kinetics and the mechanism for decomposition of the $(CH_3)_2CNF_2$ radical. Thermochimica Acta, 384:101~111

2002POU/UPS Poutsma J C, Upshaw S D, Squires R R, Wenthold P G. 2002. Absolute heat of formation and singlet-triplet splitting for HCCN. J Phys Chem A, 106:1067~1073

2002PRA/DIL Pratt D K, DiLabio G A, Valgimigli L, Pedulli G F, Ingold K U. 2002. Substituent effects on the bond dissociation enthalpies of aromatic amines. J Am Chem Soc, 124:11085~11092

2002RAM/BLA Ramond T M, Blanksby S J, Kato S, Bierbaum V M, Davico G E, Schwartz R L, Lineberger W C, Ellison G B. 2002. Heat of formation of the hydroperoxyl radical HOO via negative ion studies. J Phys Chem A, 106:9641~9647

2002REE/KAS Reed D R, Kass S R, Mondanaro K R, Daily W P. 2002. Formation of a 1-bicyclo[1.1.1]pentyl anion and experimental determination of the acidity and C–H bond dissociation energy of 3-tert-butylbicyclo[1.1.1]pentane. J Am Chem Soc, 124:2790~2795

2002ROU/TEM Roux M V, Temprado M, Davalos J Z, Jimenez P, Hosmane R S, Liebman J F. 2002. Enthalpy of formation of methyl benzoate: Calorimetry and consequences. Phys Chem Chem Phys, 4:3611~3613.

2002RUS/WAG Ruscic B, Wagner A F, Harding L B, Asher R L, Feller D, Dixon D A, Peterson K A, Song Y, Qiam X X, Ng C Y, Liu J, Chen W, Schwenke D W. 2002. On the enthalpy of formation of hydroxyl radical and gas-phase bond dissociation energies of water and hydroxyl. J Phys Chem A, 106:2727~2747

2002SAB/FUJ Sablier M, Fujii T. 2002. Mass spectrometry of free radicals. Chem Rev, 102:2855~2924

2002SAI/PEL Sailer W, Pelc A, Matejcik S, Illenberger E, Scheier P, Mark T D. 2002. Dissociative electron attachment study to nitromethane. J Chem Phys, 117:7989~7994

2002SAN/MUR dos Santos R M B, Muralha V S F, Correia C F, Guedes R C, Cabral B J C, Simoes J A M. 2002. S–H bond dissociation enthalpies in thiophenols: A time-resolved photoacoustic calorimetry and quantum chemistry study. J Phys Chem A, 106: 9883~9889

2002SEB/BOC Sebbar N, Bockhorn H, Bozzelli J W. 2002. Structures, thermochemical properties (enthalpy, entropy and heat capacity), rotation barriers, and peroxide bond energy of vinyl, allyl, ethynyl and phenyl hydroperoxides. Phys Chem Chem Phys, 4:3691~3703

2002SEE Seetula J A. 2002. Kinetics of the R + HBr = RH + Br (R = CH_2I or CH_3) reaction. An initio study of the enthalpy of formation of the CH_2I, CHI_2 and CI_3 radicals. Phys Chem Chem Phys, 4:455~460

2002SHI/BAB Shim I, Baba S M, Gingerich K A. 2002. Electronic structure of Ge2 and thermodynamic properties of Ge2 from all electron ab intio investigations and Knudsen effusion mass spectroscopic measurements. Chem Phys, 277. 9~20

2002SON/GOL Song S, Golden D M, Hanson R K, Bowman C T. 2002. A shock tube study of benzylamine decomposition: Overall rate coefficient and heat of formation of the benzyl radical. J Phys Chem A, 106:6094~6098

2002SUN/BOZ Sun H, Bozzelli, J W. 2002. Structures, rotational barriers, thermochemical properties, and additivity groups for 2-propanol, 2-chloro-2-propanol and the corresponding alkoxy and hydroxyalkyl adicals. J Phys Chem A, 106:3947~3956

2002TUM/KRO Tumanov V E, Kromkin E A, Denisov E T. 2002. Estimation of dissociation energies of

C–H bonds in oxygen-containing compounds from kinetic data for radical abstraction reactions. Russ Chem Bull 51:1641~1650.

2002VER/HEI Verevkin S P, Heintz A. 2002. Chemical equilibrium study in the reacting system of (1-alkoxyethyl) benzene synthesis from isoalkanol and styrene. J Chem Soc Perkin Trans, 2: 728~733.

2002WAL/CHE Walker B W, Check C E, Lobring K C, Pommerening C A, Sunderlin L S. 2002. The thermochemistry of group 15 tetrachloride anions. J Am Mass Spectrom, 13:469~476

2002ZHU/BOZ Zhu L, Bozzell J W. 2002. Structures, rotational barrics, and thermochemical properties of chlorinated aldehydes and the corresponding acetyl and formyl methyl radicals and additivity groups. J Phys Chem A, 106:345~355

2002ZHU/BOZ(b) Zhu L, Bozzelli J W. 2002. Thermodynamic properties of chloroacetylene, dichloroacetylene, ethynyl radical, and chloroethynyl radical. Chem Phys Lett, 362:445~452

2003AMO/LUC Amorati R, Lucarini M, Mugnaini V, Peddulli G F, Minisci F, Recupero F, Fontana F, Astolfi P, Greci L. 2003. Hydroxylamines as oxidation catalysis: Thermochemical and kinetic studies. J Org Chem, 68:1747~1754

2003AMO/LUC(b) Amorati R, Lucarini M, Mugnaini V, Peddulli G F. 2003. Antioxidant activity of o-bisphenols: The role of intramolecular hydrogen bonding. J Org Chem, 68:5198~5204

2003BLA/ELL Blanksby S J, Ellison G B. 2003. Bond dissociation energies of organic molecules. Acc Chem Res, 36:255~263

2003BRA/NES Braun M, Nestler K, Marx G. 2003. Thermochemistry of hydride and phenyl groups on the surface of amorphous silicon dioxide. Thermochimica Acta, 405:73~84

2003BUR/KHA Burcat A, Khachatryan L, Dellinger B L. 2003. Thermodynamics of chlorinated phenols, polychlorinated dibenzo-p-dioxins, polychlorinated dibenzofurans, derived radicals, and intermediate species. J Phys Chem Ref Data, 32:443~517

2003CAR/BOU Carrell T G, Bourles E, Lin M, Dismukes G C. 2003. Trasition from hydrogen atom to abstraction by $Mn_4(O_2PPh_2)_6$ versus $[Mn_4O_4(O_2PPh_2)_6]^+$: O–H bond dissociation energies and the formation of $Mn_4O_3(OH)(O_2PPh_2)_6$. Inorg Chem, 42:2849~2859

2003CHE/BOZ Chen C C, Bozzelli J W. 2003. Structures, intramolecular rotation barriers, and thermochemical properties of methyl ethyl, methyl isopropyl, and methyl tert-butyl ethers and the corresponding radicals. J Phys Chem A, 107:4531~4546

2003CHE/LI Chen H, Li G, Zhang F F, Sun L, Chen H L, Zhang S Y. 2003. Co–C bond dissociation energy and reaction volume change of 2',5'-dideoxyadenosylcobalamin studies by laser-induced time-resolved photoacoustic calorimetry. Spectrochimica Acta, Part A: Mol. Biomol. Spectroscopy, 59:2767~2774

2003DEA/LI Deakyne C A, Li L, Zheng W, Xu D, Liebman J E. 2003. Regularities in the bond dissociation enthalpies of molecules of types AB and BAB: Energetics of 10- and 16-valence electron ions of groups 13, 15, and 16. Int J Quant Chem, 95:713~718

2003DOR/IOR Dorofeeva O V, Iorish V S, Novikov V P, Neumann D B. 2003. NIST-JANAF Thermochemical table. 2. Three molecules related to atmospheric chemistry: HNO_3, H_2SO_4, and H_2O_2. J Phys Chem Ref Data, 32:879~901

2003FAT/MCC Fattahi A, McCarthy R E, Ahmad M R, Kass S R. 2003. Why does cyclopropene have the acidity of an acetylene but the bond energy of methane? J Am Chem Soc, 125:11746~11750

2003FEL/DIX Feller D, Dixon A A. 2003. Coupled cluster theory and multireference configuration interaction study of FO, F_2O, FO_2, and FOOF. J Phys Chem A, 107:9641~9651

2003FEL/DIX(b) Feller D, Dixon A A, Francisco J S. 2003. Coupled cluster theory determination of the heats of formation of combustion-related compounds: CO, HCO, CO_2, HCO_2, HOCO, HC(O)OH, and HC(O)OOH. J Phys Chem A, 107:1604~1617

2003GAR Garcia J E. 2003. Theoretical enthalpies of formation and C–H bond dissociation enthalpies of n-bromopropane and its free radicals. Chem Phys Lett, 377:607~612

2003GUE/COU Guedes R C, Coutinho K, Cabral B J C, Canuto S, Correia CF, dos Santos R M B, Simoes J A M. 2003. Solvent effects on the energetics of the phenol O–H bond: Differential solvation of phenol and phenoxt radical in benzene and acetonitrile. J Phys Chem A, 107:9197~9207

2003HIL/LAU Hildenbrand D L, Lau K H, Sanjurjo A. 2003. Experimental thermochemistry of the SiCl and SiBr radicals: Enthalpies of formation of species in the Si–Cl and S–Br systems. J Phys Chem A, 107:5448~5451

2003KHA/MUF Khatymov R V, Muftakhov M V, Schukin P V, Mazunov V A. 2003. On the structure of negative ions formed by dissociative electron attachment by monochlorophenol molecules. Russ Chem Bull, 52:1974~1981

2003KOS/CAI Koshino N, Cai Y, Espenson J H. 2003. Kinetic study of the phthalimide N-oxyl (PINO) radical in acetic acid. Hydrogen abstraction from C–H bonds and evaluation of O–H bond dissociation energy of N-hydroxyphthalimide. J Phys Chem A, 107:4262~4267

2003KRO/TUM Kromkin EA, Tumanov VE, Denisov, ET. 2003. Evaluation of the energies of dissociation of C–X bonds in monohaloalkyls according to kinetic data. Khimicheskaya Fizika, 22(11):30~36

2003LIY/STY Liyanage R, Styles M L, O'Hair R A J, Armentrout P B. 2003. Guided ion beam and ab intio studies of platinum chloride cations. J Phys Chem A, 107:10303-10310

2003LUC/MUG Lucarini M, Mugnaini V, Pedulli G F, Guerra M. 2003. Hydrogen-bonding effects on the properties of phenoxyl radicals. An EPR, kinetic, and computational study. J Am Chem Soc, 125:8318~8329

2003LUC/MUG(b) Lucarini M, Mugnaini V, Pedulli G F. 2003. Determination by the EPR radical equilibration technique of the O–H bond dissociation enthalpies in 3,5-diethylphenol. Struc Chem, 14:399~401

2003MAX/BUG Maximiliano A, Burgos P, Gustavo P G, Willner H. 2003. Kinetics of the thermal decomposition of bis(trifluoromethyl) peroxydicarbonate, $CF_3OC(O)OOC(O)OCF_3$. Int J Chem Kinet, 35:15~19

2003MIN/REC Minisci F, Recupero F, Pedulli G F, Lucarini M. 2003. Transition metal salts catalysis in the aerobic oxidation of organic compounds. Thermochemical and kinetic aspects and new synthetic developments in the presence of N-hydroxy-derivative catalysis. J Mol Catal A Chem, 204/205:63~90

2003NASA/JPL US NASA. 2003. http://jpldataeval.jpl.gov, Feb 24, 2003

2003OWE/NAU Owens N L, Nauta K, Kable S H, Haworth N L, Bacskay G B. 2003. An experimental and theoretical investigation of the triple fragmentation of $CFClBr_2$ by photolysis near 250 nm. Chem Phys Lett, 370:469~477

2003POL/KON Pollack I B, Konen I M, Li E X J, Lester M I. 2003. Spectroscopic characterrization of HOONO and its binding energy via infrared action spectroscopy. J Chem Phys, 119:9981~9984

2003REE/HAR Reed D R, Hare M C, Fattahi A, Chung G, Gordon M S, Kass S R. 2003. alpha-2,3,4-dehydrophenol radical anions: Formation, reactivity, and energetics leading to the heats of formation of alpha-2,3,4-oxocyclohexadienylidene. J Am Chem Soc, 125:4643~4651

2003ROU/TEM Roux M V, Temprado M, Jimenez P, Davalos J Z, Notario R, Guzman-Mejia R, Juaristi E. 2003. Calorimetric and computationl study of thiacylohexane 1-oxide and thiacylcyclohexane 1,1-dioxide (thiane sulfoxide and thiane sulfone). Enthalpies of formation and the energy of the S=O bond. J Org Chem, 68:1762~1770

2003SAR/ROG Saraf S R, Rogers W J, Mannan M S, Hall M B, Thomson L M. 2003. Theoretical

thermochemistry: Ab initio heat of formation for hydroxylamine. J Phys Chem A, 107:1077~1081

2003SEE Scetula J A. 2003. Kinetics of the R + HBr = RH + Br (R = CH_2Br, CHBrCl or CCl_3) equilibrium. Thermochemistry of the CH_2Br and CHBrCl radicals. Phys Chem Chem Phys, 5:849~855

2003SEN/RIV Sena M, Riveros J M. 2003. Dissociation of p-cymene molecular ions induced by thermal radiation. Int J Mass Spectrom, 227:135~145

2003SIL/SAN de Silva, M D M C R, Santos L M N B F, Silva A L R, Fernandes O, Acree W E Jr. 2003. Energetics of 6-methoxyquinoline and 6-methoxyquinoline B N-oxide: The dissociation enthalpy of the N–O bond. J Chem Thermodyn, 35:1093~1100

2003SRI/KIE Srinivasan N K, Kiefer J H, Tranter R S. 2003. Dissociation, relaxation, and incubation in the pyrolysis of neopentane: Heat of formation for tert-butyl radical. J Phys Chem A, 107:1532~1539

2003TAN/DAG Tan X, Dagdigian P J. 2003. Electronic spectrum of the gallium dimer. J Phys Chem A, 107:2642~2649

2003TUM/DEN Tumanov V E, Denisov ET. 2003. Estimation of S–H and C–H bond dissociation energies on organic compounds. Neftekhimiya, 43:406~411

2003VAL/BRI Valgimigli L, Brigati G, Pedulli G F, DiLabip G A, Mastragostino M, Arbizzani C, Pratt D A. 2003. The effect of ring nitrogen atoms on the homolytic reactivity of phenolic compounds: Understanding the radical-scavenging ability of 5-pyrimidinols. Chem Eur J, 9:4997~5010

2003VER/KRA Verevkin S P, Krasnykh E L, Wright JS. 2003. Thermodynamic properties of benzyl halides: Enthalpies of formation, strain enthalpies, and carbon-halogen bond dissiciation enthalpies. Phys Chem Chem Phys, 5:2605~2611

2003WAN/WU Wang J, Wu G H, Sheng L S, Zhang Y W. 2003. Vacuum ultraviolet photoionization and photodissociation of 1,2-dimethoxyethane, Acta Chinica Sinca, 61:989~993

2003WIJ/PRA Wijtmans M, Pratt D A, Vagimgli L, DiLabio G, Pedulli, G F, Porter N A. 2003. 6-Amino-3-pyridinols: towards diffusion-controlled chain-breaking antioxidants. Angew Chem Int Ed, 42:4370~4373

2003WU/CAR Wu F, Carr R W. 2003. Reactivity of the CF_3CHO radical: Thermal decomposition and reaction with O_2. J Phys Chem A, 107:10733~10742

2003YUN Yungman V S ed. 2003. Thermal Constants of Substances, http://www.chem.msu.su/cgi-bin/tkv.pl? show=welcome.html

2003ZAV Zavitsas A A. 2003. The relation between bond lengths and dissociation energies of carbon-carbon bonds. J Phys Chem A, 107:897~898

2003ZHE/SAE Zheng S, Saeed J L, Khan S I, Rubin Y. 2003. Synthesis, characterization, and coordination chemistry of the 2-azaphenalenyl radical. J Am Chem Soc, 125:5786~5791

2003ZHU/CAO Zhu X Q, Cao L, Liu Y, Yang Y, Lu J Y, Wang J S, Cheng J P. 2003. Thermodynamics and kinetics of the hydride-transfer cycles for 1-ary-1,4-dihydronicotinamide and its 1,2-dihydroisomer. Chem Eur J, 9:3937~3945

2003ZHU/LI Zhu X Q, Li H R, Li Q, Ai T, Lu J Y, Yang Y, Cheng J P. 2003. Determination of the C_4–H bond dissociation energies of NADH models and their radical cations in acetonitrile. Chem Eur J, 9:871~880

2003ZHU/YAN Zhu X Q, Yang Y, Zhang M, Cheng J P. 2003. First estimation of C_4–H bond dissociation energies of NADH and its radical cation in aqueous solution. J Am Chem Soc, 125:15298~15299

2004AUT/BRO Autrey T,Brown A K, Camaioni D M, Dupuis M, Foster N S, Getty A. 2004.Thermochemistry of aqueous hydroxyl radical from advances in photoacoustic calorimetry and ab initio continuum solvation theory. J Am Chem Soc, 126:3680~3681

2004CAR/KOY Caraiman D, Koyanagi G K, Bohme D K. 2004. Gas-phase reactions of transition-metal ion with hexafluorobenzenr: room-temperature kinetics and periodicities in reactivity. J Phys Chem A, 108:978~986

2004CAS http://www.cas.org/cgi-bin/regreport.pl, updated frequently

2004DEN/DEN Denisova TG, Denisov ET. 2004. Estimation of O–H bond dissociation energy in hydroperoxides with functional groups on kinetic data. Petroleum Chem, 44:278~283

2004DON/WOR Donkeers R L, Workentin M S. 2004. Elucidation of the electron transfer reduction mechanism of anthracene endoperoxides. J Am Chem Soc, 126:1688~1698

2004GRE/KRA Grebenkin S Y, Krasnoperov L N. 2004. Kinetics and thermochemistry of the hydroxycycloxadienyl radical reaction with O_2: $C_6H_6OH + O_2 = C_6H_6(OH)OO$. J Phys Chem A, 108:1953~1963

2004HIR/YAN Hirata S, Yanai T, de Jong W A, Nakajima T, Hirao K. 2004. Third-order Douglas-Kroll relativistic coupled-cluster theory through connected single, double, triple, and quadruole substitutions: Applications to diatomic and triatomic hydrides. J Chem Phys, 120:3297~3310.

2004LEW/CRA Lewin J L, Cramer C J. 2004. Rapid quantum mechanical models for the computational estimation of C–H bond dossociation energies as a measure of metabolic stability. Mol. Pharmaceutics, 1:128~135

2004LUC/PED Lucarini M, Pedulli G F, Guerra M. 2004. A critical evaluation of the factors determining the effect of intramolecular hydrogen bonding on the O–H bond dissociatio enthalpy of catechol and of flavonoid antioxidants. Chem. Eur J, 10:933~939

2004MUR/SAN Muralha V S F, dos Santos R M B, Simoes J A M. 2004. Energetics of alkylbenzyl radicals: A time-resolved photoacoustic calorimetry study. J Phys Chem A, 108:936~942

2004POS/SHA Poskrebyshev G.A, Shafirovich V and Lymar S L. 2004. Hyponitrite radical, a stable adduct of nitric oxide and nitroxyl. J Am Chem Soc, 126:891~899

2004SIL/MAT da Silva D M C R, Matos M A R, Miranda M S, Morais V M F., Acree W E Jr. 2004. Experimental and theoretical study of the dissociation enthalpy of the N–O bond on 2-hydroxypyridine N-oxide: Theoretical analysis of the energetics of the N–O bond for hydroxypyrydine N-oxide isomers. J Chem Thermodyn, 35:107~113

2004SUN/BOZ Sun H, Bozzelli J W. 2004. Thermochemical and kinetic analysis on the reactions of neopentyl and hydroperoxy-neopentyl radicals with oxygen. 1. OH and initial stable HC product formation. J Phys Chem A, 108:1694~1711

2004ZHA/CHE Zhang Y P, Cheng C H, Kim J T, Stanojevic J, Eyler E E. 2004. Dissociation energies of molecular hydrogen and the hydrogen molecular ion. Phy Rev Lett, 92:203003~203004

附　录

能量转换因子: SI 能量单位与传统单位之间的转换

	cm^{-1}	eV	au	K	kcal/mol	kJ/mol
1 cm^{-1} = (for spectrometry)	1	1.2399(–4)	4.556(–6)	1.4388	2.859(–3)	1.1963(–2)
1 eV = (for mass spectrometry)	8.065(+3)	1	3.675(–2)	1.1605(+4)	2.306(+1)	9.648(+1)
1 hartree (au) = (for theoretical calculations)	2.195(+5)	2.721(+1)	1	3.158(+5)	6.275(+2)	2.626(+3)
1 K = (for theoretical physics)	6.950(–1)	8.617(–5)	3.167(–6)	1	1.9871(–3)	8.314(–3)
1 kcal/mol = (for calorimetry)	3.498(+2)	4.336 (–2)	1.5936(–3)	5.032(+2)	1	4.184
1 kJ/mol = (SI unit)	8.359(+1)	1.0364(–2)	3.809(–4)	1.2027(+2)	2.390(–1)	1

注：括号内的数字表示 10 的幂方次。

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