

Bibliography

- [1] J. J. Klicic, R. A. Friesner, S.-Y. Liu, W. C. Guida, *J. Phys. Chem. A* **2002**, *106*, 1327.
- [2] E. Riedel, fourth ed., de Gruyter, Bln, **2002**.
- [3] H. R. Christen, F. Voegtle, *Grundlagen der organischen Chemie, Vol. Vol.1*, Otto Salle Verlag: Frankfurt, Germany, **1988**.
- [4] J. Crystal, R. A. Friesner, *J. Phys. Chem. A* **2000**, *104*, 2362.
- [5] M.-H. Baik, R. A. Friesner, *J. Phys. Chem. A* **2002**, *106*, 7407.
- [6] A. Warshel, S. T. Russel, *Q. Rev. Biophys* **1984**, *17*, 283.
- [7] T. Simonson, J. Carlsson, D. A. Case, *J. Am. Chem. Soc.* **2004**, *126*, 4167.
- [8] D. M. Popovic, A. Zmiric, S. D. Zaric, E. W. Knapp, *J. Am. Chem. Soc.* **2002**, *124*, 3775.
- [9] K. A. Sharp, B. Honig, *Annu. Rev. Biophys. Chem* **1990**, *19*, 301.
- [10] B. Honig, A. Nicholls, *Science* **1995**, *268*, 1144.
- [11] B. Rabenstein, G. M. Ullmann, E. W. Knapp, *Biochemistry* **1998**, *37*, 2488.
- [12] B. Rabenstein, G. M. Ullmann, E. W. Knapp, *Biochemistry* **2000**, *39*, 10487.
- [13] D. Voet, J. G. Voet, *Biochemistry*, second ed., **1995**.
- [14] W. Bauer, K. Khüren, *Methoden der Organischen Chemie, Vol. 832-890*, fifth ed., Georg Thieme Publishers: Stuttgart, Germany, **1985**.
- [15] A. Harriman, *J. Phys. Chem.* **1987**, *91*, 6102.
- [16] C. Li, M. Z. Hoffman, *J. Phys. Chem B.* **1999**, *103*, 6653.
- [17] C. Saby, J. H. T. Luong, *Electroanalysis* **1997**, *10*, 7.
- [18] P. Hapiot, P. Neta, J. Pinson, C. Rolando, S. Schneider, *New J. Chem.* **1993**, *17*, 211.

- [19] Z. Zhu, M. R. Gunner, *Biochemistry* **2005**, *44*, 82.
- [20] R. A. Wheeler, *J. Am. Chem. Soc.* **1994**, *116*, 11048.
- [21] J. E. Leffler, *An introduction to free radicals, Vol. 123*, John Wiley & Sons: New York, **1993**.
- [22] J. Fossey, D. Lefort, J. Sorba, *Free radicals in organic chemistry, Vol. 109*, Masson: Paris, **1995**.
- [23] R. Zhao, J. Lind, G. Merenyi, T. E. Eriksen, *J. Am. Chem. Soc.* **1998**, *120*, 2811.
- [24] R. Zhao, J. Lind, G. Merenyi, T. E. Eriksen, *J. Phys. Chem.* **1999**, *103*, 71.
- [25] R. Zhao, J. Lind, G. Merenyi, M. Jonsson, T. E. Eriksen, *J. Phys. Chem.* **2000**, *104*, 8524.
- [26] K. S. Raymond, A.K.Grafton, R. A. Wheeler, *J.Phys. Chem. B* **1997**, *101*, 623.
- [27] D. Meisel, R. W. Fessenden, *J. Am. Chem. Soc.* **1975**, 7505.
- [28] M. E. Peover, *Journal of the Chemical Society* **1962**, *Nov*, 4540.
- [29] J. G. Smith, M.Fieser, *Reagents for Organic Synthesis, Vol. 12*, Wiley-Interscience: New-York, **1990**.
- [30] P. R. Rich, D. S. Bendall, *Febs. Lett.* **1979**, *105*, 189.
- [31] M. Y. Okamura, G. Feher, *Annu. Rev. Biochem* **1992**, *61*, 861.
- [32] H. Ishikita, G. Morra, E. W. Knapp, *Biochemistry* **2003**, *42*, 3882.
- [33] G. Cecchini, E. Maklashina, V. Yankovskaya, T. M. Iverson, S. Iwata, *FEBS Lett.* **2003**, *545*, 31.
- [34] H. Ishikita, E. W. Knapp, *J. Biol. Chem.* **2003**, *278*, 5202.
- [35] M. Schmidt am Busch, E. W. Knapp, *J. Am. Chem. Soc.* **2005**, *127*, 15730.
- [36] T. C. Bruice, G. L. Schmir, *J. Am. Chem. Soc.* **1958**, *80*, 148.
- [37] M. Tanokura, *Biochim.Biophys.Acta* **1983**, *742*, 576.

- [38] J. Lind, X. Shen, T. E. Eriksen, G. Merenyi, *J. Am. Chem. Soc.* **1990**, *112*, 479.
- [39] P. Wardman, *J. Phys. Chem. Ref. Data* **1989**, *18*, 1637.
- [40] M. D. Liptak, K. C. Cross, P. G. Seybold, S. Feldgus, G. C. Shields, *J. Am. Chem. Soc.* **2002**, *124*, 6421.
- [41] M. Schmidt am Busch, E. W. Knapp, *ChemPhysChem* **2004**, *5*, 1513.
- [42] J. Quenneville, D. M. Popovic, A. L. Stuchebrukhov, *J. Phys. Chem. B* **2004**, *108*, 18283.
- [43] M. D. Liptak, G. C. Shields, *J. Am. Chem. Soc.* **2001**, *123*, 7314.
- [44] P. Winget, C. J. Cramer, D. G. Truhlar, *Theor. Chem. Acc.* **2004**, *112*, 217.
- [45] A. I. Topol, G. J. Tawa, S. K. Burt, *J. Phys. Chem. A* **1997**, *101*, 10075.
- [46] W. H. Richardson, C. Peng, D. Bashford, L. Noodleman, D. A. Case, *Int. J. Quantum Chem.* **1997**, *61*, 207.
- [47] C. Lim, D. Bashford, M. Karplus, *J. Phys. Chem.* **1991**, *95*, 5610.
- [48] G. Schüürmann, M. Cossi, V. Barone, J. Tomasi, *Phys. Chem. A* **1998**, *102*, 6706.
- [49] Y. H. Jang, L. C. Sowers, T. Cagin, W. A. Goddard III, *J. Phys. Chem. A* **2001**, *105*, 274.
- [50] P. Winget, E. J. Weber, C. J. Cramer, D. G. Truhlar, *PhysChemChemPhys* **2000**, *2*, 1231.
- [51] I.-J. Chen, A. D. MacKerell, *Theor. Chem. Acc.* **2000**, *103*, 483.
- [52] Y. Fu, L. Liu, R.-Q. Li, R. Liu, Q.-X. Guo, *J. Am. Chem. Soc.* **2004**, *126*, 814.
- [53] Y. Fu, L. Liu, H.-Z. Yu, Y.-M. Wang, Q.-X. Guo, *J. Am. Chem. Soc.* **2005**, *127*, 7227.
- [54] B. Kallies, R. Mitzner, *J. Phys. Chem. B* **1997**, *101*, 2959.
- [55] J. Li, C. L. Fisher, J. L. Chen, D. Bashford, L. Noodleman, *Inorg. Chem.* **1997**, *35*, 4694.
- [56] A. Klamt, F. Eckert, M. Diedenhofen, M. E. Beck, *J. Phys. Chem. A* **2003**, *107*, 9380.
- [57] E. Demchuk, R. C. Wade, *J. Phys. Chem.* **1996**, *100*, 17373.

- [58] D. Bashford, *Curr. Opin. Struct. Biol.* **1991**, *1*, 175.
- [59] M. Strajbl, A. Shurki, A. Warshel, *Proc. Natl. Acad. Sci. USA* **2003**, *100*, 14834.
- [60] G. M. Ullmann, *J. Phys. Chem. B.* **2000**, *104*, 6293.
- [61] P. Voigt, E. W. Knapp, *J. Biol. Chem.* **2003**, *278*, 51993.
- [62] T. Simonson, G. Archontis, M. Karplus, *J. Phys. Chem. B.* **1999**, 6142.
- [63] D. M. Popovic, A. A. Stuchebrukhov, *J. Am. Chem. Soc.* **2004**, *126*, 1858.
- [64] G. M. Ullmann, *J. Phys. Chem. B* **2002**, 1263.
- [65] M. Garcia-Viloca, J. Gao, M. Karplus, D. G. Truhlar, *Science* **2004**, *303*, 186.
- [66] A. Warshel, *Nature* **1987**, *330*, 15.
- [67] G. M. Ullmann, E. W. Knapp, *Eur. Biophys. J.* **1999**, *28*, 533.
- [68] W. C. Still, A. Tempczyk, R. C. Hawley, T. Hendrickson, *J. Am. Chem. Soc.* **1990**, *112*, 6127.
- [69] B. H. Besler, K. M. Merz, P. A. Kollman, *J. Comp. Chem.* **1990**, *11*, 431.
- [70] C. I. Bayly, P. Cieplak, W. D. Cornell, P. A. Kollman, *J. Phys. Chem.* **1993**, *97*, 10269.
- [71] U. C. Sing, P. A. Kollmann, *J. Comp. Chem* **1984**, *5*, 129.
- [72] L. E. Chirlain, M.M. Francl, *J. Comput. Chem.* **1987**, *6*, 894.
- [73] E. Sigfridson, U. Ryde, *J. Comput. Chem* **1998**, *19*, 377.
- [74] E. Sigfridsson, U. Ryde, B. L. Bush, *J. Comput. Chem* **2002**, *23*, 351.
- [75] A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 1372.
- [76] A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648.
- [77] C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785.

- [78] L. A. Curtiss, P. C. Redfern, K. Raghavachari, V. Rassolov, J. A. Pople, *J. Chem. Phys.* **1999**, *110*, 4703.
- [79] T. H. Dunning-Jr., *J. Chem. Phys.* **1989**, *90*, 1007.
- [80] R. A. Kendall, T. H. Dunning-Jr., R. J. Harrison, *J. Chem. Phys.* **1992**, *96*, 6796.
- [81] J. C. Rienstra-Kiracofe, G. S. Tschumper, H. F. Schaefer, S. Nandi, G. B. Ellison, *Chemical Reviews* **2002**, *102*, 231.
- [82] J. Warwicker, H. C. Watson, *J. Mol. Biol.* **1982**, *157*, 671.
- [83] A. S. Galstyan, S. D. Zaric, E.-W. Knapp, *J. Biol. Inorg. Chem.* **2005**, *10*, 343.
- [84] R. M. Noyes, *J. Am. Chem. Soc.* **1962**, *84*, 513.
- [85] M. D. Tissandier, K. A. Cowen, W. Y. Feng, E. Gundlach, M. H. Cohen, A. D. Earhart, J. V. Coe, T. R. Tuttle Jr., *J. Phys. Chem. A* **1998**, *102*, 7787.
- [86] J. Florian, A. Warshel, *J. Phys. Chem. B* **1997**, *101*, 5583.
- [87] C. E. Klots, *J. Phys. Chem.* **1981**, *85*, 3585.
- [88] S. Trasatti, *J. Electroanal. Chem* **1982**, *139*, 1.
- [89] G. J. Tawa, A. Topol, S. K. Burt, R. A. Caldwell, A. A. Rashin, *J. Chem. Phys.* **1998**, *4852-4863*, 109.
- [90] H. Reiss, A. Heller, *J. Phys. Chem.* **1985**, *89*, 4207.
- [91] A. Szabo, N. S. Ostlund, *Modern Quantum Chemistry*, first (revised) ed., Dover, **1996**.
- [92] I. A. Levine, *Quantum Chemistry*, fifth ed., Prentice-Hall, Inc, **2000**.
- [93] V. May, O. Kuehn, *Charge and Energy Transfer Dynamics in Molecular Systems*, first (reprint) ed., Wiley-VCH, **2000**.
- [94] K. Wolfram, M. C. Holthausen, *A Chemist's Guide to Density Functional Theory*, second ed., Wiley-VCH, **2001**.

- [95] C. W. Bauschlicher, A. Ricca, H. Partridge, S. R. Langhoff, "*Chemistry by Density Functional Theory*" in *Recent Advances in Density Functional Methods Part II*, Chong, D.P. (ed), World Scientific, Singapore, **1997**.
- [96] J. M. L. Martin,, (Eds.: P. Geerlings, F. D. Proft, F. Langenaeker), VUB Press, Brussels, **2000**.
- [97] K. S. Raymond, R. A. Wheeler, *J.Comp. Chem* **1999**, 20, 207.
- [98] S. J. Vosko, L. Wilk, M. Nussair, *Canadien Journal of Chemistry* **1980**, 58, 1200.
- [99] R. Colle, O. Salvetti, *Theor. Chim. Acta.* **1975**, 37, 329.
- [100] J. P. Perdew, Y. Wang, *Phys. Rev.B.* **1992**, 45, 13244.
- [101] J. P. Perdew, *Phys. Rev.B.* **1986**, 33, 8822.
- [102] A. D. Becke, *Phys. Rev.* **1988**, 38, 3098.
- [103] A. D. Becke, *J.Chem.Phys.* **1995**, 104, 1041.
- [104] P. J. Stevens, J. F. Devlin, C. F. Chabalowski, M. J. Frisch, *J.Phys. Chem.* **1994**, 98, 11623.
- [105] F. Herman, J. P. V. Dyke, I. B. Ortenburger, *Phys. Rev.Lett.* **1969**, 22, 807.
- [106] L. A. Curtiss, K. Raghavachari, P. C. Redfern, V. Rassolov, J. A. Pople, *J.Chem.Phys.* **1998**, 109, 7764.
- [107] L. A. Curtiss, K. Raghavachari, G. W. Trucks, J. A. Pople, *J.Chem.Phys.* **1991**, 94, 7221.
- [108] A. L. Leach, *Molecular Modeling*, first (reprinted) ed., **1998**.
- [109] C. M. Breneman, K. B. Wiberg, *J. Comp. Chem.* **1990**, 11, 361.
- [110] E. Sigfridsson, U. Ryde, *J.Comp. Chem* **1997**, 19, 377.
- [111] D. A. McQuarrie, *Statistical Mechanics*, Harber&Row, New York, **1976**.
- [112] T. L. Hill, *An Introduction to Statistical Thermodynamics*, Dover Publications, New York, **1986**.

- [113] D. Bashford, K. Gerwert, *J. Mol. Biol.* **1992**, *33*, 473.
- [114] D. Bashford, D. A. Case, C. Dalvit, L. Tennant, P. E. Wright, *Biochemistry* **1993**, *32*, 8045.
- [115] A. Nicolls, B. Honig, *J. Comp. Chem.* **1991**, *12*, 435.
- [116] W. Press, S. Teukolsky, W. Vetterling, B. Flannery, *Numerical Recipes in C*, second ed., Cambridge University Press, **1992**.
- [117] M. Schaefer, M. Karplus, *J. Phys. Chem.* **1996**, *100*, 1578.
- [118] M. Schaefer, M. Sommer, M. Karplus, *J. Phys. Chem. B.* **1997**, *101*, 1663.
- [119] M. Schaefer, C. Frömmel, *J. Mol. Biol.* **1990**, *216*, 1045.
- [120] J. V. Coe, *Chem. Phys. Lett.* **1994**, *229*, 161.
- [121] R. Gomer, G. Tryson, *J. Chem. Phys.* **1977**, *66*, 4413.
- [122] B. Wilson, R. Georgiadis, J. E. Bartmess, *J. Am. Chem. Soc.* **1991**, *113*, 1762.
- [123] J. E. B. Randles, *Trans. Faraday Soc.* **1956**, *52*, 1573.
- [124] Y. Gurevich, V. Pleskov, *Sov. Electrochem.* **1982**, *18*, 1315.
- [125] F. Lohmann, *Z. Naturforsch. A.* **1967**, *22*, 843.
- [126] C.-G. Zhan, D. A. Dixon, *J. Phys. Chem. A.* **2001**, *105*, 11534.
- [127] J. Florian, A. Warshel, *J. Phys. Chem. B* **1999**, *103*, 10282.
- [128] P. JAGUAR 4.2 Schrödinger Inc, OR. 2002.
- [129] A. Bondi, *J. Phys. Chem.* **1964**, 441-551.
- [130] I. Tunon, E. Silla, J.-L. Pascual-Ahuir, *J. Am. Chem. Soc.* **1993**, *115*, 2226.
- [131] GAUSSIAN03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, B. P. M. W. Gill, G. Johnson, M. A. Robb, J. R. Cheeseman, T. A. Keith, G. A. Petersson, J. A. Montgomery, K. Raghavachari, M. A. Al-Laham, V. G. Zakrzewski, J. V. Ortiz, J. B. Foresman, J. Cioslowski, B. B. Stefanov, A. Nanayakkara, M. Challacombe, C. Y. Peng, P. Y. Ayala, W. Chen, M. W. Wong, J. L. Andres, E. S. Replogle, R. Gomperts, R. L. Martin, D. J. Fox,

- J. S. Binkley, D. J. Defrees, J. Baker, J. P. Stewart, M. Head-Gordon, C. Gonzales, J. A. Pople, *Gaussian, Inc., Pittsburgh, PA* **2003**.
- [132] D. C. R. Guide, http://www.clippercontrols.com/info/dielectric_constants.html.
- [133] J. E. Bartmess, "Negative Ion Energetics Data" in *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*, Eds. P.J. Linstrom and W.G. Mallard, March 2003, National Institute of Standards and Technology, Gaithersburg MD, 20899 (<http://webbook.nist.gov>).
- [134] E. P. Hunter, S. G. Lias, in *NIST Chemistry WebBook, NIST Standard Reference Database, Number 69: Negative Ion Energetics Data*(Eds.:P.J. Linstrom, W.G. Mallard), National Institute of Standards and Technology, Gaithersburg MD, March 2003, 20899 (<http://webbook.nist.gov>).
- [135] E. P. Hunter, S. G. Lias, *J. Phys. Chem. Ref. Data* **1998**, 27, 413.
- [136] G. Caldwell, R. Renneboog, P. Kebarle, *Canadian Journal of Chemistry* **1989**, 67, 611.
- [137] T. B. McMahon, P. Kebarle, *J. Am. Chem. Soc.* **1977**, 99, 2222.
- [138] M. Fujio, R. T. McIver, R. W. Taft, *J. Am. Chem. Soc.* **1981**, 103, 4017.
- [139] D. H. Aue, H. M. Webb, W. R. Davidson, P. Toure, H. P. Hopkins-Jr, S. P. Moulik, D. V. Jahagirdar, *J. Am. Chem. Soc.* **1991**, 113, 1770.
- [140] A. Mackerell, D. Bashford, M. Bellott, R. Dunbrack, J. Evanseck, M. Field, S. Fischer, J. Guo, S. Ha, D. Joseph, L. Kuchnir, K. Kuczera, F. Lau, C. Mattos, S. Michnick, T. Ngo, D. Nguyen, B. Prodhom, W. Reiher, B. Roux, J. Smith, R. Stote, J. Straub, M. Watanabe, M. Wiorcikiewicz-Kuczera, D. Yin, M. Karplus, *J. Phys. Chem. B.* **1998**, 102, 3586.
- [141] S. Steenken, P. Neta, *J. Phys. Chem.* **1982**, 86, 3661.
- [142] D. A. Armstrong, Q. Sun, R. H. Schuler, *J. Phys. Chem.* **1996**, 100, 9892.
- [143] G. A. Larsen, H. A. Holm, M. Roberson, K. Daasbjerg, *J. Am. Chem. Soc.* **2001**, 123, 1723.
- [144] J. Robert, M. Anouti, J. Paris, *J. Chem. Soc. Perkin. Trans. 2* **1997**, 473.
- [145] R. Gunion, M. Gilles, M. Polak, W. Lineberger, *International Journal of Mass Spectrometry and Ion Processes* **1992**, 117, 601.

- [146] J. H. Richardson, L. M. Stephenson, J. I. Brauman, *J. Am. Chem. Soc.* **1975**, *28*, 2967.
- [147] J. Schiedt, R. Weinkauf, *J. Chem. Phys.* **1999**, 304.
- [148] T. Heinis, S. Chowdbury, S. L. Scott, P. Kebarle, *J. Am. Chem. Soc.* **1988**.
- [149] J. Marks, P. B. Comita, J. I. Brauman, *J. Am. Chem. Soc.* **1985**, *107*, 3718.
- [150] R. W. Taft, F. G. Bordwell, *Acc. Chem. Res.* **1988**, *21*, 463.
- [151] C. F. Ding, X. B. Wang, L. S. Wang, *J. Phys. Chem. A.* **1998**, *102*, 8633.
- [152] A. Rauk, D. A. Armstrong, *J. Am. Chem. Soc.* **1994**, *116*, 8222.
- [153] M. Kieninger, O. N. Ventura, A. Suhai, *Int. J. Quantum Chem.* **1998**, *70*, 253.
- [154] M. Jonsson, A. Houmam, G. Jocys, D. D. M. Wayner, *J. Chem. Soc. Perkin. Trans. 2* **1999**, 425.
- [155] S. Miertus, E. Scrocco, J. Tomasi, *J. Chem. Phys.* **1981**, *55*, 117.
- [156] S. Miertus, J. Tomasi, *J. Chem. Phys.* **1982**, *65*, 239.
- [157] M. Cossi, V. Barone, J. Tomasi, *J. Chem. Phys.* **1997**, *107*, 3210.
- [158] V. Barone, M. Cossi, *J. Phys. Chem. A.* **1998**, *102*, 1995.
- [159] *Handbook of chemistry and physics*, 73 ed., CRC Press, Boca Raton, **1992-1993**.
- [160] A. J. Swallow, *Functions of Quinones in Energy Conserving Systems*, Academic Press, **1982**.
- [161] J. A. Montgomery, M. J. Frisch, J. W. Ochterski, G. A. Peterson, *J. Chem. Phys.* **1999**, *110*, 2822.
- [162] B. H. Greely, T. V. Russo, D. T. Mainz, R. A. Friesner, J. M. Langlois, W. A. Goddard III, R. E. Donnelly, M. N. Ringalda, *J. Chem. Phys.* **1994**, *101*, 10075.
- [163] P. JAGUAR 3.5 Schrödinger Inc, OR. 1998.

- [164] C.R. Ganellin, *Molecular and Quantum Pharmacology*, Proceedings of the Seventh Jerusalem Symposium on Quantum and Biochemistry; Bergmann, E. D.; Pullman, B.; Eds.; D. Reidel Publishing Co.: Dordrecht/Boston, **1974**, pp. 43-55.