REFERENCES

1. Bernal, J. D., and Fowler, R. H. (1933). A Theory of Water and Ionic Solution with Particular Reference to Hydrogen and Hydroxyl Ions. J. Chem. Phys. 1: 515-548.
2. Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., and Teller, E. (1953). Equation of State Calculation by Computing Machines. J. Chem. Phys. 21(6): 1087-1092.
3. Alder, B. J., and Wainwight, T. E. (1960). Studied in Molecular Dynamics. II. Behavior of a Small Number of Elastic Spheres. J. Chem. Phys. 33: 1439-1451.
4. 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: 679-692.
5. Hannongbua, S., Ishida, T., Spohr, E., and Heinzinger, K. (1988). Molecular Dynamics Study of a Lithium Ion in Ammonia. Z. Naturforsch. 43a: 572-582.
6. Kheawsrikul, S., Hannongbua, S. V., Kokpol, S. U. and Rode, B. M. (1989). A Monte Carlo Study on Preference Solvation of Lithium(I) in Aqueous Ammonia. J. Chem. Soc. Faraday. Trans. II 85: 643-649.
7. Hannongbua, S., Kerdcharoen, T., and Rode, B. M. (1992). Zinc(II) in Liquid Ammonia: Intermolecular Potential Including Three-Body Terms and Monte Carlo Simulation. J. Chem. Phys. 96: 6945-6949.
8. 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: 2229-2238.
9. Muzzarelli, R. (1994). Polymeric Biomaterials. New York: Marcel Dekker.
10. Hirano, S., Seiono, H., Akiyama, Y., and Nonaka, I. (1990). Progress in Biomedical Polymers. New York: Plenum Press.

11. Deuchi, K., Kanauchi, O., Imasato, Y., and Kobayashi, E. (1994) Decreasing Effect of Chitosan on the Apparent Fat Digestibility by Rats Fed on a High-Fat Diet. Biosci. Biotechnol. and Biochem. 58: 1613-1616.

12. Trautwein, E. A., Jurgensen, U., and Erbersdobler, H. F. (1997) Cholesterol-Lowering and Gallstone-Preventing Action of Chitosans with Different Degrees of Deacetylation in Hamsters Fed Cholesterol-Rich Diets. Nutrition Research 17: 1053-1065.

13. Fattah, E. I., Grant, D. J. W., Gabr, K. E., and Meshali, M. M. (1998). Physical Characteristics and Release Behavior of Salbutamol Sulfate Beads Prepare with Different Ionic Polysaccharides. Drug Development and Industrial Pharmacy 24: 541-547.

14. Bonvin, M. M., and Debertorello, M. M. (1994). In-Vitro Drug-Release from Chitosan Membranes: Study of the Mechanisms of Permeation. Polymer Bulletin 32: 69-75.

15. Needleman, G., and Smales, F. C. (1995). In-Vitro Assessment of Bioadhesion for Periodontal and Buccal Drug-Delivery. Biomaterials 16: 617-624.

16. Wan, L. S. C., Lim, L. Y., and Soh, B. L. (1994). Drug-Release from Chitosan Beads. STP Pharma Sciences 4: 195-200.

17. Giunchedi, P., Genta, I., Conti, B., Muzzarelli, R. A. A., and Conte, U. (1998). Preparation and Characterization of Ampicilin Loaded Methylpyrrolidinone Chitosan and Chitosan Microspheres. Biomaterials 19: 157-161.

18. Thacharodi, D., and Rao, K. P. (1993). Propranolol Hydrochloride Release Behaviour of Crosslinked Chitosan Membranes. J. Chem. Tech. Biotechnol. 58: 177-181.

19. Fang, Y.-E., Cheng, Q., and Lu, X.-B. (1998). Kinetics of In Vitro Drug Release from Chitosan/Gelatin Hybrid Membranes. J. Appl. Polym. Sci. 68: 1751-1758.

20. Genta, I., Perugini, P., and Pavanetto, F. (1998). Different Molecular Weight Chitosan Microspheres: Influence on Drug Loading and Drug Release. Drug Development and Industrial Pharmacy 24: 779-784.

21. Nakatsuka, S., and Andrady, A. L. (1992). Permeability of Vitamin B-12 in Chitosan Membranes: Effect of Crosslinking and Blending with Poly (vinyl alcohol) on Permeability. J. Appl. Polym. Sci. 44, 17-28.

22. Kubota, N. (1993). Molecular Weight Dependence of the Properties of Chitosan Hydrogel for Use in Sustained-Release Drug. Bull. Chem. Soc. Jpn. 66: 1807-1812.

23. Al-Angary, A. A., Al-Helw, A. A. M., Al-Dardiri, M. M., and Mahrous, G. M. (1998). Release and Bioavailability of Diclofenac Sodium from Low Molecular Weight Chitosan Microspheres treated with Japan and Carnauba Wax. Pharmazeutische Industrie 60: 629-634.

24. Hsien, T.-Y., and Rorrer, G. L. (1997). Heterogeneous Cross-Linking of Chitosan Gel Beads: Kinetics, Modeling, and Influence on Cadmium Ion Adsorption Capacity. Ind. Eng. Chem. Res. 36: 3631-3638.

25. Cardinal, J. R., Curatolo, W. J., and Ebert, C. D. (1990). Chitosan Compositions for Controlled and Prolonged Release of Macromolecules. U. S. Patent 4,895,724.

26. Hannongbua, S., and Rode, B. M. (1992). Monte Carlo Simulations of a Magnesium Ion in Liquid Ammonia. Chemical Physics 162: 257-263.

27. Hannongbua, S. (1996). Solvation of 1,4,7,10-Tetraazacyclododecane in Aqueous Solution As Studied by the Monte Carlo Method. J. Phys. Chem. 100: 17655-17661.

28. Udomsub, S., and Hannongbua, S. (1997). Solvation of a Macrocyclic Compound in a Water-Ammonia Mixture: Monte Carlo Simulations. J. Chem. Soc., Faraday Trans. 93: 3045-3052.

29. Merzbacher, E. (1961). Quantum Mechanics. New York: John Wiley & Sons.

30. Leach, A. R. (1996). Molecular Modelling: Principles and Applications. 1st ed. Essex: Addison Wesley Longman Limited.

31. Hehre, W. J., Radom, L., Schleyer, P. V. R., and Pople, J. A. (1986). AB Initio Molecular Orbital Theory. New York: John Wiley & Sons.

32. Parasuk, V. (1991). Electronic and Molecular Structeres of Medium-Sized Carbon Clusters. Doctoral dissertation, Department of Chemistry, Graduate School, University of Minnesota.

33. Szabo, A., and.Ostlund, N. S. (1989). Modern Quantum Chemistry. 1st ed. Revised, USA: McGraw-Hill Publishing.

34. Slater, J. S. (1930). Atomic Shielding Constant. Phys. Rev. 36: 57-64.

35. Aree, T. (1996). Study of Optimized and Electronic Structures of Endohedral and Exohedral Lithium-Buckminsterfullerene Complexes by Quantum Chemical Calculations. Master's Thesis, Department of Chemistry, Graduate School, Chulalongkorn University.

36. Roothaan, C. C. J. (1951). New Developments in Molecular Orbital Theory. Rev. Mod. Phys. 23: 69-89.

37. Hall, G. G. (1951). The Molecular Orbital Theory of Chemical Valency VIII. A Method for Calculating Ionization Potentials. Proc. Roy. Soc. (London) A205: 541-552.

38. Mulliken, R. S. (1955). Electronic Population Analysis on LCAO-MO Molecular Wave Functions I. J. Chem. Phys. 23:1833-1846.

39. Boys, S. F. (1951). Electronic Wave Function .IV. Some General Theorems for the Calculation of Schrödinger Integral Between Complicated Vector-Coupled Functions for Many-Electron Atoms. Proc. Roy. Soc. (London) A207: 181-197.

40. Whitten, J. C. (1963). Gaussian Expansion of Hydrogen Atom Wave Functions. J. Chem. Phys. 39: 349-352.

41. Whitten, J. C. (1966). Gaussian Lobe Function Expansions of Hartree Fock Solution for the First Row Atoms and Ethylene. J. Chem. Phys. 44: 359-364.

42. Davidson, E. R., and Feller, D. (1986). Basis Set Selection for Molecular Calculations. Chem. Rev. 86: 681-696.

43. Clementi, E., and Popkie, H. (1972). Study of the Structure of Molecular Complexes. I. Energy Surface of a Water Molecule in the Field of a Lithium Positive Ion. J. Chem. Phys. 57: 1077-1094.

44. Boys, S. F., and Bernardi, F. (1970). The Calculation of Small Molecular Interactions by the Differences of Separate Total Energies: Some Procedures with Reduced Errors. Mol. Phys. 19: 553-566.

45. Ewald, P. (1921). Due Berechnung Optischer und Elektrostatischer Gitterpotentiale. Ann. Phys. 64: 253-287.

46. Friedman, H. L. (1975). Image Approximation to the Reaction Field. Molecular Physics 29: 1533-1543.

47. Benedict, W. S., Gailar, N., and Plyler, E. K. (1956). Rotation-Vibration Spectra of Deuterated Water Vapour. J. Chem. Phys. 24: 1139-1165.

48. Cambridge Crystallographic Data Center, Cambridge, UK. (http://www.ccdc.cam.ac.uk)

49. Dunning, T. H. (1970). Gaussian Basis Functions for Use in Molecular Calculations. I. Contraction of (9s5p) Atomic Basis Sets for First-Row Atoms. J. Chem. Phys. 53: 2823-2883.

50. Reed, A. E., Weinstock, R. B., and Weinhold, F. (1985). Natural Population Analysis. J. Chem. Phys. 83: 735-1985.

51. Hehre, W. J., Stewart, R. F., and Pople, J. R. (1969). Self- Consistent Molecular Orbital Methods. I. Use of Gaussian Expansions of Slater-Type Atomic Orbitals. J. Chem. Phys. 51: 2657-2664.

52. Collins, J. B., Schleyer, P. V. R., Binkley, J. S., and Pople, J. A. (1976). Self-Consistent Molecular Orbital Methods. XVII. Geometries and Binding

Energies of Second-Row Molecule. A Comparison of Three Basis Sets. J. Chem. Phys. 64: 5142-5151.

53. Levine, I. N. (1991). Quatum Chemistry. 4th ed. New Jersey: Prentice-Hall.

54. Binkley, J. S., Pople, J. A., and Hehre, W. J. (1980). Self-Consistent Molecular Orbital Methods. 21. Small Split-Valence Basis Sets for First-Row Elements. J. Am. Chem. Soc. 102: 939-947.

55. Gardon, M. S., Binkley, J. S., Pople, J. A., Pietro, W. J., and Hehre, W. J. (1982). Self-Consistent Molecular Orbital Methods. 22. Small Split-Valence Basis Sets for Second-Row Elements. J. Am. Chem. Soc. 104: 2797-2803.

56. Hehre, W. J., Ditchfield, R., and Pople, J. A. (1972). Self-Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian-Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules. J. Chem. Phys. 56: 2257-2261.

57. Dunning, T. H., and Hay, P. J. (1977). Methods of Electronic Structure Theory. vol. 3. New York: Plenum Press.

58. Dunning, T. H. (1989). Gaussian Basis Sets for Use in Correlated Molecular Calculations. I. The Atoms Boron through Neon and Hydrogen. J. Chem. Phys. 90: 1007-1023.

59. Matsuoka, O., Clementi, E., and Yoshimine, M. (1976). CI Study of the Water Dimer Potential Surface. J. Chem. Phys. 64: 1351-1361.

60. Perera, L., Essmann, U., and Berkowitz, M. L. (1995). Effect of the Treatment of Long-Range Forces on the Dynamics of Ions in Aqueous Solutions. J. Chem. Phys. 102: 450-456.

61. Lie, G. C., Clementi, E., and Yoshimine, M. (1976). Study of the Structure of Molecular Complexes. XIII. MonteCarlo Simulation of Liquid Water with a Configuration Interaction Pair Potential. J. Chem. Phys. 64: 2314-2323.

62. Caffarena, E. R., and Grigera, J. R. (1999). Hydration of Glucose in the Rubbery and Glassy States Studied by Molecular Dynamics Simulation. Carbohydrate Res. 315: 63-69.

63. Molteni, C., and Parrinello, M. (1998). Glucose in Aqueous Solution by First Principles Molecular Dynamics. J. Am. Chem. Soc. 120: 2168-2171.

APPENDICES

Appendix I

Exponents and Coefficients for STO-3G Basis Set

Atom	Shell	Exponent	Coefficient	
H	S 3 1.00	3.42525091E+00	1.54328970E-01	
		6.23913730E-01	5.35328140E-01	
		1.68855400E-01	4.44634540E-01	
C	S 3 1.00	7.16168370E+01	1.54328970E-01	
		1.30450960E+01	5.35328140E-01	
		3.53051220E+00	4.44634540E-01	
	SP 3 1.00	2.94124940E+00	-9.99672300E-02	1.55916270E-01
		6.83483100E-01	3.99512830E-01	6.07683720E-01
		2.22289900E-01	7.00115470E-01	3.91957390E-01
N	S 3 1.00	9.91061690E+01	1.54328970E-01	
		1.80523120E+01	5.35328140E-01	
		4.88566020E+00	4.44634540E-01	
	SP 3 1.00	3.78045590E+00	-9.99672300E-02	1.55916270E-01
		8.78496600E-01	3.99512830E-01	6.07683720E-01
		2.85714400E-01	7.00115470E-01	3.91957390E-01
O	S 3 1.00	1.30709320E+02	1.54328970E-01	
		2.38088610E+01	5.35328140E-01	
		6.44360830E+00	4.44634540E-01	
	SP 3 1.00	5.03315130E+00	-9.99672300E-02	1.55916270E-01
		1.16959610E+00	3.99512830E-01	6.07683720E-01
		3.80389000E-01	7.00115470E-01	3.91957390E-01

Exponents and Coefficients for 3-21G Basis Set

Atom	Shell	Exponent	Coefficient	
H	S 2 1.00	5.44717800E+00	1.56285000E-01	
		8.24547000E-01	9.04691000E-01	
	S 1 1.00	1.83192000E-01	1.00000000E+00	
C	S 3 1.00	1.72256000E+02	6.17669000E-02	
		2.59109000E+01	3.58794000E-01	
		5.53335000E+00	7.00713000E-01	
	SP 2 1.00	3.66498000E+00	-3.95897000E-01	2.36460000E-01
		7.70545000E-01	1.21584000E+00	8.60619000E-01
	SP 1 1.00	1.95857000E-01	1.00000000E+00	1.00000000E+00
N	S 3 1.00	2.42766000E+02	5.98657000E-02	
		3.64851000E+01	3.52955000E-01	
		7.81449000E+00	7.06513000E-01	
	SP 2 1.00	5.42522000E+00	-4.13301000E-01	2.37972000E-01
		1.14915000E+00	1.22442000E+00	8.58953000E-01
	SP 1 1.00	2.83205000E-01	1.00000000E+00	1.00000000E+00
O	S 3 1.00	3.22037000E+02	5.92394000E-02	
		4.84308000E+01	3.51500000E-01	
		1.04206000E+01	7.07658000E-01	
	SP 2 1.00	7.40294000E+00	-4.04453000E-01	2.44586000E-01
		1.57620000E+00	1.22156000E+00	8.53955000E-01
	SP 1 1.00	3.73684000E-01	1.00000000E+00	1.00000000E+00

Exponents and Coefficients for 6-31G Basis Set

Atom	Shell	Exponent	Coefficient	
H	S 3 1.00	1.87311370E+01	3.34946000E-02	
		2.82539370E+00	2.34726950E-01	
		6.40121700E-01	8.13757330E-01	
	S 1 1.00	1.61277800E-01	1.00000000E+00	
C	S 6 1.00	3.04752490E+03	1.83470000E-03	
		4.57369510E+02	1.40373000E-02	
		1.03948690E+02	6.88426000E-02	
		2.92101550E+01	2.32184400E-01	
		9.28666300E+00	4.67941300E-01	
		3.16392700E+00	3.62312000E-01	
	SP 3 1.00	7.86827240E+00	-1.19332400E-01	6.89991000E-02
		1.88128850E+00	-1.60854200E-01	3.16424000E-01
		5.44249300E-01	1.14345640E+00	7.44308300E-01
	SP 1 1.00	1.68714400E-01	1.00000000E+00	1.00000000E+00
N	S 6 1.00	4.17351100E+03	1.83480000E-03	
		6.27457900E+02	1.39950000E-02	
		1.42902100E+02	6.85870000E-02	
		4.02343300E+01	2.32241000E-01	
		1.28202100E+01	4.69070000E-01	
		4.39043700E+00	3.60455000E-01	
	SP 3 1.00	1.16263580E+01	-1.14961000E-01	6.75800000E-02
		2.71628000E+00	-1.69118000E-01	3.23907000E-01
		7.72218000E-01	1.14585200E+00	7.40895000E-01
	SP 1 1.00	2.12031300E-01	1.00000000E+00	1.00000000E+00
O	S 6 1.00	5.48467170E+03	1.83110000E-03	
		8.25234950E+02	1.39501000E-02	
		1.88046960E+02	6.84451000E-02	
		5.29645000E+01	2.32714300E-01	
		1.68975700E+01	4.70193000E-01	
		5.79963530E+00	3.58520900E-01	
	SP 3 1.00	1.55396160E+01	-1.10777500E-01	7.08743000E-02
		3.59993360E+00	-1.48026300E-01	3.39752800E-01
		1.01376180E+00	1.13076700E+00	7.27158600E-01
	SP 1 1.00	2.70005800E-01	1.00000000E+00	1.00000000E+00

Exponents and Coefficients for DZ Basis Set

Atom	Shell	Exponent	Coefficient
H	S 3 1.00	1.92406000E+01	3.28280000E-02
		2.89920000E+00	2.31208000E-01
		6.53400000E-01	8.17238000E-01
	S 1 1.00	1.77600000E-01	1.00000000E+00
C	S 6 1.00	4.23261000E+03	2.02900000E-03
		6.34882000E+02	1.55350000E-02
		1.46097000E+02	7.54110000E-02
		4.24974000E+01	2.57121000E-01
		1.41892000E+01	5.96555000E-01
		1.96660000E+00	2.42517000E-01
	S 1 1.00	5.14770000E+00	1.00000000E+00
	S 1 1.00	4.96200000E-01	1.00000000E+00
	S 1 1.00	1.53300000E-01	1.00000000E+00
	P 4 1.00	1.81557000E+01	1.85340000E-02
		3.98640000E+00	1.15442000E-01
		1.14290000E+00	3.86206000E-01
		3.59400000E-01	6.40089000E-01
	P 1 1.00	1.14600000E-01	1.00000000E+00
N	S 6 1.00	5.90944000E+03	2.00400000E-03
		8.87451000E+02	1.53100000E-02
		2.04749000E+02	7.42930000E-02
		5.98376000E+01	2.53364000E-01
		1.99981000E+01	6.00576000E-01
		2.68600000E+00	2.45111000E-01
	S 1 1.00	7.19270000E+00	1.00000000E+00
	S 1 1.00	7.00000000E-01	1.00000000E+00
	S 1 1.00	2.13300000E-01	1.00000000E+00
	P 4 1.00	2.67860000E+01	1.82570000E-02
		5.95640000E+00	1.16407000E-01
		1.70740000E+00	3.90111000E-01
		5.31400000E-01	6.37221000E-01
	P 1 1.00	1.65400000E-01	1.00000000E+00

(Continued)

Atom	Shell	Exponent	Coefficient
O	S 6 1.00	7.81654000E+03	2.03100000E-03
		1.17582000E+03	1.54360000E-02
		2.73188000E+02	7.37710000E-02
		8.11696000E+01	2.47606000E-01
		2.71836000E+01	6.11832000E-01
		3.41360000E+00	2.41205000E-01
	S 1 1.00	9.53220000E+00	1.00000000E+00
	S 1 1.00	9.39800000E-01	1.00000000E+00
	S 1 1.00	2.84600000E-01	1.00000000E+00
	P 4 1.00	3.51832000E+01	1.95800000E-02
		7.90400000E+00	1.24189000E-01
		2.30510000E+00	3.94727000E-01
		7.17100000E-01	6.27375000E-01
	P 1 1.00	2.13700000E-01	1.00000000E+00

Exponents and Coefficients for DZP Basis Set

Atom	Shell	Exponent	Coefficient
H	S 3 1.00	1.92406000E+01	3.28280000E-02
		2.89920000E+00	2.31208000E-01
		6.53400000E-01	8.17238000E-01
	S 1 1.00	1.77600000E-01	1.00000000E+00
	P 1 1.00	1.00000000E+00	1.00000000E+00
C	S 6 1.00	4.23261000E+03	2.02900000E-03
		6.34882000E+02	1.55350000E-02
		1.46097000E+02	7.54110000E-02
		4.24974000E+01	2.57121000E-01
		1.41892000E+01	5.96555000E-01
		1.96660000E+00	2.42517000E-01
	S 1 1.00	5.14770000E+00	1.00000000E+00
	S 1 1.00	4.96200000E-01	1.00000000E+00
	S 1 1.00	1.53300000E-01	1.00000000E+00

(Continued)

Atom	Shell	Exponent	Coefficient
	P 4 1.00	1.81557000E+01	1.85340000E-02
		3.98640000E+00	1.15442000E-01
		1.14290000E+00	3.86206000E-01
		3.59400000E-01	6.40089000E-01
	P 1 1.00	1.14600000E-01	1.00000000E+00
	D 1 1.00	7.50000000E-01	1.00000000E+00
N	S 6 1.00	5.90944000E+03	2.00400000E-03
		8.87451000E+02	1.53100000E-02
		2.04749000E+02	7.42930000E-02
		5.98376000E+01	2.53364000E-01
		1.99981000E+01	6.00576000E-01
		2.68600000E+00	2.45111000E-01
	S 1 1.00	7.19270000E+00	1.00000000E+00
	S 1 1.00	7.00000000E-01	1.00000000E+00
	S 1 1.00	2.13300000E-01	1.00000000E+00
	P 4 1.00	2.67860000E+01	1.82570000E-02
		5.95640000E+00	1.16407000E-01
		1.70740000E+00	3.90111000E-01
		5.31400000E-01	6.37221000E-01
	P 1 1.00	1.65400000E-01	1.00000000E+00
	D 1 1.00	8.00000000E-01	1.00000000E+00
O	S 6 1.00	7.81654000E+03	2.03100000E-03
		1.17582000E+03	1.54360000E-02
		2.73188000E+02	7.37710000E-02
		8.11696000E+01	2.47606000E-01
		2.71836000E+01	6.11832000E-01
		3.41360000E+00	2.41205000E-01
	S 1 1.00	9.53220000E+00	1.00000000E+00
	S 1 1.00	9.39800000E-01	1.00000000E+00
	S 1 1.00	2.84600000E-01	1.00000000E+00
	P 4 1.00	3.51832000E+01	1.95800000E-02
		7.90400000E+00	1.24189000E-01
		2.30510000E+00	3.94727000E-01
		7.17100000E-01	6.27375000E-01
	P 1 1.00	2.13700000E-01	1.00000000E+00
	D 1 1.00	8.50000000E-01	1.00000000E+00

Appendix II

The MCY Potential for Water-Water Interactions [60]

(ΔE in kcal/mol, r in Å)

$$\Delta E(W,W) = \frac{Q^2}{4\pi\varepsilon_0}\left[\left(\frac{1}{r_{13}}+\frac{1}{r_{23}}+\frac{1}{r_{14}}+\frac{1}{r_{24}}\right)+\frac{4}{r_{78}}-2\left(\frac{1}{r_{18}}+\frac{1}{r_{28}}+\frac{1}{r_{37}}\frac{1}{r_{47}}\right)\right]$$
$$+ a_1 \exp(-b_1 r_{56})$$
$$+ a_2[\exp(-b_2 r_{13}) + \exp(-b_2 r_{14}) + \exp(-b_2 r_{23}) + \exp(-b_2 r_{23})]$$
$$+ a_3[\exp(-b_3 r_{16}) + \exp(-b_3 r_{26}) + \exp(-b_3 r_{35}) + \exp(-b_3 r_{45})]$$
$$- a_4[\exp(-b_4 r_{16}) + \exp(-b_4 r_{26}) + \exp(-b_4 r_{35}) + \exp(-b_4 r_{45})]$$

Parameter	Coefficient
$Q_2/4\pi\varepsilon_0$	170.9389
a_1	1088213.2
a_2	666.3373
a_3	1455.427
a_4	273.5954
b_1	5.152712
b_2	2.760844
b_3	2.961895
b_4	2.233264

Appendix III

Source Codes for Program Fortran77

1. Program for Generating Coordination of Water Molecule

```
**********************************************************
*        PROGRAM : Generation of Coordination of Water        *
**********************************************************
C       Generation coordinate of water in Quadrant 2 (-,+,+)
        REAL SINALP,SINBET,SINGAM,COSALP,COSBET,COSGAM,
      + A21,A22,A23,A31,A32,A33
        REAL*8 X,Y,Z,DIST,u,v,w,r,s,t
        CHARACTER*3 O, H1, H2
        PARAMETER(YH1ST=0.75669,YH2ST=-0.75669,ZHST=0.58589)
C       IA is alpha, IB is beta, IC is gramma ***
        OPEN (1,FILE='coorQ2')
        PI=4.*ATAN(1.)
C
C       alpha=180, beta=0, gramma=0-90
        IB= 0
        IA= 180
        DO  11  IC= 0,90,90
           DO  11  IZ= 1,7
             DO  11  IY= 1,7
               DO  11  IX= 1,7
                 XO  = REAL(IX)*(-1.)
                 YO  = REAL(IY)
                 ZO  = REAL(IZ)
                 ALP = REAL(IA)*(PI/180.0)
                 BET = REAL(IB)*(PI/180.0)
                 GAM = REAL(IC)*(PI/180.0)
C
                 SINALP=SIN(ALP)
                 COSALP=COS(ALP)
                 SINBET=SIN(BET)
                 COSBET=COS(BET)
                 SINGAM=SIN(GAM)
                 COSGAM=COS(GAM)
C
```

```
      A21=COSALP*SINGAM+SINALP*SINBET*COSGAM
      A22=COSALP*COSGAM-SINALP*SINBET*SINGAM
      A23=-SINALP*COSBET
      A31=SINALP*SINGAM-COSALP*SINBET*COSGAM
      A32=SINALP*COSGAM+COSALP*SINBET*SINGAM
      A33=COSALP*COSBET
C
      XH1=A21*YH1ST+A31*ZHST + XO
      YH1=A22*YH1ST+A32*ZHST + YO
      ZH1=A23*YH1ST+A33*ZHST + ZO
      XH2=A21*YH2ST+A31*ZHST + XO
      YH2=A22*YH2ST+A32*ZHST + YO
      ZH2=A23*YH2ST+A33*ZHST + ZO
C
      DIST = SQRT((XO**2)+(YO**2)+(ZO**2))
      WRITE(1,70) XO,YO,ZO,DIST,XH1,YH1,ZH1,XH2,YH2,ZH2
11    CONTINUE
C
C     alpha=90, beta=0, gamma=90
      IA= 90
      IB= 0
      IC= 90
      DO 22 IZ= 1,7
        DO 22 IY= 1,7
          DO 22 IX= 1,7
            XO  = REAL(IX)*(-1.)
            YO  = REAL(IY)
            ZO  = REAL(IZ)
            ALP = REAL(IA)*(PI/180.0)
            BET = REAL(IB)*(PI/180.0)
            GAM = REAL(IC)*(PI/180.0)
C
            SINALP=SIN(ALP)
            COSALP=COS(ALP)
            SINBET=SIN(BET)
            COSBET=COS(BET)
            SINGAM=SIN(GAM)
            COSGAM=COS(GAM)
C
            A21=COSALP*SINGAM+SINALP*SINBET*COSGAM
            A22=COSALP*COSGAM-SINALP*SINBET*SINGAM
            A23=-SINALP*COSBET
            A31=SINALP*SINGAM-COSALP*SINBET*COSGAM
            A32=SINALP*COSGAM+COSALP*SINBET*SINGAM
```

```
                A33=COSALP*COSBET
C
                XH1=A21*YH1ST+A31*ZHST + XO
                YH1=A22*YH1ST+A32*ZHST + YO
                ZH1=A23*YH1ST+A33*ZHST + ZO
                XH2=A21*YH2ST+A31*ZHST + XO
                YH2=A22*YH2ST+A32*ZHST + YO
                ZH2=A23*YH2ST+A33*ZHST + ZO
C
                DIST = SQRT((XO**2)+(YO**2)+(ZO**2))
                WRITE(1,70) XO,YO,ZO,DIST,XH1,YH1,ZH1,XH2,YH2,ZH2
22      CONTINUE
C
C       alpha=0, beta=90, gramma=90-270
        IB= 90
        IA= 0
        DO 33 IC= 90,270,90
          DO 33 IZ= 2,5
            DO 33 IY= 1,3
              DO 33 IX= 2,5
                XO  = REAL(IX)*(-1.)
                YO  = REAL(IY)
                ZO  = REAL(IZ)
                ALP = REAL(IA)*(PI/180.0)
                BET = REAL(IB)*(PI/180.0)
                GAM = REAL(IC)*(PI/180.0)
C
                SINALP=SIN(ALP)
                COSALP=COS(ALP)
                SINBET=SIN(BET)
                COSBET=COS(BET)
                SINGAM=SIN(GAM)
                COSGAM=COS(GAM)
C
                A21=COSALP*SINGAM+SINALP*SINBET*COSGAM
                A22=COSALP*COSGAM-SINALP*SINBET*SINGAM
                A23=-SINALP*COSBET
                A31=SINALP*SINGAM-COSALP*SINBET*COSGAM
                A32=SINALP*COSGAM+COSALP*SINBET*SINGAM
                A33=COSALP*COSBET
C
                XH1=A21*YH1ST+A31*ZHST + XO
                YH1=A22*YH1ST+A32*ZHST + YO
                ZH1=A23*YH1ST+A33*ZHST + ZO
```

```
                XH2=A21*YH2ST+A31*ZHST + XO
                YH2=A22*YH2ST+A32*ZHST + YO
                ZH2=A23*YH2ST+A33*ZHST + ZO
C
                DIST = SQRT((XO**2)+(YO**2)+(ZO**2))
                WRITE(1,70) XO,YO,ZO,DIST,XH1,YH1,ZH1,XH2,YH2,ZH2
33      CONTINUE
C
70      FORMAT('O  ',3F12.5,F8.2/,'H  ',3F12.5/,'H  ',3F12.5)
        CLOSE(1)
        OPEN (1,FILE='coorQ2')
        OPEN (2,FILE='coorQ2.bak')
60      READ (1,80,END=94) O,X,Y,Z,DIST,H1,u,v,w,H2,r,s,t
        IF (DIST.GE.3.4 .AND. DIST.LT.10.) THEN
           WRITE (2,80) O,X,Y,Z,DIST,H1,u,v,w,H2,r,s,t
        END IF
        GO TO 60
94      CLOSE (2)
        CLOSE (1)
80      FORMAT(A3,3F12.5,F8.2/,A3,3F12.5/,A3,3F12.5)
        END
```

2. Program for Automatically Running Gaussian98 and Getting Output

```
**** PROGRAM COMP : GLUCOSAMINE-WATER  ***
        REAL*8 EHF, DeltaE, DIST,r,s,t, u,v,w, x,y,z
        real*8 Emono, Hartree
        CHARACTER TEXT*9,SCF*9,PROB*9,STOP*9,ERROR*9,
      + O*3,H1*3,H2*3,line*20
        OPEN (1,FILE='energy')
        OPEN (7,FILE='coord')
        open (2,file='const')
        read (2,55) Emono, Hartree
C       Hartree = 627.5, Emono = Emono(Glu)+Emono(Water)
55      format(F16.9,F8.2)
        line = '----------'
        WRITE (1,'(T1,A41)')'   ***  Energy of Glucosamine + H2O  ***'
        WRITE (1,'(T1,4A20)') line,line,line,line
        WRITE (1,'(T1,A75)')'ATOM      X         Y         Z      DI
      + ST       EHF        DeltaE'
        WRITE (1,'(T1,4A20)') line,line,line,line
```

```
      NCONF=50
      DO 70 I= 1,NCONF
      READ (7,10) O,r,s,t, H1,u,v,w, H2,x,y,z
10    FORMAT(A3,3F12.5/,A3,3F12.5/,A3,3F12.5)
      DIST = SQRT((r**2)+(s**2)+(t**2))
      OPEN (8,FILE='Water')
      WRITE(8,11) O,r,s,t, H1,u,v,w, H2,x,y,z
11    FORMAT(A3,3F12.5/,A3,3F12.5/,A3,3F12.5/)
      CLOSE(8)
      CALL SYSTEM ('cat head Water > wg.inp')
C     head is head of the input Gaussian file
      CALL SYSTEM ('g98 < wg.inp > wg.out')
      OPEN (9,FILE='wg.out')
15    READ (9,20,END=99) TEXT
20    FORMAT (A9)
      SCF = ' SCF Done'
      PROB = ' Problem '
      STOP = '    STOP'
      ERROR = '    core'
      IF (TEXT.EQ.SCF) THEN
         BACKSPACE (UNIT=9)
         READ (9,30) EHF
30       FORMAT (20X,F16.9)
         DeltaE = Hartree * (EHF - Emono)
         WRITE (1,40) O,r,s,t,DIST,EHF,DeltaE,H1,u,v,w,H2,x,y,z
40       FORMAT (A3,3F12.5,F10.5,2F16.9/,A3,3F12.5/,A3,3F12.5)
         CLOSE (9)
         GO TO 70
      END IF
      IF (TEXT.EQ.PROB) THEN
         WRITE (1,50) O, r, s, t, DIST, ERROR,H1,u,v,w,H2,x,y,z
50       FORMAT (A3,3F12.5,F10.5,A9/,A3,3F12.5/,A3,3F12.5)
         CLOSE (9)
         GO TO 70
      END IF
      GO TO 15
99    WRITE (1,50) O, r, s, t, DIST, STOP,H1,u,v,w,H2,x,y,z
70    CONTINUE
      CLOSE (7)
      CLOSE (1)
      END
```

Appendix IV

Input Files for Gaussian98 Program

1. Optimization of Glucosamine Structure

```
$RunGauss
#HF/D95* scf=direct optcyc=999 popt

Glucosamine Optimization

0  1
H1
O2   H1 r2
C3   O2 r3   H1 a3
C4   C3 r4   O2 a4   H1 d4
N5   C4 r5   C3 a5   O2 d5
H6   N5 r6   C4 a6   C3 d6
H7   N5 r7   C4 a7   C3 d7
C8   C4 r8   C3 a8   O2 d8
O9   C8 r9   C4 a9   C3 d9
H10   O9 r10   C8 a10   C4 d10
C11   C8 r11   C4 a11   C3 d11
O12   C11 r12   C8 a12   C4 d12
H13   O12 r13   C11 a13   C8 d13
C14   C11 r14   C8 a14   C4 d14
C15   C14 r15   C11 a15   C8 d15
O16   C15 r16   C14 a16   C11 d16
H17   O16 r17   C15 a17   C14 d17
O18   C3 r18   O2 a18   H1 d18
H19   C3 r19   O2 a19   H1 d19
H20   C4 r20   C3 a20   O2 d20
H21   C8 r21   C4 a21   C3 d21
H22   C11 r22   C8 a22   C4 d22
H23   C14 r23   C11 a23   C8 d23
H24   C15 r24   C14 a24   C11 d24
H25   C15 r25   C14 a25   C11 d25
Variables:
d4=  160.0000000
d10=  -55.1809684
```

d13= 65.3990185
d17= -284.2960206
Constants:
r2= 0.8719969
r3= 1.3984393
r4= 1.5291429
r5= 1.4437478
r6= 0.9049919
r7= 0.9057244
r8= 1.5343384
r9= 1.4251882
r10= 0.7936508
r11= 1.5222113
r12= 1.4407029
r13= 0.8023056
r14= 1.5343415
r15= 1.5154879
r16= 1.4211470
r17= 0.8966384
r18= 1.4082009
r19= 0.9709391
r20= 1.0457743
r21= 1.0606668
r22= 1.0593746
r23= 1.0657942
r24= 1.0458814
r25= 1.0773269
a3= 107.0002873
a4= 105.7385685
a5= 110.5074557
a6= 113.6001523
a7= 113.5194933
a8= 110.3986089
a9= 110.5366633
a10= 113.5970767
a11= 108.9352193
a12= 108.4701334
a13= 121.9268115
a14= 109.6102878
a15= 115.5051439
a16= 113.9834004
a17= 123.0757485
a18= 107.7372813
a19= 103.8283705

a20= 112.4443428
a21= 110.1063949
a22= 107.7373748
a23= 105.7528325
a24= 100.3697534
a25= 103.8821473
d5= -64.3750894
d6= 109.7327354
d7= -49.9277388
d8= 171.8609814
d9= -173.8526647
d11= -53.3456585
d12= 174.9480087
d14= 55.9780277
d15= 179.5229541
d16= 55.4258471
d18= -81.0000049
d19= 36.7415416
d20= 51.8620269
d21= 66.5390537
d22= -72.5162642
d23= 57.4738128
d24= -65.5554123
d25= -162.2956507

2. Single Point Energy of Glucosamine-Water

$RunGauss
#HF/D95** scf=direct

Glucosamine+Water

0 1
H -0.53119 3.14992 0.45062
O 0.00333 2.56802 0.81949
C 0.00017 1.43384 0.00143
C 1.27971 0.67058 0.34564
N 2.44337 1.44807 -0.00907
H 2.90230 1.76013 0.70577
H 2.41728 1.77272 -0.85422
C 1.28778 -0.69914 -0.34574

O 2.40751 -1.46927 0.08351
H 3.10409 -1.10457 -0.02441
C -0.00016 -1.43384 -0.00142
O -0.03704 -2.66506 -0.74866
H 0.52110 -3.23403 -0.65676
C -1.20626 -0.57172 -0.39676
C -2.56470 -1.18445 -0.12125
O -2.75826 -1.57599 1.23112
H -2.89345 -0.98955 1.89578
O -1.15147 0.68485 0.31090
H -0.05259 1.79639 -0.89774
H 1.38113 0.50408 1.37309
H 1.35160 -0.57640 -1.39735
H 0.06382 -1.74041 1.01060
H -1.09530 -0.37953 -1.43919
H -2.54262 -1.99568 -0.78101
H -3.23735 -0.60826 -0.73458
O -3.15147 0.28485 0.42090
H -2.05259 1.80639 -0.29774
H -1.38113 0.71408 1.11309

3. Basis Set Superposition Error: Glucosamine as a Ghost Atom

$RunGauss
#HF/D95** scf=direct Massage

Glucosamine+H2O : Glucosamine is a Ghost atom

0 1
H
O 1 r2
C 2 r3 1 a3
C 3 r4 2 a4 1 d4
N 4 r5 3 a5 2 d5
H 5 r6 4 a6 3 d6
H 5 r7 4 a7 3 d7
C 4 r8 3 a8 2 d8
O 8 r9 4 a9 3 d9
H 9 r10 8 a10 4 d10
C 8 r11 4 a11 3 d11
O 11 r12 8 a12 4 d12

H 12 r13 11 a13 8 d13
C 11 r14 8 a14 4 d14
C 14 r15 11 a15 8 d15
O 15 r16 14 a16 11 d16
H 16 r17 15 a17 14 d17
O 3 r18 2 a18 1 d18
H 3 r19 2 a19 1 d19
H 4 r20 3 a20 2 d20
H 8 r21 4 a21 3 d21
H 11 r22 8 a22 4 d22
H 14 r23 11 a23 8 d23
H 15 r24 14 a24 11 d24
H 15 r25 14 a25 11 d25
O 18 r26 3 a26 2 d26
H 26 r27 18 a27 3 d27
H 26 r28 18 a28 3 d28

Variables:

r2= 0.8720
r3= 1.3984
a3= 107.00
r4= 1.5291
a4= 105.74
d4= 159.46
r5= 1.4438
a5= 110.51
d5= 295.63
r6= 0.9050
a6= 113.60
d6= 109.73
r7= 0.9057
a7= 113.52
d7= 310.07
r8= 1.5343
a8= 110.40
d8= 171.86
r9= 1.4252
a9= 110.54
d9= 186.15
r10= 0.7936
a10= 113.60
d10= 304.40
r11= 1.5222
a11= 108.93
d11= 306.65

r12= 1.4407
a12= 108.47
d12= 174.95
r13= 0.8023
a13= 121.93
d13= 61.19
r14= 1.5343
a14= 109.61
d14= 55.98
r15= 1.5155
a15= 115.51
d15= 179.52
r16= 1.4212
a16= 113.98
d16= 55.43
r17= 0.8966
a17= 123.08
d17= 73.58
r18= 1.4082
a18= 107.74
d18= 279.00
r19= 0.9709
a19= 103.83
d19= 36.74
r20= 1.0458
a20= 112.44
d20= 51.86
r21= 1.0607
a21= 110.11
d21= 66.54
r22= 1.0594
a22= 107.74
d22= 287.48
r23= 1.0658
a23= 105.75
d23= 57.47
r24= 1.0459
a24= 100.37
d24= 294.44
r25= 1.0773
a25= 103.88
d25= 197.70
r26= 2.5464
a26= 93.36

d26= 322.46
r27= 0.9570
a27= 42.57
d27= 339.21
r28= 0.9570
a28= 144.03
d28= 309.67

1 0 0.0
2 0 0.0
3 0 0.0
4 0 0.0
5 0 0.0
6 0 0.0
7 0 0.0
8 0 0.0
9 0 0.0
10 0 0.0
11 0 0.0
12 0 0.0
13 0 0.0
14 0 0.0
15 0 0.0
16 0 0.0
17 0 0.0
18 0 0.0
19 0 0.0
20 0 0.0
21 0 0.0
22 0 0.0
23 0 0.0
24 0 0.0
25 0 0.0

4. Basis Set Superposition Error: Water as a Ghost Atom

$RunGauss
#HF/D95** scf=direct Massage

Glucosamine+H2O : Water is Ghost atom

0 1

H
O 1 r2
C 2 r3 1 a3
C 3 r4 2 a4 1 d4
N 4 r5 3 a5 2 d5
H 5 r6 4 a6 3 d6
H 5 r7 4 a7 3 d7
C 4 r8 3 a8 2 d8
O 8 r9 4 a9 3 d9
H 9 r10 8 a10 4 d10
C 8 r11 4 a11 3 d11
O 11 r12 8 a12 4 d12
H 12 r13 11 a13 8 d13
C 11 r14 8 a14 4 d14
C 14 r15 11 a15 8 d15
O 15 r16 14 a16 11 d16
H 16 r17 15 a17 14 d17
O 3 r18 2 a18 1 d18
H 3 r19 2 a19 1 d19
H 4 r20 3 a20 2 d20
H 8 r21 4 a21 3 d21
H 11 r22 8 a22 4 d22
H 14 r23 11 a23 8 d23
H 15 r24 14 a24 11 d24
H 15 r25 14 a25 11 d25
O 18 r26 3 a26 2 d26
H 26 r27 18 a27 3 d27
H 26 r28 18 a28 3 d28

Variables:
r2= 0.8720
r3= 1.3984
a3= 107.00
r4= 1.5291
a4= 105.74
d4= 159.46
r5= 1.4438
a5= 110.51
d5= 295.63
r6= 0.9050
a6= 113.60
d6= 109.73
r7= 0.9057
a7= 113.52
d7= 310.07

r8= 1.5343
a8= 110.40
d8= 171.86
r9= 1.4252
a9= 110.54
d9= 186.15
r10= 0.7936
a10= 113.60
d10= 304.40
r11= 1.5222
a11= 108.93
d11= 306.65
r12= 1.4407
a12= 108.47
d12= 174.95
r13= 0.8023
a13= 121.93
d13= 61.19
r14= 1.5343
a14= 109.61
d14= 55.98
r15= 1.5155
a15= 115.51
d15= 179.52
r16= 1.4212
a16= 113.98
d16= 55.43
r17= 0.8966
a17= 123.08
d17= 73.58
r18= 1.4082
a18= 107.74
d18= 279.00
r19= 0.9709
a19= 103.83
d19= 36.74
r20= 1.0458
a20= 112.44
d20= 51.86
r21= 1.0607
a21= 110.11
d21= 66.54
r22= 1.0594
a22= 107.74

d22= 287.48
r23= 1.0658
a23= 105.75
d23= 57.47
r24= 1.0459
a24= 100.37
d24= 294.44
r25= 1.0773
a25= 103.88
d25= 197.70
r26= 2.5464
a26= 93.36
d26= 322.46
r27= 0.9570
a27= 42.57
d27= 339.21
r28= 0.9570
a28= 144.03
d28= 309.67

26 0 0.0
27 0 0.0
28 0 0.0

5. Natural Population Analysis of Glucosamine

$RunGauss
#HF/D95** scf=direct pop=NPA

Glucosamine, Natural Population Analysis

0	1		
H	-0.53119	3.14992	0.45062
O	0.00333	2.56802	0.81949
C	0.00017	1.43384	0.00143
C	1.27971	0.67058	0.34564
N	2.44337	1.44807	-0.00907
H	2.90230	1.76013	0.70577
H	2.41728	1.77272	-0.85422
C	1.28778	-0.69914	-0.34574
O	2.40751	-1.46927	0.08351

H	3.10409	-1.10457	-0.02441
C	-0.00016	-1.43384	-0.00142
O	-0.03704	-2.66506	-0.74866
H	0.52110	-3.23403	-0.65676
C	-1.20626	-0.57172	-0.39676
C	-2.56470	-1.18445	-0.12125
O	-2.75826	-1.57599	1.23112
H	-2.89345	-0.98955	1.89578
O	-1.15147	0.68485	0.31090
H	-0.05259	1.79639	-0.89774
H	1.38113	0.50408	1.37309
H	1.35160	-0.57640	-1.39735
H	0.06382	-1.74041	1.01060
H	-1.09530	-0.37953	-1.43919
H	-2.54262	-1.99568	-0.78101
H	-3.23735	-0.60826	-0.73458

CURRICULUM VITAE

Khatcharin Siriwong

1972	Born February 7th, in Udon Thani, Thailand Father : Mr. Kian Siriwong Mother : Mrs. Lun Siriwong
1979-1985	Elementary School (Ban Dongtat School, Udon Thani)
1985-1988	Primary School (Kutchabprachasan School, Udon Thani)
1988-1991	High School (Kutchabprachasan School, Udon Thani)
1991-1995	Bachelor of Science (Chemistry),] Khon Kaen University, Khon Kaen (Scholarship awarded by the Development and Promotion of Science and Technology Talents Project, DPST)
1998-2000	Master degree student at Department of Chemistry, Chulalongkorn University, Bangkok
1995-Present	Lecturer at Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen