Table 2.1 (continued) A Summary of Main Experimental Methods for Measuring BDEs

Experimental Methods	Measured Quantities	Applications	References
Calorimetry			
• Microcalorimetrc	Heats of combustion, vaporization, and formation	Species in solid, solution, or gas–solid surface	(1) 1995LEB/CHI (2) 2004SIL/MAT
• Solution titration	Reaction heats		(3) 1992BUR (3) 1992HOF (4) 1995NOL
• Gas–solid surface	Femtomole adsorption heats on single-crystal surface		(5) 1998BRO/KOS (6) 1998CER
Thermal desorption spectroscopy (TDS) Temperature programmed-desorption (TPD)	An adsorbed surface is heated and desorbing species are detected with MS, IR or others	Gas–solid interface	(1) 1986WOO/DEL (2) 1990JON/NIE
Helium atom scattering (HAS)	Monoenergetic beam of helium atoms are scattered from ordered surfaces and detected	Gas–solid interface	1996HOF/TOE

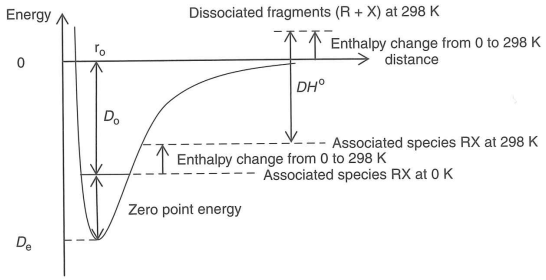
The readers may find more methods for determining the BDEs in e-publication (2002SIL).

2.2 *The conversion between D_0, D_e, and DH^0*

Related energies are often encountered when searching for experimental BDE data.

D_0 the bond dissociation energy at 0 K
D_e the electronic energy, i.e., the minimum on the potential energy curve or surface or the well depth.

D_0(R−X) may be determined from D_e, as shown in figure:



$$D_0 = D_e - \Delta(\text{ZPE}) \tag{2.1}$$

Here Δ(ZPE) is the change of the zero point vibrational energies in the species involved in the bond dissociation processes, the dissociating state as the energy reference.

For diatomic molecules and Morse potential, the approximate relationship follows:

$$\begin{aligned} D_0 &\simeq \frac{\omega_e^2}{4\omega_e x_e} - \frac{\omega_e}{2} + \frac{\omega_e x_e}{4} \\ D_e &\simeq \frac{\omega_e^2}{4\omega_e x_e} \\ \Delta(\text{ZPE}) &= \frac{\omega_e}{2} - \frac{\omega_e x_e}{4} \end{aligned} \tag{2.2}$$

Here ω_e and x_e are the spectroscopic parameters.

In general, the relationship between the dissociation enthalpy change and temperature must be determined to make the conversion from D_0 to DH^0. There are four methods for this conversion.

1. Thermochemical calculations (2005RUS/BOG).
2. Calculations by quantum chemistry (1997CUR/RAG; 2000CIO/SCH; 2002NIST/COM).
3. Using NIST-JANAF Thermochemical Tables (1998CHA).
4. Simple approximation. This is good for biatomic, triatomic, and tetraatomic species. This method is reviewed below.

2.2.1 *Diatomic molecules*

From thermodynamics, the enthalpy change, ΔH, and internal energy change, ΔE, for the bond dissociation processes is described as

$$\Delta H = \Delta E + \Delta(PV) \tag{2.3}$$

Where Δ(PV) is the molar work that is equal to Δ(RT), assuming 1 molar ideal gas. For diatomic species, a vibrational free degree becomes a translational one because of the bond dissociation. An approximate equation is obtained as

$$\Delta H = \Delta E + RT \approx D_0 + \frac{3}{2}RT \tag{2.4}$$

For T=298.15 K, the BDE is derived based on the experimental D_0 at 0 K

$$\begin{aligned} \text{BDE} \equiv DH^0 &\approx D_0 + \frac{3}{2}RT \\ &= D_0 + 0.8886 \text{ kcal/mol} = D_0 + 3.7181 \text{ kJ/mol} \end{aligned} \tag{2.5}$$

Here the R is the gas constant; the H in the nomenclature DH^0 emphasizes that the BDE is the enthalpy change of the dissociation processes. The superscript '0' denotes the standard conditions of thermodynamics.

Table 4.5.3 (continued) C–C BDEs in Organic Compounds Containing Sulfur Atom(s)

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; reference in parentheses) kcal/mol	kJ/mol	Methods (reference in parentheses)	References
3-Methyl-1-butanethiol *iso*-$\mathbf{C_4H_9}$–CH_2SH	80.5±2.5	336.8±10.5	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY
2,2-Dimethyl-1-propanethiol *tert*-$\mathbf{C_4H_9}$–CH_2SH	78.7±2.5	329.3±10.5	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY
1-Hexanethiol $n\mathbf{C_5H_{11}}$–CH_2SH	80.3±2.5	336.0±10.5	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY
1-Heptanethiol $n\mathbf{C_6H_{13}}$–CH_2SH	80.2±2.5	335.6±10.5	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY
Phenylmethane-1-thiol $\mathbf{C_6H_5}$–CH_2SH	93.2±2.5	389.9±10.5	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY
1,2-Ethanethiol $\mathbf{HSCH_2}$–CH_2SH	74.9±2.8	313.4±11.7	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY
Ethyl methyl sulphide $\mathbf{CH_3}$–CH_2SCH_3	82.0±2.0	343.1±8.4	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY
Methyl propyl sulphide $\mathbf{C_2H_5}$–CH_2SCH_3	80.8±2.0	338.1±8.4	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY
Ethyl phenyl sulphide $\mathbf{CH_3}$–$CH_2SC_6H_5$	80.9±2.0	338.5±8.4	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY
Dibenzyl sulphide $\mathbf{C_6H_5}$–$CH_2SC_6H_5$	97.1±2.0	406.3±8.4	Derived from $\Delta_f H^0$ in ref.	1986PED/NAY

4.6 C–C BDEs in radicals

Table 4.6 C–C BDEs in Radicals

The broken bonds (**boldface** = dissociated group)	BDEs (**boldface** = recommended data; reference in parentheses) kcal/mol	kJ/mol	Methods (reference in parentheses)	References
C–C	(1) 142.36	595.63	(1) Derived from $\Delta_f H^0$ in ref.	(1) 1998CHA
	(2) **147.8±3.7**	**618.3±15.4**	(2) Spectroscopy	(2) 2000LU/TOS
C–C_x				
x=2	(1) 175.5	734	(1) Derived from $\Delta_f H^0$ in ref.	(1) 1998CHA
	(2) **167.9**	**703**	(2) Derived from $\Delta_f H^0$ in ref.	(2) 1994GIN/FIN
3	(1) 135.3	566		
	(2) **118.5**	**496**		
	(3) 108.6±3.5	454.4±14.5	(3) PD	(3) 2000CHO/BIS
4	(1) 169.3	708		
	(2) **164.4**	**688**		
5	(2) 116.1	486		
6	(2) 168.2	704		
C^+–C (also see Chapter 24)	143.9±4.6	601.9±19.3	GIB MS	1999LU/TOS
C^-–C (also see Chapter 24)	188.7±0.2	789.6±1.0	Derived from EA in ref.	1996NIST
C_2–C_2	(1) **139.1**	**582**	Derived from $\Delta_f H^0$ in ref.	(1) 1994GIN/FIN
	(2) 168.4	705		(2) 1998CHA
C_2–C_3	(1) **135.5**	**567**	(1) Derived from $\Delta_f H^0$ in ref.	(1) 1994GIN/FIN
	(2) 162.2	679	(2) Derived from $\Delta_f H^0$ in ref.	(2) 1998CHA
	(3) 137.4±3.5	575.0±14.5	(3) PD	(3) 2000CHO/BIS

(continued)

1997YAN/LIN Yang, Y., Linnert, H. V. et al., *J. Phys. Chem. A*, 101, 2371–2378, 1997.
1997YEO/VAT Yeo, Y. Y., Vattuone, L., and King, D. A., *J. Chem. Phys.*, 106, 1990–1996, 1997.
1997YEO/VAT(b) Yeo, Y. Y., Vattuone, L., and King, D. A., *J. Chem. Phys.*, 106, 392–401, 1997.
1997ZAN/TAY Zanni, M. T., Taylor, T. R. et al., *J. Chem. Phys.*, 107, 7613–7619, 1997.
1997ZHA/BAR Zhang, C. M., Bartelt, M. C. et al., *J. Crys. Growth*, 174, 851–857, 1997.
1997ZHA/BOR Zhao, Y., Bordwell, F. D. et al., *J. Am. Chem. Soc.*, 119, 9125–9129, 1997.
1997ZHA/CHE Zhao, H. Q., Cheung, Y. S. et al., *J. Chem. Phys.*, 107, 7230–7241, 1997.
1997ZHA/CHE(b) Zhao, H. Q., Cheung, Y. S. et al., *J. Chem. Phys.*, 106, 86–93, 1997.
1997ZHA/LIN Zhao, R., Lind, J. et al., *J. Chem. Soc. Perkin Trans.* 2, 569–574, 1997.
1997ZHU/ZHA Zhu, Q., Zhang, X. M., and Fry, A. J., *Polymer Degrad Stability*, 57, 43–50, 1997.
1997ZOL/BLA Zolfaghari, A., Blais, S., and Jerkiewicz, G., *Proceedings-Electrochem. Soc.*, 97–16, *Electrochemical Surface Science of Hydrogen Adsorption and Absorption*, 88–100, 1997.
1997ZOL/CHA Zolfaghri, A., Chayer, M., and Jerkiewicz, G., *J. Electrochem. Soc.*, 144, 3034–3041, 1997.
1998ALI/KLO Ali, T., Klotzer, B. et al., *J. Chem. Phys.*, 109, 10996–11009, 1998.
1998ALI/WAL Ali, T., Walker, A. V. et al., *Surf. Sci.*, 414, 304–314, 1998.
1998ALL/VER Allouche, A., Verlaque, P., and Pourcin, J., *J. Phys. Chem. B*, 102, 89–98, 1998.
1998ALM/MAC Almazouzi, A., Macht, M. P. et al., *Phys. Stat. Sol.*, 167, 15–28, 1998.
1998ANN/FRA Anne, A., Fraoua, S. et al., *J. Am. Chem. Soc.*, 120, 2951–2958, 1998.
1998AQU/ASC Aquilanti, V., Ascenzi, D. et al., *J. Chem. Phys.*, 109, 3898–3910, 1998.
1998ASM/TAY Asmis, K. R., Taylor, T. R. et al., *J. Chem. Phys.*, 109, 4389–4395, 1998.
1998ASM/TAY(b) Asmis, K. R., Taylor, T. R., and Neumark, D. M., *Chem. Phys. Lett.*, 295, 75–81, 1998.
1998AUB/HOL Aubry, C., Holmes, J. C., and Walton, J. C., *J. Phys. Chem. A*, 102, 1389–1393, 1998.
1998BAL/GIG Balducci, G., Gigli, G., and Meloni, G., *J. Chem. Phys.*, 109, 4384–4388, 1998.
1998BAR/STO Bardotti, L., Stoldt, C. R. et al., *Phys. Rev. B*, 57, 12544–12549, 1998.
1998BEA/MAC Beattie, D. A., MacLeod, N. A. et al., *J. Electron Spectrosc. Relat. Phenom.*, 97, 191–196, 1998.
1998BEC/BOG Becerra, R., Boganov, S. E. et al., *J. Am. Chem. Soc.*, 120, 12657–12665, 1998.
1998BEC/WAL Becerra, R. and Walsh, R., In *The Chemistry of Organic Silicon Compounds*, Vol. 2, Rappoport, Z. et al., Eds. Wiley, New York, pp. 153–180, 1998, Chap. 4.
1998BEN/LES Bencze, L., Lesar, A., and Popovic, A., *Rapid Commun. Mass Spectrom.*, 12, 917–930, 1998.
1998BER/CAR Berho, F., Caralp, F. et al., *J. Phys. Chem. A*, 102, 1–8, 1998.
1998BOL/CER Bolis, V., Cerrato, G. et al., *Thermochim. Acta*, 312, 63–77, 1998.
1998BOR/LIU Bordwell, F. G. and Liu, W. Z., *J. Phys. Org. Chem.*, 11, 397–406, 1998.
1998BOR/ZHA Bordwell, F. G., Zhao, Y., and Cheng, J. P., *J. Phys. Org. Chem.*, 11, 10–14, 1998.
1998BRA/GRE Braun, J. E., Grebner, T. H., and Neusser, H. J., *J. Phys. Chem. A*, 102, 3273–3278, 1998.
1998BRE/CAH Brechignac, C., Cahuzac, P. et al., *Phys. Rev. Lett.*, 81, 4612–4515, 1998.
1998BRI/DIE Brinkley, D., Dietrich, M. et al., *Surf. Sci.*, 395, 292–306, 1998.
1998BRI/PIC Briquez, S., Picaud, S. et al., *J. Chem. Phys.*, 109, 6435–6449, 1998.
1998BRO/BEC Brocks, J., Beckhaus, H. D. et al., *J. Org. Chem.*, 63, 1935–1943, 1998.
1998BRO/KOS Brown, W. A., Kose, R., and King, D. A., *Chem. Rev.*, 98, 797–831, 1998.
1998BRO/KRE Broenstrup, M., Kretzschmar, I. et al., *Halv. Chim. Acta*, 81, 2348–2369, 1998.
1998BRO/MOF Brown, D. E., Moffatt, D. J., and Wolkow, R. A., *Science*, 279, 542–544, 1998.
1998BRU Brune, H., *Surf. Sci. Rep.*, 31, 121–229, 1998.
1998CAM/BIE Campargue, A., Biennier, L. et al., *Chem. Phys. Lett.*, 288, 734–742, 1998.
1998CAM/FAV Caminati, W., Favero, P. G., and Velino, B., *Chem. Phys.*, 239, 223–227, 1998.
1998CAM/MEL Caminati, W., Melandri, S. et al., *Chem. Phys. Lett.*, 294, 377–380, 1998.
1998CAO/PET Cao, Y., Petersen, J. L., and Stolzenberg, A. M., *Inorg. Chem.*, 37, 5173–5179, 1998.
1998CAP/WIX Capps, K. B., Wixmerten, B. et al., *Inorg. Chem.*, 37, 2861–2864, 1998.

1998CER Cerny, S., *Thermochim. Acta*, 312, 3–16, 1998.
1998CER/HOY Cerda, B. A., Hoyau, S. et al., *J. Am. Chem. Soc.*, 120, 2437–2448, 1998.
1998CHA Chase, M. W. Jr., *NIST-JANAF Thermochemical Table*, 4th ed., *J. Phys. Chem. Ref. Data*, Monograph 9, 1998.
1998CHA/BRA Chabinyc, M. L. and Brauman, J. I., *J. Am. Chem. Soc.*, 120, 10863–10870, 1998.
1998CHE/AUB Chen, Q., Auberry, K. J., and Freiser, B. S., *Int. J. Mass Spectrom. Ion Proc.*, 175, 1–14, 1998.
1998CHE/CHE Chen, E. S. D., Chen, E. C. M., and Sana, N., *Biochem. Biophys. Res. Commun.*, 246, 228–230, 1998.
1998CHE/FRE Chen, Q., Frederick, B. Q., and Richardson, N. V., *J. Chem. Phys.*, 108, 5942–5947, 1998.
1998CHE/FRE(b) Chen, Q. and Freiser, B. S., *J. Phys. Chem. A*, 102, 3343–3351, 1998.
1998CHE/HEA Chen, Y. and Heaven, M. C., *J. Chem. Phys.*, 109, 5171–5174, 1998.
1998CHE/LIU Cheng, J. P., Liu, B., and Zhang, X. M., *J. Org. Chem.*, 63, 7574–7575, 1998.
1998CHE/LIU(b) Cheng, J. P., Liu, B. et al., *J. Org. Chem.*, 63, 7072–7077, 1998.
1998CHE/LU Cheng, J. P., Lu, Y. et al., *Science China Ser. B*, 41, 215–224, 1998.
1998CHE/WAN Cheng, J. P., Wang, K. et al., *Tetrahedron Lett*, 39:7925–7928, 1998.
1998CHE/WON Chen, J., Wong, T. H. et al., *J. Chem. Phys.*, 108, 2285–2296, 1998.
1998CHE/WON(b) Chen, J., Wong, T. H., and Kleiber, P. D., *J. Chem. Phys.*, 109, 8311–8318, 1998.
1998CHE/XIA Cheng, J. P., Xian, M. et al., *J. Am. Chem. Soc.*, 120, 10266–10267, 1998.
1998CHO/MOR Choi, H., Mordaunt, D. H. et al., *J. Chem. Phys.*, 108, 4070–4078, 1998.
1998CHR Christmann, K., In *Electrocatalysis*, Lipkowski, J. et al, Eds., Wiley, New York, pp. 1–41, 1998.
1998CLI/WEN Clifford, E. P., Wenthold, P. G. et al., *J. Chem. Phys.*, 109, 10293–10310, 1998.
1998CLI/WEN(b) Clifford, E. P., Wenthold, P. G. et al., *J. Phys. Chem. A*, 102, 7100–7112, 1998.
1998CLI/WEN(c) Clifford, E. P., Wenthold, P. G. et al., *J. Chem. Soc. Perkin Trans.* 2, No. 5, 1015–1022, 1998.
1998COL/GRE Colussi, A. J. and Grela, M. A., *Int. J. Chem. Kinet.*, 30, 41–45, 1998.
1998COU/MON Courty, A., Mons, M. et al., *J. Phys. Chem. A*, 102, 4890–4898, 1998.
1998COU/MON(b) Courty, A., Mons, M. et al., *J. Phys. Chem. A*, 102, 6590–6600, 1998.
1998DEC/KLO Decker, S. A. and Klobukowski, M., *J. Am. Chem. Soc.*, 120, 9342–9355, 1998.
1998DEN Denisov, E. T., *Russ. Chem. Bull.*, 47, 1274–1279, 1998.
1998DEN/KEB Deng, H. and Kebarle, P., *J. Phys. Chem. A*, 102, 571–579, 1998.
1998DEN/KEB(b) Deng, H. and Kebarle, P., *J. Am. Chem. Soc.*, 120, 2925–2931, 1998.
1998DET/ERV DeTuri, V. F. and Ervin, K. M., *Int. J. Mass Spectrom. Ion Proc.*, 175, 123–132, 1998.
1998DIN/WAN Ding, C. F., Wang, X. B., and Wang, L. S., *J. Phys. Chem. A*, 102, 8633–8636, 1998.
1998DON/WOR Donkers, R. L. and Workentin, M. S., *J. Phys. Chem. B*, 102, 4061–4063, 1998.
1998DOS/SIM dos Santos, R. M. B., and Simoes, J. A. M., *J. Phys. Chem. Ref. Data*, 27, 707–739, 1998.
1998DUN/ROS Dunphy, J. C., Rose, M. et al., *Phys. Rev. B*, 57, R12705–R12708, 1998.
1998EBI/ARN Ebinger, H. D., Arnolds, H. et al., *Surf. Sci.*, 412/413, 586–615, 1998.
1998ELL/AHL Elliott, S. D. and Ahlrichs, R., *J. Chem. Phys.*, 109, 4267–4280, 1998.
1998EPS/SHU Epstein, L. M., Shubina, E. S. et. al., *Inorg. Chem.*, 37, 3013–3017, 1998.
1998FAN/LIU Fan, W. Y., Liu, Z., and Davies, P. B., *J. Mol. Spectrosc.*, 191, 98–107, 1998.
1998FRA/PUL France, M. R., Pullins, S. H., and Duncan, M. A., *J. Chem. Phys.*, 109, 8842–8850, 1998.
1998FUH/WAC Fuhrmann, D., Wacker, D. et al., *J. Chem. Phys.*, 108, 1651–2658, 1998.
1998FUK/MIY Fukuzumi, S., Miyamoto, K. et al., *J. Am. Chem. Soc.*, 120, 2880–2889, 1998.
1998GAL/PAU Galli, C. and Pau, T., *Tetrahedron*, 54, 2893–2904, 1998.
1998GEE/BOI Gee, C., Boissel, P., and Phanessian, G., *Chem. Phys. Lett.*, 298, 85–92, 1998.
1998GER/GRA Gerlach, R., Graham, A. P., and Toennies, J. P., *J. Chem. Phys.*, 109, 5319–5326, 1998.

2000CHE/LEE Cheng, K., Lee, J., and Lyding, J. W., *App. Phys. Lett.*, 77, 3388–3390, 2000.
2000CHE/LIU Cheng, J. P., Liu, B. et al., *J. Am. Chem. Soc.*, 122, 9987–9992, 2000.
2000CHE/LU Cheng, J. P., Lu, Y. et al., *J. Org. Chem.*, 65, 3853–3857, 2000.
2000CHO/BIS Choi, H., Bise, R. T. et al., *J. Phys. Chem. A*, 104, 2025–2032, 2000.
2000CIO/SCH Cioslowski, J., Schimeczek, M. et al., *J. Chem. Phys.*, 113, 9377–9389, 2000.
2000CON/LIY Conceicao, J., Liyanage, R., and Armentrout, P. B., *Chem. Phys.*, 262, 115–130, 2000.
2000COO/LAN Cook, P. A., Langford, S. R. et al., *J. Chem. Phys.*, 113, 994–1004, 2000.
2000CUI/HE Cui, J., He, Y. et al., *Huaxue Wuli Xuebao*, 13, 649–653. 2000.
2000DAH/TOR Dahl, S., Tornqvis, E., and Chorkendorff, I., *J. Catal.*, 192, 381–390, 2000.
2000DAV/GOO Davis, K. K. and Goodman, D. W., *J. Phys. Chem. B*, 104, 8557–8562, 2000.
2000DEN/DEN Denisov, E. T. and Denisova, T. G., *Handbook of Antioxidants*, CRC Press, Boca Raton, 2000.
2000DEN/KHU Denisov, E. T. and Khursan, S. L., *Russ. J. Phys. Chem.*, 74, Suppl. 3, S491–S497, 2000.
2000DIS/BOE Distelrath, V. and Boesl, U., *Faraday Discuss.*, 115, 161–174, 2000.
2000DOP/ROT Dopfer, O., Roth, D., and Maier, J. P., *J. Phys. Chem. A*, 104, 11702–11713, 2000.
2000DUC/GOE Duckworth, D. C., Goeringer, D. E. et al., *J. Am. Soc. Mass Spectrom.*, 11, 1072–1078, 2000.
2000DYA Dyall, K. G., *J. Phys. Chem. A*, 104, 4077–4083, 2000.
2000EIC/ZIM Eicher, B., Zimmermann, H. P., and Gaggeler, H. W., *J. Phys. Chem. A*, 104, 3126–3131, 2000.
2000ESP Espinosa-Garcia J., *Chem. Phys. Lett.*, 316, 563–568, 2000.
2000EVA/GER Evans, C. J. and Gerry, M. C. L., *J. Mol. Spectrosc.*, 203, 105–117, 2000.
2000FAN/CHE Fang, L., Chen, X. et al., *Low Tem. Phys.*, 26, 752–755, 2000.
2000FAN/CHE(b) Fang, L., Chen, X. et al., *J. Phys. Chem. A*, 104, 9153–9155, 2000.
2000FAN/CHE(c) Fang, L., Chen, X. et al., *J. Chem. Phys.*, 113, 10202–10206, 2000.
2000FAR/BUR Farrell, G. L. and Burkey, T. J., *J. Photochem, Photobiol. A Chem.*, 137, 135–139, 2000.
2000FER/ALC Fernandez-Morata, F., Alcami, M. et al., *J. Phys. Chem. A*, 104, 8075–8080, 2000.
2000FOC/LI Focsa, C., Li, H., and Bernath, P. D., *J. Mol. Spectrosc.*, 200, 104–119, 2000.
2000FRE Freund, H. J., *Faraday Discuss.*, 114, 1–31, 2000.
2000FRE/LEM Freeman, S. T. N., Lemke, F. R. et al., *Organometallics*, 19, 4828–4833, 2000.
2000FRI/ZAN Frischkorn, C., Zanni, M. T. et al., *Faraday Discuss.*, 115, 49–62, 2000.
2000GAI/POM Gailbreath, B. D., Pommerening, C. A. et al., *J. Phys. Chem. A*, 104, 2958–2961, 2000.
2000GAP/DUN Gapeev, A. and Dunbar, R. C., *J. Phys. Chem. A*, 104, 4084–4088, 2000.
2000GAP/YAN Gapeev, A., Yang, C. N. et al., *J. Phys. Chem. A*, 104, 3246–3256, 2000.
2000GAS/LAW Gascooke, J. R. and Lawrance, W. D., *J. Phys. Chem. A*, 104, 10328–10335, 2000.
2000GE/KOS Ge, Q., Kose, R., and King, D. A., *Adv. Cataly.*, 45, 207–259, 2000.
2000GIL/TAL Gilles, M. K., Talukdar, R. K., and Ravishankara, A. R., *J. Phys. Chem., A* 104, 8945–8950, 2000.
2000GIN/BAB Gingerich, K. A., Baba, M. S. et al., *Chem. Phys.*, 262, 65–72, 2000.
2000GIN/SCH Gingerich, K. A., Schmude, R. W. et al., *J. Chem. Phys.*, 112, 7443–7448, 2000.
2000GLA/MAK Glasovac, Z. and Maksic, M. E., *J. Org. Chem.*, 65, 1818–1824, 2000.
2000GOL/SMI Golden, D. M. and Smith, G. P., *J. Phys. Chem. A*, 104, 3991–3997, 2000.
2000GRI/SCH Grisenti, R. E., Schollkopf, W. et al., *Phys. Rev. Lett.*, 85, 2284–2287, 2000.
2000GUT/GAL Guthrie, J. P. and Gallant, R. T., *Can. J. Chem.*, 78, 1295–1298, 2000.
2000HAA/MEN Haas, G., Menck, A. et al., *Phys. Rev. B*, 61, 11105–11108, 2000.
2000HAM/WEN Hammad, L. A. and Wenthold, P. W, *J. Am. Chem. Soc.*, 122, 11203–11211, 2000.
2000HAN/CHU Han, S. Y., Chu, I. et al., *J. Chem. Phys.*, 113, 596–601, 2000.
2000HAR/HWA Harich, S. A., Hwang, D. W. H. et al., *J. Chem. Phys.*, 113, 10073–10090, 2000.

2000HIL Hilpert, K., *Fresenius J., Anal. Chem.*, 370, 471–478, 2000.
2000HIL/LAU Hildenbrand, D. L. and Lau, K. H., *Chem. Phys. Lett.*, 319, 95–98, 2000.
2000HIR/NAS Hiraoka, K., Nasu, M. et al., *J. Phys. Chem. A*, 104, 8353–8359, 2000.
2000HIR/IIN Hiraoka, K., Iino, T. et al., *Chem. Phys. Lett.*, 323, 155–159, 2000.
2000HIR/PIN Hirao, T., Pinchemel, B., and Bernath, P. F., *J. Mol. Spectrosc.*, 202, 213–222, 2000.
2000HOF Hoff, C. D., *Coordin. Chem. Rev.*, 206/207, 451–467, 2000.
2000HOP/NIE Hopstaken, M. J. P. and Niemantsverdriet, J. W., *J. Phys. Chem. B*, 104, 3058–3066, 2000.
2000HOP/SAU Hop, C. E. C. A., Saulys, D. A. et al., *J. Mass Spectrom.*, 35, 1003–1010, 2000.
2000HOV/KOL Hovel, S., Kolczewski, C. et al., *J. Chem. Phys.*, 112, 3906–3816, 2000.
2000HUS/AGU Husband, J., Aguirre, F. et al., *J. Phys. Chem. A*, 104, 2020–2024, 2000.
2000ING/BUS Ingolfsson, O., Busolt, U., and Sugawara, K., *J. Chem. Phys.*, 112, 4613–4620, 2000.
2000JAR/MIL Jarek, R. L., Miles, T. D. et al., *J. Phys. Chem. A*, 104, 2230–2237, 2000
2000KIM Kimura, K., In *Photoionization and Photodetachment, Part 1*, Ng, C. Y. Ed., World Science, Singapore, pp. 246–295, 2000, Chap. 6.
2000KIM/CHE Kim, Y. M. and Chen, P., *Int. J. Mass Spectrom.*, 202, 1–7, 2000.
2000KIR/KOR Kiraly, Z., Kortvelyesi, T., and Seres, L., *Phys. Chem. Chem. Phys.*, 3, 349–354, 2000.
2000KOD/PET Kodambaka, S., Petrova, V. et al., *Surf. Rev. Lett.*, 7, 589–593, 2000.
2000KOP/CZA Koperski, J. and Czajkowski, M., *Phys. Rev. A*, 62, 012505/1–012505/9, 2000.
2000KOP/KIE Koperski, J., Kielbasa, S. M., and Czajkowski, M., *Spectrochim. Acta Part A*, 56, 1613–1626, 2000.
2000KOS/MIR Kostikova, L. M., Miroshnichemko, E. A., and Matyushin, Y. N., *Inter Ann Conf. of ICT*, Karlsruhe, Germany, 31st. pp. 50/1–50/11, 2000.
2000KRA/CIR Kranenburg, M., Ciriano, M. V. et al., *J. Phys. Chem. A*, 104, 915–921, 2000.
2000KRE/SCH Kretzschmar, I., Schroder, D. et al., *J. Phys. Chem. A*, 104, 5046–5058, 2000.
2000LAF/SZA Lafleur, R. D., Szatary, B., and Baer, T., *J. Phys. Chem. A*, 104, 1450–1455, 2000.
2000LAT/SAT Latini, A., Satta, M. et al., *Chem. Eur. J.*, 6, 1042–10949, 2000.
2000LEE/AHN Lee, J. G., Ahner, J. et al., *J. Chem. Phys.*, 112, 3351–3357, 2000.
2000LEE/WAN Lee, Y. R., Wang, L. D. et al., *J. Chem. Phys.*, 113, 6107–6112, 2000.
2000LEI/DAG Lei, J. and Dagdigian, P. J., *J. Chem. Phys.*, 113, 602–610, 2000.
2000LI/KOV Li, R., Kovacs, A. D., and North, S. W., *Chem. Phys.*, 254, 309–317, 2000.
2000LIA/HU Liang, F. P., Hu, R. X. et al., *Wuji Xuaxue Xuebao*, 16, 144–145, 2000.
2000LIB/SCO Libuda, J. and Scoles, G., *J. Chem. Phys.*, 112, 1522–1530, 2000.
2000LIU/GOM Liu, Z., Gomez, H., and Neumark, D. M., *Chem. Phys. Lett.*, 332, 65–72, 2000.
2000LON/WEI Long, G. T. and Weitz, E., *J. Am. Chem. Soc.*, 122, 1431–1442, 2000.
2000LOP/FAV Lopez, J. C., Favero, P. G. et al., *Chem. Phys. Lett.*, 316, 81–87, 2000.
2000LOV/BIA Lovejoy, E. R. and Bianco, R., *J. Phys. Chem. A*, 104, 10280–10287, 2000.
2000LU/TOS Lu, W., Tosi, P. et al., *J. Chem. Phys.*, 112, 1330–1334, 2000.
2000LU/ZHU Lu, J. M., Zhu, X. Q. et al., *Chem. J. Chin. Univ.*, 21, 570–572, 2000.
2000MAG/FRE Magnusson, O. T. and Frey, P. A., *J. Am. Chem. Soc.*, 122, 8807–8813, 2000.
2000MAN/ROU Manca, C., Roubin, P., and Martin, C., *Chem. Phys. Lett.*, 330, 21–26, 2000.
2000MAR/HEP Martin, J. D. D. and Hepburn, J. W., *Faraday Diss.*, 115, 407, 2000.
2000MAR/SUG Markin, E. M. and Sugawara, K. I., *J. Phys. Chem. A*, 104, 1416–1422, 2000.
2000MAT/LEB Matyushin, Y. N., Lebedev, V. P. et al., *Inter Ann Conf of ICT, 31st* pp. 51/1–51/8, Karlsruhe, Germany, 2000.
2000MCK McKellar, A. R. W., *J. Chem. Phys.*, 112, 9282–9288, 2000.
2000MCM McMahon, T. B., *Int. J. Mass Spectrom.*, 200, 187–199, 2000.
2000MEL/BAB Meloni, G., Baba, M. S., and Gingerich, K. A., *J. Chem. Phys.*, 113, 8995–8999, 2000.
2000MEL/GIN Meloni, G. and Gingerich, K. A., *J. Chem. Phys.*, 113, 10978–10982, 2000.
2000MEL/PIM Melkhanova, S. V., Pimenova, S. M. et al., *J. Chem. Thermodyn.*, 32, 1311–1317, 2000.