

REFERENCES

1. Bernal, J.D. and King, S.V. 1968. Experimental studies of a simple liquid model. In H.N.V. Temperley, J.S. Rowlinson, and G.S. Rushbrooke (ed.), Physics of simple liquids, pp. 231-252. Amsterdam: North-Holland press.
2. Pieranski, P., Malecki, J., Kuczynski, W. and Wojciechowski, K. 1978. A hard disc system, an experimental model. Phil.Mag. A37: 107-115.
3. White, T.R., Hsu, S.P., Mobley, M.J. and Glaunsinger, W.S. 1984. Magnetic properties of metal-ammonia compound. J.Phys.Chem. 88: 3890-3895.
4. Glausinger, W.S., Von Dreele, R.B., Marzke, R.F., Hanson, R.C., Chieuk, P., Damay, P. and Catterall, R. 1984. Structure and properties pf metal-ammonia compounds on the trial of a new ammonia geometry. J.Phys.Chem. 88: 3860.
5. Ohtaki, H., Yamaguchi, T. and Maeda, M. 1976. Bull.Che.Soc.Japan 49: 701-708.
6. Maeda, M. and Ohtaki, H. 1975. Bull.Chem.Soc.Japan. 48: 3755-3756.
7. Narten, A.H. 1977. J.Chem.Phys. 66: 3117-3120
8. Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N., Teller, A.H. and Teller E. 1953. Equation of state calculation by computing machine. J.Chem.Phys. 21(6): 1087-1092.
9. Alder, B.J. and Wainwright, T.E. 1960. Studied in molecular dynamics II:

- Behaviour of a small number of elastic sphere. J.Chem.Phys.
33(5): 1439-1451.
10. Lie, G.C., Clementi, E. and Yoshimine, M. 1975. Study of the structural
of molecular complexes XIII: Monte Carlo simulation of liquid
water with a configuration interaction pair potential.
J.Chem.Phys. 64(6): 2314-2323.
11. Swaminathan, S., Harrison, S.W. and Beveridge, D.L. 1977. Monte Carlo
studies on the structure of a dilute aqueous solution of
methane. J.Am.Chem.Soc. 100(8): 5705-5712.
12. Hagler, A.T. and Moult, J. 1978. Computer simulation of the solvent
structure around biological macromolecules. Nature 272(16):
1978.
13. Jorgensen, W.L. and Ibrahim, M. 1980. Structure and properties of
liquid ammonia. J.Am.Chem.Soc. 102(10): 3309-3315.
14. Jorgensen, W.L. 1981. Simulation of liquid ethanol including internal
rotation. J.Am.Chem.Soc. 103(2): 345-350.
15. Bolis, G., Corongiu, G. and Clementi, E. 1981. Methanol in water
solution at 300 K. Chem.Phys.Lett. 6(3): 299-306.
16. Jorgensen, W.L. and Madura, J.D. 1983. Solvation and conformation
of methanol in water. J.Am.Chem.Soc. 105(6):
17. Linse, P., Karlstrom, G. and Jonsson, B. 1984. Monte Carlo studies
of a dilute aqueous solution of benzene. J.Am.Chem.Soc.
106(15): 4096-4102.
18. Byrnes, J.M. and Sandler, S.I. 1984. Monte Carlo simulation of
liquid ethane. J.Chem.Phys. 80(2): 881-885.
19. Dietz, W. and Heinzinger, K. 1984. Structure of liquid chloroform:



- A comparison between computer simulation and neutron scattering results. Ber.Bunsenges.Phys.Chem. 88: 543-546.
20. Okazaki, S., Touhara, H. and Nakanishi, K. 1984. Computer experiments of aqueous solutions V: Monte Carlo calculation on the hydrophobic interaction in 5 mol % methanol solution. J.Chem.Phys. 81(2): 890-894.
21. Alagona, G., Ghio, C. and Kollman, P.A. 1985. Monte Carlo simulations of the solvation of the dimethyl phosphate anion. J.Am.Chem.Soc. 107(8): 2229-2238.
22. Hannongbua, S.S. and Rode, B.M. 1985. A Monte Carlo study on the influence of macrocyclic compounds on the structure of water. J.Sci.Soc.Thailand 11: 135-139.
23. Hannongbua, S.S. and Rode, B.M. 1986. Monte Carlo simulations of a cyclen molecule in water. J.Chem.Soc.Faraday.Trans. II 82: 1021-1031.
24. Bounds, D.G. 1985. A molecular dynamics study of the structure of water around the ions Li(I), Na(I), K(I), Ca(I), Ni(I) and Cl(I). Mol.Phys. 54(6): 1335-1355.
25. Rahman, A., Stillinger, F.H. and Lemberg, H.L. 1975. Study of a central force model for liquid water by molecular dynamics. J.Chem.Phys. 63(12): 5223-5230.
26. Narusawa, H. and Nakanishi, K. 1980. A simulation of preferential solvation in ternary Lennard-Jones liquid mixtures by the molecular dynamics method. J.Chem.Phys. 73(8): 4066-4070.
27. Tanaka, H., Nakanishi, K. and Touhara, H. 1985. Computer experiments on aqueous solutions VII: Potential energy function for urea

- dimer and molecular dynamics calculation of 8 mol % aqueous solution of urea. J.Chem.Phys. 82: 5184-5190.
28. Sphor, E. and Heinzinger, K. 1986. Molecular dynamics simulation of a water/metal interface. Chem.Phys.Lett. 123(3): 218-220.
29. Probst, M.M., Radnai, T., Heinzinger, K., Bopp, P. and Rode, B.M. Molecular dynamics and X-ray investigation of an aqueous CaCl_2 solution. J.Phys.Chem. 89(5):.
30. Palinkas, G. and Heinzinger, K. 1986. Hydration shell structure of the calcium ion. Chem.Phys.Lett. 126(3): 251-254.
31. Migliore, M. and Fornili, S.L., Spohr, E., Palinkas, G., and Heinzinger, K. 1986. A molecular dynamics study of the structure of an aqueous KCl solution. Z.Naturforsch. 41a: 826-834.
32. Limtrakul, J.P., Fujiwara, S. and Rode, B.M. 1985. A quantum chemical analysis of the structural entities in aqueous sodium chloride solution and their concentration dependence. Anal.Sci. 1: 29-32.
33. Hannongbua, S.S., Ishida, T., Spohr, E. and Heinzinger, K. 1988. Molecular dynamics study of a lithium ion in ammonia. Z.Naturforsch. 43a: 572-582.
34. Tanabe, Y. and Rode, B.M. 1988. Monte Carlo simulation of an 18.45 mol % aqueous ammonia solution. J.Chem.Soc.Faraday Trans. II 84(6): 679-692.
35. Rode, B.M. and Tanabe, Y. 1988. A Monte Carlo study on preferential solvation of sodium(I) in aqueous ammonia. J.Chem.Soc.Faraday Trans. II 84:.

36. Czerwan, H.J. and Peinel, G. 1990. Molecular dynamics method :
 Publication and citation patterns of a research specialty
 of computer simulation. Information Quarterly for Computer
 Simulation of condensed phases 32, 51.
37. Allen, M.P. and Tildesley, D.J. 1987. Computer Simulation of Liquids.
 New York: Oxford University Press.
38. Benjamin, W.A. 1964. Metal ammonia solutions. In Lepoutre and Spienko,
 M.J. (ed.), Colloque Weyl I, New York: New York press.
39. Lagowski, J.J. and Spienko, M.J. 1970. Metal ammonia solutions.
Colloque Weyl II. London: Butterworths.
40. Jortner, J. and Kesner, N.R. 1973. Electrons in fluids.
Colloque Weyl III, New York: Springer-Verlag.
41. Rahman, A. 1964. Phys.Rev. 98: 159.
42. Morukuma, K. 1971. Molecular orbital studies of hydrogen bonds III.
 C=O...H-O hydrogen bond in $\text{H}_2\text{CO} \dots \text{H}_2\text{O}$ and $\text{H}_2\text{CO} \dots 2\text{H}_2\text{O}$.
J.Chem.Phys. 55: 1971.
43. Williams, D.E. and Craycroft, D.J. 1987. Non-bonded H...H repulsion
 energy from ab initio SCF calculations of methane, ammonia,
 water and methanol dimers. J.Phys.Chem. 91: 6365.
44. Alder, B.J. and Wainwright, T.E. 1958. In Prigogine, I. (ed.),
Transport processes in statistical mechanics, New York:
 Interscience.
45. Alder, B.J. and Wainwright, T.E. 1957. J.Chem.Phys. 27: 1208.
46. Metropolis, N., Rosenbluth, A.W., Teller, A.H. and Teller, E.
J.Chem.Phys. 21: 1087.
47. Wood, W.W. and Jacobson, J.D. 1957. J.Chem.Phys. 27: 1207.

48. Bernal, J.D. 1964. Proc.Roy.Soc. A280: 299.
49. Hirschfelder, J.O., Curtiss, C.F. and Bird, R.B. 1964. Molecular theory of gases and liquids rev.ed. New York: Wiley.
50. Hagler, A.T. and Lifson, S. 1974. Energy functions for peptides and proteins II: The amide hydrogen bond and calculation of amide crystal properties. J.Am.Chem.Soc. 96: 5327.
51. Lifson, S. and Warshel, A. 1968. Consistent force field for calculations of conformations, vibrational spectra, and enthalpies of cycloalkane and n-alkane molecules. J.Chem.Phys. 49: 5116.
52. Warshel, A. and Lifson, S. 1970. Consistent force field calculations vibrations, molecular conformations and enthalpies of alkanes. J.Chem.Phys. 53: 582.
53. Roothaan, C.C.J. 1951. Self consistent field theory for opened shell of electronic systems. Rev.Mod.Phys. 23: 69.
54. Roothaan, C.C.J. 1960. Self consistent field theory for opened shell of electronic systems. Rev.Mod.Phys. 32: 179.
55. Slater, J.S. 1930. Atomic shielding constant. Phys.Rev. 36: 57-64.
56. Boys, S.F. 1951. Electronic wave functions IV: Some general theorems for the calculation of Schrodinger integral between complicated vector. Coupled functions for many electron atoms. Proc.Roy.Soc. A207: 181-197.
57. Whitten, J.C. 1963. Gaussian expansion of hydrogen atom wave functions. J.Chem.Phys. 39: 349-352.
58. Whitten, J.C. 1966. Gaussian lobe function expansion of Hartree Fock solution for the first row atoms and ethylene.

- J.Chem.Phys. 44: 359-364.
59. Spirko, V. 1983. Vibrational anharmonicity and the inversion potential function of NH₃. J.Mol.Spectrosc. 101: 30.
60. Benedict, W.S. and Plyler, E.K. 1985. Can.J.Phys. 82: 890.
61. Dupuis, M. Watts, J.D., Villar H.O. and Hurst, G.T. 1988. HONDO version 7.0 (1987) Documentation. KGN 169. Kingston: IBM Corporation.
62. Hay, P.J. and Wadt, W.R. 1985. J.Chem.Phys. 82: 270.
63. Dunning T.H. 1970. J.Chem.Phys. 53: 2823.
64. Stevens, W.J., Basch, H. and Kraus, M. J.Chem.Phys. 81: 6026.
65. Huzinaga, S. 1985. Gaussian basis set for molecular calculations. Physical Science Data 16. Amsterdam: Elsevier.
66. Swaminathan, R.J., Whitehead, E. and Beveridge, D.L. J.Am.Chem.Soc. 99: 7817.
67. Jorgensen, W.L. and Cournoyer, N.E. 1978. J.Am.Chem.Soc. 100: 4942.
68. Wood, W.W. and Parker, F.R. 1957. J.Chem.Phys. 27: 720.
69. Verlet, L. 1967. Phys.Rev. 98: 159.
70. Verlet, L. 1967. Computer experiments on classical fluids I: Thermodynamical properties of Lennard-Jones molecules. Phys.Rev. 159: 98
71. Gear, C.W. 1966. The numerical integration of ordinary differential equations of various orders. Report ANL. pp. 7126, Argonne National Laboratory.
72. Gear, C.W. 1971. Numerical initial value problems in ordinary differential equations. NJ.: Prentice Hall.
73. Narten, A.H. 1977. Liquid ammonia: Molecular correlation functions

- from X-ray diffraction. J.Chem.Phys. 66: 3117.
74. Yongyai, Y.P., Kokpol, S.U. and Rode, B.M. 1991. Chem.Phys. : 403.
75. Probst M.M. 1987. Chem.Phys.Lett. 137: 229.
76. Hannongbua, S.S. 1991. A molecular dynamics simulation of the structure of sodium ion in liquid ammonia. Aust.J.Chem. 44: 447.
77. Klein, M.L., and McDonald, I.R. 1981. J.Chem.Phys. 74: 4214.
78. Rode, B.M., Islam, S.M. and Yongyai, Y. 1991. Pure Appl.Chem. 63: 1894.
79. Yongyai, Y., Kokpol, S. and Rode, B.M. 1991. Chem.Phys. 156: 403
80. Rode, B.M. and Islam, S.M. J.Chem.Soc.Faraday Trans. Submitted for publication.
81. Rode, B.M. and Islam, S.M. 1991. Z.Naturforsch 46a: 357.
82. Jancso, G., Heinzinger, K. and Bopp, P. 1985. Z.Naturforsch. 40a: 1235.
83. Szasz, Gy.I. and Heinzinger, K. 1983. Earth Planet Sci.Lett. 64: 163.
84. Palinkas, G., Bopp, P., Jancso, G. and Heinzinger, K. 1984. Z.Naturforsch. 39a: 179.
85. Probst, M.M., Bopp, P., Heinzinger, K. and Rode, B.M. 1984. Chem.Phys.Lett. 106: 317.
86. Szasz, Gy.I., Heinzinger, K. and Riede, W.O. 1981. Ber.Bunsenges.Phys.Chem. 85: 1056.
87. Geiger, A. 1981. Ber.Bunsenges.Phys.Chem. 85: 52.

V I T A

1968 Born on January, 7th in Chachoengsao
Father : Nong Kerdcharoen
Mother : Taweewan Kerdcharoen
1985 March : High School graduation (Trium Udom Sueksa, Bangkok)
1989 April : Bachelor of Science (Chemistry), Chulalongkorn University
1990 June : Begin of Master studies at Department of Chemistry,
Chulalongkorn University.

A publication is coming out of my Master's thesis work. It is "Zinc(II) in Liquid Ammonia : Intermolecular Potential Including 3-body Terms, and Monte Carlo Simulation", which is during publication in J.Chem.Phys.. During the study towards the Master's degree of science, I was supported by the Austrian On-Place Scholarship, and my thesis was supported by the Graduate School Fund.

