

# Bibliography

- [1] G. A. Jeffrey, *An Introduction to Hydrogen Bonding* (Oxford University Press, New York, 1997)
- [2] F. S. Dainton (chair), *The Kinetics of Proton Transfer Processes*, Faraday Discuss. Chem. Soc. **39** (1965)
- [3] D. H. Whiffen (chair), *Electron and Proton Transfer*, Faraday Discuss. Chem. Soc. **74** (1982)
- [4] A. Douhal, F. Lahmani, A. H. Zewail, Chem. Phys. **207**, 477 (1996)
- [5] T. Elsaesser, H. J. Bakker (eds.), *Ultrafast Hydrogen Bonding Dynamics and Proton Transfer Processes in the Condensed Phase* (Kluwer Academic Publ., Dordrecht, 2003)
- [6] S. Mukamel, *Principles of Nonlinear Optical Spectroscopy* (Oxford University Press, Oxford, 1995)
- [7] R. P. Bell, *The Tunnel Effect in Chemistry* (Chapman and Hall, London, 1980)
- [8] V. A. Benderskii, V. I. Goldanskii, D. E. Makarov, Phys. Rep. **233**, 195 (1993)
- [9] A. Kohen, J. P. Klinman, *Enzyme Catalysis: Beyond Classical Paradigms*, Acc. Chem. Res. **31**, 397 (1998)
- [10] P. R. Bunker, *Molecular Symmetry and Spectroscopy* (Academic Press, New York, 1979)
- [11] J. M. Hollas, *High Resolution Spectroscopy* (John Wiley & Sons, New York, 1998)
- [12] F. Madeja, M. Havenith, J. Chem. Phys. **117**, 7162 (2002)
- [13] A. J. Horsewill, N. H. Jones, R. Caciuffo, Science **291**, 100 (2001)

- [14] R. J. Abraham, P. Loftus, J. P. Fisher, *Introduction to NMR Spectroscopy* (John Wiley & Sons Ltd., New York, 1988)
- [15] M. Pettersson, E. M. S. Maçôas, L. Khriachtchev, J. Lundell, R. Fausto, M. Räsänen, *J. Chem. Phys.* **117**, 9095 (2002)
- [16] L. D. Landau, E. M. Lifschitz, *Lehrbuch der theoretischen Physik - Band III - Quantenmechanik* (Akademie-Verlag, Berlin, 1979)
- [17] M. Born, R. Oppenheimer, *Ann. Phys.* **84**, 457 (1927)
- [18] W. Domcke, H. Koppel, L. S. Cederbaum, *Mol. Phys.* **43**, 851 (1981)
- [19] E. B. Wilson, J. C. Decius, P. C. Cross, *Molecular Vibrations - The Theory of Infrared and Raman Vibrational Spectra* (Dover Publications, New York, 1955)
- [20] T. Uzer, *Phys. Rep.* **199**, 73 (1991)
- [21] M. Gruebele, *Adv. Chem. Phys.* **114**, 193 (2000)
- [22] P. M. Felker, A. H. Zewail, *J. Chem. Phys.* **82**, 2961 (Paper I to IV)
- [23] D. L. Thompson (Editor), *Modern Methods for Multidimensional Dynamics Computations in Chemistry* (World Scientific, Singapore, 1998)
- [24] O. Kühn, J. Manz, W. H. Miller (guest editors), *Towards Multidimensional Quantum Reaction Dynamics*, special issue, *Chem. Phys.* **304**, no. 1-2 (2004)
- [25] M. H. Beck, A. Jäckle, G. A. Worth, H.-D. Meyer, *Phys. Rep.* **324**, 1 (2000)
- [26] H.-D. Meyer, G. A. Worth, *Theor. Chem. Acc.* **109**, 251 (2003)
- [27] K. Takatsuka, H. Ushiyama, *Phys. Rev. A* **51**, 4353 (1995)
- [28] K. Takatsuka, H. Ushiyama, A. Inoue-Ushiyama, *Phys. Rep.* **322**, 347 (1999)
- [29] N. Makri, W. H. Miller, *J. Chem. Phys.* **91**, 4026 (1989)
- [30] S. Takada, H. Nakamura, *J. Chem. Phys.* **100**, 98 (1994)
- [31] M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, first edition (Springer-Verlag, New York, NY, 1990)
- [32] F. Grossmann, *Comments At. Mol. Phys.* **34**, 141 (1999)
- [33] M. Baranger, M. A. M. de Aguiar, F. Keck, H. J. Korsch, B. Schellhaß, J. *Phys. A: Math. Gen.* **34**, 7227 (2001)

- [34] M. F. Herman, E. Kluk, Chem. Phys. **91**, 27 (1984)
- [35] E. J. Heller, J. Chem. Phys. **75**, 2923 (1981)
- [36] V. A. Mandelshtam, J. Chem. Phys. **108**, 9999 (1998)
- [37] V. A. Mandelshtam, H. S. Taylor, J. Chem. Phys. **107**, 6756 (1997)
- [38] V. A. Mandelshtam, Progress in Nuclear Magnetic Resonance Spectroscopy **38**, 159 (2001)
- [39] V. A. Mandelshtam, M. Ovchinnikov, J. Chem. Phys. **108**, 9206 (1998)
- [40] R. L. Redington, R. L. Sams, J. Phys. Chem. A **106**, 7494 (2002).
- [41] M. E. Tuckerman, D. Marx, Phys. Rev. Lett. **86**, 4946 (2001)
- [42] B. A. Ruf, W. H. Miller, J. Chem. Soc., Faraday Trans. 2 **84**, 1523 (1988).
- [43] K. Yagi, T. Taketsugu, K. Hirao, J. Chem. Phys. **115**, 10647 (2001)
- [44] I. N. Levine, *Quantum Chemistry*, 4th edition (Prentice-Hall Int., Inc., 1991)
- [45] W. Kohn, Rev. Mod. Phys. **71**, 1253 (1999); references therein
- [46] J. A. Pople, Rev. Mod. Phys. **71**, 1267 (1999); references therein
- [47] R. L. Redington, J. Chem. Phys. **113**, 2319 (2000)
- [48] R. L. Redington, T. E. Redington, J. M. Montgomery, J. Chem. Phys. **113**, 2304 (2000).
- [49] I. C. Percival, *Semiclassical theory of bound states*, Adv. Chem. Phys. **36**, 1 (1977)
- [50] J. Ford, Adv. Chem. Phys. **24**, 155 (1973)
- [51] H. Goldstein, *Klassische Mechanik* (Akad. Verlagsgesellschaft, Wiesbaden, 7. Auflage)
- [52] V. P. Maslov, M. V. Fedoriuk, *Semi-classical Approximation in Quantum Mechanics* (D. Reidel Publishing Company, Dordrecht, Holland, 1981)
- [53] J. B. Delos, Adv. Chem. Phys. **65**, 161-214 (1985)
- [54] S. K. Knudson, J. B. Delos, D. W. Noid, J. Chem. Phys. **84**, 6886 (1986)
- [55] M. Wilkinson, Physica **21D**, 341 (1986)

- [56] Z. H. Huang, T. E. Feuchtwang, P. H. Cutler, E. Kazes, Phys. Rev. A **41**, 32 (1990)
- [57] S. Takada, J. Chem. Phys. **104**, 3742 (1996)
- [58] V. A. Benderskii, S. Yu. Grebenschchikov, G. V. Mil'nikov, Chem. Phys. **194**, 1 (1995)
- [59] G. V. Mil'nikov, H. Nakamura, J. Chem. Phys. **115**, 6881 (2001)
- [60] H. Ushiyama, K. Takatsuka, J. Chem. Phys. **109**, 9664 (1998)
- [61] K. Takatsuka, *private communication*, 01/2003
- [62] K. Giese, unpublished, 04/2003
- [63] D. W. Noid, M. L. Koszykowski, R. A. Marcus, J. Chem. Phys. **67**, 404 (1977)
- [64] V. I. Arnold, *Mathematical Methods of Classical Mechanics* (Springer, New York, Second Edition, 1989)
- [65] R. T. Skodje, F. Borondo, W. P. Reinhardt, J. Chem. Phys. **82**, 4611 (1985)
- [66] L. M. Raff, D. L. Thompson, in *Theory of Chemical Reaction Dynamics*, edited by M. Baer, Vol. III, p. 1 (CRC, Boca, Raton, FL, 1985)
- [67] D. Heidrich (Ed.), *The Reaction Path in Chemistry: Current Approaches and Perspectives* (Kluwer Academic Publishers, Dordrecht, 1995)
- [68] A. Tachibana, K. Fukui, Theor. Chim. Acta (Berlin) **51**, 189 (1979).
- [69] E. J. Heller, J. Phys. Chem. **99**, 2625 (1995)
- [70] C. Herring, Rev. Mod. Phys. **34**, 631 (1962)
- [71] V. A. Benderskii, S. Yu. Grebenschchikov, G. V. Mil'nikov, E. V. Vetoshkin, Chem. Phys. **188**, 19 (1994)
- [72] V. A. Benderskii, S. Yu. Grebenschchikov, E. V. Vetoshkin, G. V. Mil'nikov, D. E. Makarov, J. Phys. Chem. **98**, 3300 (1994)
- [73] D. G. Truhlar, A. D. Isaacson, B. C. Garrett, in *Theory of Chemical Reaction Dynamics*, edited by M. Baer, Vol. IV, p. 65 (CRC, Boca, Raton, FL, 1985)
- [74] E. Bosch, M. Moreno, J. M. Lluch, J. Bertrán, J. Chem. Phys. **93**, 5685 (1990)

- [75] S. Takada, H. Nakamura, J. Chem. Phys. **102**, 3977 (1995)
- [76] M. J. Wójcik, H. Nakamura, S. Iwata, W. Tatara, J. Chem. Phys. **112**, 6322 (2000).
- [77] N. Makri, W. H. Miller, J. Chem. Phys. **87**, 5781 (1987)
- [78] H.-D. Meyer, U. Manthe, L. S. Cederbaum, Chem. Phys. Lett. **165**, 73 (1990)
- [79] G. Worth, H.-D. Meyer, L. S. Cederbaum, J. Chem. Phys. **109**, 3518 (1998)
- [80] J. C. Light, I. P. Hamilton, J. V. Lill, J. Chem. Phys. **82**, 1400 (1985)
- [81] D. T. Colbert, W. H. Miller, J. Chem. Phys. **96**, 1982 (1992)
- [82] M. Nest, H.-D. Meyer, J. Chem. Phys. **117**, 10499 (2002)
- [83] G. A. Worth, J. Chem. Phys. **114**, 1524 (2001)
- [84] H. Wang, M. Thoss, J. Chem. Phys. **119**, 1289 (2003)
- [85] W. H. Miller, Adv. Chem. Phys. **25**, 69 (1974)
- [86] M. C. Gutzwiller, J. Math. Phys. **8**, 1979 (1967)
- [87] H. Kleinert, *Pfadintegrale in Quantenmechanik, Statistik und Polymerphysik* (BI-Wissenschaftsverlag, Mannheim, 1993)
- [88] W. H. Miller, J. Phys. Chem. A **105**, 2942 (2001)
- [89] K. G. Kay, J. Chem. Phys. **100**, 4377 (1994)
- [90] N. Metropolis, A. Rosembluth, M. Rosembluth, A. Teller, E. Teller, J. Chem. Phys. **21**, 1087 (1953)
- [91] K. G. Kay, J. Chem. Phys. **101**, 2250 (1994)
- [92] X. Sun, W. H. Miller, J. Chem. Phys. **108**, 8870 (1998)
- [93] T. Yamamoto, W. H. Miller, J. Chem. Phys. **118**, 2135 (2003)
- [94] S. Garashchuk, D. Tannor, Chem. Phys. Lett. **262**, 477 (1996)
- [95] F. Grossmann, V. A. Mandelshtam, H. S. Taylor, J. S. Briggs, Chem. Phys. Lett. **279**, 355 (1997)
- [96] E. Kluk, M. F. Herman, H. L. Davis, J. Chem. Phys. **84**, 326 (1986)
- [97] Y. Weissman, J. Chem. Phys. **76**, 4067 (1982)

- [98] J. Ankerhold, M. Saltzer, E. Pollak, *J. Chem. Phys.* **116**, 5925 (2002)
- [99] Y. Guo, S. Li, D. L. Thompson, *J. Chem. Phys.* **107**, 2853 (1997)
- [100] T. D. Sewell, Y. Guo, D. L. Thompson, *J. Chem. Phys.* **103**, 8557 (1995)
- [101] Y. Guo, D. L. Thompson, *J. Phys. Chem. A* **106**, 8374 (2002)
- [102] V. Guallar, B. F. Gherman, W. H. Miller, S. J. Lippard, R. A. Friesner, *J. Am. Chem. Soc.* **124**, 3377 (2002)
- [103] M. Ben-Nun, T. J. Martínez, *J. Phys. Chem. A* **103**, 6055 (1999)
- [104] V. A. Benderskii, E. V. Vetoshkin, S. Yu. Grebenschikov, L. von Laue, H. P. Trommsdorff, *Chem. Phys.* **219**, 119 (1997)
- [105] G. V. Mil'nikov, H. Nakamura, *J. Chem. Phys.* **122**, 124311 (2005)
- [106] G. V. Mil'nikov, K. Yagi, T. Taketsugu, H. Nakamura, K. Hirao, *J. Chem. Phys.* **120**, 5036 (2004)
- [107] G. V. Mil'nikov, O. Kühn, H. Nakamura, *J. Chem. Phys.* **123**, 074308 (2005)
- [108] C. S. Tautermann, A. F. Voegele, T. Loerting, K. R. Liedl, *J. Chem. Phys.* **117**, 1962 (2002)
- [109] T. C. Allison, D. G. Truhlar, in: *Modern Methods for Multidimensional Dynamics Computations in Chemistry*, edited by D. L. Thompson, p. 618 (World Scientific, Singapore, 1998)
- [110] Y.-P. Liu, G. C. Lynch, T. N. Truong, D.-h. Lu, D. G. Truhlar, B. C. Garrett, *J. Am. Chem. Soc.* **115**, 2408 (1993)
- [111] W. H. Miller, N. C. Handy, J. E. Adams, *J. Chem. Phys.* **72**, 99 (1980)
- [112] R. A. Marcus, M. E. Coltrin, *J. Chem. Phys.* **67**, 2609 (1977)
- [113] B. C. Garrett, D. G. Truhlar, *J. Chem. Phys.* **79**, 4931 (1983)
- [114] C. S. Tautermann, A. F. Voegele, T. Loerting, K. R. Liedl, *J. Chem. Phys.* **117**, 1967 (2002)
- [115] M. Razavy, A. Pimpale, *Phys. Rep.* **168**, 305 (1988)
- [116] S. K. Gray, D. W. Noid, B. G. Sumpter, *J. Chem. Phys.* **101**, 4062 (1994)
- [117] J.-H. Lim, E. K. Lee, Y. Kim, *J. Phys. Chem. A* **101**, 2233 (1997)

- [118] Y. Kim, J. Am. Chem. Soc. **118**, 1522 (1996)
- [119] N. Shida, P. F. Barbara, J. Almlöf, J. Chem. Phys. **94**, 3633 (1991)
- [120] M. V. Vener, O. Kühn, J. M. Bowman, Chem. Phys. Lett. **349**, 562 (2001)
- [121] H. Ushiyama, K. Takatsuka, J. Chem. Phys. **115**, 5903 (2001)
- [122] S. Miura, M. E. Tuckerman, M. L. Klein, J. Chem. Phys. **109**, 5290 (1998)
- [123] K. Wolf, A. Simperler, W. Mikenda, Monatshefte für Chemie **130**, 1031 (1999)
- [124] M. J. Frisch *et al.*, Gaussian 98 (Revision A.7), Gaussian, Inc., Pittsburgh, 1998
- [125] Ch. Rambaud, H. P. Trommsdorff, Chem. Phys. Lett. **306**, 124 (1999)
- [126] C. S. Tautermann, A. F. Voegele, K. R. Liedl, J. Chem. Phys. **120**, 631 (2004)
- [127] W.-T. Chan, I. P. Hamilton, J. Chem. Phys. **105**, 5907 (1996)
- [128] W.-T. Chan, I. P. Hamilton, Chem. Phys. Lett. **292**, 57 (1998)
- [129] W.-T. Chan, *private communication*
- [130] J. Main, K. Weibert, V. A. Mandelshtam, G. Wunner, Phys. Rev. E **60**, 1639 (1999)
- [131] N. T. Maitra, E. J. Heller, Phys. Rev. Lett. **78**, 3035 (1997)
- [132] B. Spath, W. H. Miller, J. Chem. Phys. **104**, 95 (1996)
- [133] F. Grossmann, E. J. Heller, Chem. Phys. Lett. **241**, 45 (1995)
- [134] K. G. Kay, J. Chem. Phys. **107**, 2313 (1997)
- [135] J. Main, Phys. Rep. **316**, 233 (1999)
- [136] M. R. Wall, D. Neuhauser, J. Chem. Phys. **102**, 8011 (1995)
- [137] V. A. Mandelshtam, H. S. Taylor, Phys. Rev. Lett. **78**, 3274 (1997)
- [138] T. Bartsch, J. Main, G. Wunner, Phys. Rev. E **64**, 056705 (2001)
- [139] J. Chen, V. A. Mandelshtam, A. J. Shaka, J. Magn. Reson. **146**, 363 (2000)

- [140] G. A. Worth, M. Beck, A. Jäckle, H.-D. Meyer, *The MCTDH Package*, Version 8.2 (University of Heidelberg, Heidelberg, 2002)
- [141] O. Kühn, D. Lahav, *private communication*, 2002
- [142] W. H. Miller, in *Potential Energy Surfaces and Dynamics Calculations*, edited by D. G. Truhlar, p. 265 (Plenum Press, New York, 1981)
- [143] T. Carrington, Jr., W. H. Miller, *J. Chem. Phys.* **81**, 3942 (1984)
- [144] D. Lauvergnat, A. Nauts, Y. Justum, X. Chapuisat, *J. Chem. Phys.* **114**, 6592 (2001).
- [145] T. Carrington, Jr., W. H. Miller, *J. Chem. Phys.* **84**, 4364 (1986)
- [146] N. Shida, P. F. Barbara, J. E. Almlöf, *J. Chem. Phys.* **91**, 4061 (1989)
- [147] D. Babic, S. D. Bosanac, N. Doslić, *Chem. Phys. Lett.* **358**, 337 (2002)
- [148] M. V. Vener, S. Scheiner, N. D. Sokolov, *J. Chem. Phys.* **101**, 9755 (1994)
- [149] H. Naundorf, J. A. Organero, A. Douhal, O. Kühn, *J. Chem. Phys.* **110**, 11286 (1999).
- [150] M. Petković, O. Kühn, *J. Phys. Chem. A* **107**, 8458 (2003).
- [151] T. Hayashi, S. Mukamel, *J. Phys. Chem. A* **107**, 9113 (2003).
- [152] M. J. Frisch *et al.* Gaussian 03 (Revision B.04), Gaussian, Inc., Pittsburgh PA, 2003
- [153] T. Taketsugu, N. Watanabe, K. Hirao, *J. Chem. Phys.* **111**, 3410 (1999).
- [154] C. Gonzalez, H. B. Schlegel, *J. Phys. Chem.* **94**, 5523 (1990)
- [155] A. C. P. Alves, J. M. Hollas, *Mol. Phys.* **23**, 927 (1972).
- [156] A. C. P. Alves, J. M. Hollas, *Mol. Phys.* **25**, 1305 (1973).
- [157] H. Sekiya, Y. Nagashima, Y. Nishimura, *J. Chem. Phys.* **92**, 5761 (1990)
- [158] H. Sekiya, T. Tsuji, S. Ito, A. Mori, H. Takeshita, Y. Nishimura, *J. Chem. Phys.* **101**, 3464 (1994)
- [159] R. K. Frost, F. C. Hagemeister, C. A. Arrington, T. S. Zwier, *J. Chem. Phys.* **105**, 2595 (1996).

- [160] K. Tanaka, H. Honjo, T. Tanaka, H. Kohguchi, Y. Ohshima, Y. Endo, J. Chem. Phys. **110**, 1969 (1999).
- [161] Y. Guo, T. D. Sewell, D. L. Thompson, J. Phys. Chem. A **102**, 5040 (1998)
- [162] L. A. Curtiss, K. Raghavachari, P. C. Redfern, V. Rassolov, J. A. Pople, J. Chem. Phys. **110**, 4703 (1999)
- [163] P. L. Fast, D. G. Truhlar, J. Phys. Chem. A **104**, 6111 (2000)
- [164] B. Hartke, J. Manz, J. Am. Chem. Soc. **110**, 3063 (1988)
- [165] K. Yagi, G. V. Mil'nikov, T. Taketsugu, K. Hirao, H. Nakamura, Chem. Phys. Lett. **397**, 435 (2004)
- [166] R. L. Redington, T. E. Redington, J. Mol. Spec. **78**, 229 (1979)
- [167] L. M. Jackman, J. C. Trewella, R. C. Haddon, J. Am. Chem. Soc. **102**, 2519 (1980).
- [168] V. May, O. Kühn, *Charge and Energy Transfer Dynamics in Molecular Systems* (Wiley-VCH, Weinheim, 2004)
- [169] E. J. Heller, J. Phys. Chem. A **103**, 10433 (1999)
- [170] O. Bohigas, S. Tomsovic, D. Ullmo, Phys. Rep. **223**, 43 (1993)
- [171] M. Wilkinson, J. Phys. A: Math. Gen. **20**, 635 (1987)
- [172] T. J. Minehardt, J. D. Adcock, R. E. Wyatt, C. Iung, Chem. Phys. Lett. **303**, 347 (1999)
- [173] K. Heyne, E. T. J. Nibbering, T. Elsaesser, M. Petković, O. Kühn, J. Phys. Chem. A **108**, 6083 (2004)

