References

Alder, B. J. and Wainwright, T. E. 1957. **J. Chem. Phys.** 27: 1208.

Alder, B. J. and Wainwright, T. E. 1959. **J. Chem. Phys.** 31: 459.

Allgaier, R. S. 1970. **Phys. Rev. B** 2: 2257.

Benedict, W. S. and Plyler, E. K. 1985. **Can. J. Phys.** 35: 890.

Birchall, T., Drummond, I. 1970. **J. Chem. Soc.** 1859.

Bopp, P. 1986. **Chem. Phys.** 196: 205.

Born, M. and Karman, V. 1912. **Physik. Z.** 13: 297.

Born, M. and Oppenheimer 1927. **Ann. Physik.** 84: 457.

Boys, S. F. 1950. **Proc. Roy. Soc. A** 200: 542.

Boys, S. F. and Bernardi, F. 1970. **Mol. Phys.** 19: 553.

Burow, D. F. and Lagowski, J. J. 1965. **Adv. Chem. Ser.** 50: 125.

Cusack, N. E. 1963. **Rep. Prog. Phys.** 26: 361.

Dang, L. X. 1992. **J. Chem. Phys.** 96: 6970.

Deng, Z., Martyna, G. J., and Klien M. L. 1992 **Phys. Rev. Lett.** 68: 2496.

Deng, Z., Martyna, G. J., and Klien M. L. 1994 **J. Chem. Phys.** 100: 7590.

Elrod, M. J. and Saykally, R. J. 1994. **Chem. Rev.** 94: 1975.

Ewald, P. P., 1921. **Ann, Phys**. 64: 253.

Faber, T. E. 1972. **Introduction to the theory of liquid metals.** Cambridge University Press.

Frenke, D. and Smit, B. 1996. **Understanding Molecular Simulation.** CA: Academic Press.

Frenkel, J. 1946. **Kinetic theory of liquids.** Oxford: Clarendon Press.

Garroway, A. N. and Cotts, R. M. 1973. **Phys. Rev. A** 7: 635.

Gear, C. W. 1966. **The numerical integration of ordinary differential equations of various orders.** Report ANL 7126, Argonne National Laboratory.

Gear, C. W. 1971. **Numerical initial value problems in ordinary differential equations.** NJ: Prentice-Hall.

Glaunsinger, W. S., Von Dreele, R. B., Marzke, R. F., and Hanson, R. C. 1984. **J. Phys. Chem.** 88: 3860.

Gurskii, Z., Hannongbua, H., Heinzinger, K. 1993. **Mol. Phys.** 78: 461.

Hall, G. G. 1951. **Proc. Roy. Soc. A** 205: 541.

Hallada, C. J. and Jolly, W. L. 1963. **J. Inorg. Chem.** 2: 1076.

Hannongbua, S. 1991. **Aust. J. Chem.** 44: 447.

Hannongbua, S. 1997. **J. Chem. Phys.** 106: 6076.

Hannongbua, S. 1998. **Chem. Phys. Lett.** in press.

Hannongbua, S. V., Ishida T., Spohr, E., and Heinzinger, K. 1988. **Z. Naturforsch.** 43a: 572.

Hannongbua, S., Kerdcharoen, T., and Rode, B. M. 1992. **J. Chem. Phys.** 96: 6945

Harrison, W. 1963. **Phys. Rev.** 131: 2433.

Hodgman, C. D. 1959. **Handbook of Chemistry and Physics** 41th ed., Ohio: Chemical Rubber.

Ichimaru, S. and Utsumi, K. 1981. **Phys. Rev. B** 24: 7385.

Impey, R. W. and Klein, M. L. 1984. **Chem. Phys. Lett.** 104: 579.

Jansen, L. 1962. **Phys. Rev.** 125: 1798.

Kelterbaum, R., Turki, N., Rahmouni, A., and Kochanski E. 1994 **J. Chem. Phys.** 100: 1589.

Kim, J., Lee, S., Cho, S. J., Mhin, B. J., and Kim, K. S. **J. Chem. Phys.** 102: 839.

Klein, M. L. 1994. http://www.psc.edu/MetaCenter/MetaScience/Articles/Klein/Klein.html University of Pennsylvania, Michael L. Klein.

Lucas, K. 1991. **Applied Statistical Thermodynamics** Berlin: Springer-Verlag.

Lynbrand, T. P. and Kollman, P. A. 1985. **J. Chem. Phys.** 83: 2923.

Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N. Teller, A. H. and Teller, E. 1953. **J. Chem. Phys**. 21: 1087.

Moissan, H. 1904. **Bull. Soc. Chim. Paris** 331: 549.

Naiditch, S. 1964. **Metal-ammonia solutions**. New York: W. A. Benjamin.

Narten, A. H. 1977. **J. Chem. Phys.** 66: 3117.

Nasby, R. D. and Thomson, J. C. 1970. **J. Chem. Phys.** 53, 109.

O'Reilly, D. E., Peterson, E. M., and Scheie, C. E. 1973. **J. Chem. Phys.** 58: 4072.

Onsager, L. 1936. **J. Am. Chem. Soc.** 58: 1486.

Polymeropoulos, E. E. and Brickmann, J. 1982. **Chem. Phys. Lett.** 96: 273.

Roothaan, C. C. J. 1951. **Rev. Mod. Phys.** 23: 69.

Sagarik, K., Ahlrichs, R., and Brode, S. 1986. **Mol. Phys.** 6: 1247.

Schroeder, R. L., Thompson, J. C., and Oertel, P. L. 1969. **Phys. Rev.** 178: 298.

Seely, C. A. 1871. **Chem. News** 23: 169.

Slater, J. C. 1930. **Phys. Rev.** 35: 509.

Spirko, V. 1983. **J. Mol. Spectrosc.** 101: 30.

Strett, W. B., Tildesley, D. J., and Saville, G. 1978. **ACS Symp. Ser** 86: 144.

Taft, R. 1933. **J. Chem. Educ.** 10: 196.

Teoh , H., Antoniewich, P. R., and Thompson, J. C. 1971. **J. Phys. Chem.** 75: 399.

Thompson, J. C. 1976. **Electron in Liquid Ammonia**. Oxford: Clarendon Press.

Tongraar, A., Hannongbua, S., and Rode, B. M. 1997. **Chem. Phys.** 219: 279.

Weast, R. C. 1976. **Handbook of Chemistry and Physics.** 57th ed., Ohio: CRC.

Weast, R. C. 1977. **Handbook of Chemistry and Physics.** 57th ed., Ohio: CRC.

Weyl, W. 1864. **Poggendorffs Annln**. 121: 601.

Whitten, J. C. 1963. **J. Chem. Phys.** 44(1): 359.

Wong, W. S. 1966. **Ph.D. Dissertation.** University of California at Berkeley.

Yongyai, Y., Kokpol, S., and Rode, B. M. 1991. **Chem. Phys.** 156: 403.

Appendices

Appendix A : basis set

Exponent and coefficient for basis set of H

shell	*exponent*	*coefficient*
S 3 1.00	.3386500000D+02	.2549380000D-01
	.5094790000D+01	.1903730000D+00
	.1158790000D+01	.8521610000D+00
S 1 1.00	.3258400000D+00	.1000000000D+01
S 1 1.00	.1027410000D+00	.1000000000D+01
P 1 1.00	.7500000000D+00	.1000000000D+01

Exponent and coefficient for basis set of N

shell	*exponent*	*coefficient*
S 6 1.00	.5909440000D+04	.2004000000D-02
	.8874510000D+03	.1531000000D-01
	.2047900000D+03	.7429300000D-01
	.5983760000D+02	.2533640000D+00
	.1999810000D+02	.6005760000D+00
	.2686000000D+01	.2451110000D+00
S 1 1.00	.7192700000D+01	.1000000000D+01
S 1 1.00	.7000000000D+00	.1000000000D+01
S 1 1.00	.2133000000D+00	.1000000000D+01
P 4 1.00	.2678600000D+02	.1825700000D-01
	.5956400000D+01	.1164070000D+00
	.1707400000D+01	.3901110000D+00
	.5314000000D+00	.6372210000D+00
P 1 1.00	.1654000000D+00	.1000000000D+01
D 1 1.00	.8000000000D+00	.1000000000D+01

Exponent and coefficient for basis set of Ca

shell	*exponent*	*coefficient*
S 1 1.00	.2260900200D+06	.1000000000D+01
S 1 1.00	.3390447600D+05	.1000000000D+01
S 1 1.00	.7719622900D+04	.1000000000D+01
S 1 1.00	.2192246900D+04	.1000000000D+01
S 1 1.00	.7193664100D+03	.1000000000D+01
S 1 1.00	.2621894800D+03	.1000000000D+01
S 1 1.00	.1036953100D+03	.1000000000D+01
S 1 1.00	.4326127000D+02	.1000000000D+01
S 1 1.00	.1349212600D+02	.1000000000D+01
S 1 1.00	.5569443000D+01	.1000000000D+01
S 1 1.00	.1429822200D+01	.1000000000D+01
S 1 1.00	.5840690900D+00	.1000000000D+01
S 1 1.00	.9131598000D-01	.1000000000D+01
S 1 1.00	.3512626000D-01	.1000000000D+01
P 1 1.00	.1397334100D+04	.1000000000D+01
P 1 1.00	.3316781200D+03	.1000000000D+01
P 1 1.00	.1070755000D+03	.1000000000D+01

P	1	1.00	.4033535300D+02	.1000000000D+01
P	1	1.00	.1647589000D+02	.1000000000D+01
P	1	1.00	.7023515800D+01	.1000000000D+01
P	1	1.00	.2755287700D+01	.1000000000D+01
P	1	1.00	.1154607400D+01	.1000000000D+01
P	1	1.00	.4405384500D+00	.1000000000D+01
D	1	1.00	.2998230700D+02	.1000000000D+01
D	1	1.00	.8300332300D+01	.1000000000D+01
D	1	1.00	.2740691800D+01	.1000000000D+01
D	1	1.00	.9548327300D+00	.1000000000D+01
D	1	1.00	.2900331000D+00	.1000000000D+01

CONSTANT

The physical constants and widely used variables are set in this subroutine

INPUT

This routine read all information necessary to perform the simulation from the input file, and convert them to unit used in the program.

POWTPRP

Since the shift-force potential method have been applied to the intermolecular interaction calculations, the necessary value used in the method were prepared in thin subroutine.

OUTPUT

this subroutine simply writes the data used in program to an appropriate output files.

HISTSTRT

the actual simulation begin with reading the starting configuration, positions and velocities, from configuration file, performing by this HISTSTRT subroutine.

NEBR

Since potential and the forces become zero beyond the cutoff distance, due to shift-force potential method. Only the neighbor on the distance not longer than cutoff radius need to account in calculation. This subroutine count for the neighbor list, containing a list of effective particles, and update them at specified intervals.

POWT

The force and potential on each particles in simulations system are calculated in this subroutine. Each pairs of interaction were calculated by the specific subroutines called by this subroutine.

PSEUDO_FORCE & PSEUDO_POTENTIAL

The routine used for calculate the indirect interaction function, (equation 4.32)

$$V_{ind}(R) = \frac{\Omega_0}{\pi^2}\int_0^\infty F(q)\frac{\sin qR}{R} q\, dq\,.$$

EPSILON

The routine used for calculate the temperature dependent dielectric function, (detail in section 4.3.5.2)

$$\varepsilon(q) = 1 + \frac{4\pi}{q^2}\Pi(q)\,.$$

PRED

The predicted $\vec{r}(t)$, $\vec{v}(t)$, $\vec{a}(t)$, and $\vec{b}(t)$ for the next timestep of nitrogen atoms, hydrogen atoms and calcium ions were calculated in this subroutine. The periodic boundary conditions were also taken care.

CORR

after the predicted $\vec{r}(t)$, $\vec{v}(t)$, $\vec{a}(t)$, and $\vec{b}(t)$ have been calculated, they were corrected in this subroutine by equation (3.12).

RUNTEST

This routine is used for observed any properties the simulations system and insert required condition into the system. Any subroutine used for observe and for control system properties were attached with this routine.

HISTOUT

At every specified timesteps, this routine write the system configuration, positions and velocities to the history files for later used.

HISTEND

Before the program terminated normally, this routine write the system last configuration, positions and velocities to the appropriate files for later used.

Appendix C : Intramolecular Potential

The intramolecular potential surfaces for the ammonia molecule is given by

$$V_{intra} = \sum_{i=1}^{4} k_u h^{2u} + k_1' h^2 s_1 + k_2' h^4 s_1 + \frac{1}{2}\sum_{i=1}^{5}\sum_{j=i}^{5} F_{ij} s_i s_j + \sum_{i=1}^{5}\sum_{j=i}^{5}\sum_{k=j}^{5} F_{ijk} s_i s_j s_k + \sum_{i=1}^{5}\sum_{j=i}^{5}\sum_{k=j}^{5}\sum_{l=k}^{5} F_{ijkl} s_i s_j s_k s_l$$

The symmetry coordinates is

$$s_1 = \frac{1}{\sqrt{3}}\left(\Delta r_1 + \Delta r_2 + \Delta r_3\right),$$

$$s_2 = \frac{1}{\sqrt{6}}\left(2\Delta r_1 - \Delta r_2 - \Delta r_3\right),$$

$$s_3 = \frac{1}{\sqrt{6}}\left(2\Delta \alpha_1 - \Delta \alpha_2 - \Delta \alpha_3\right),$$

$$s_4 = \frac{1}{\sqrt{2}}\left(\Delta r_2 - \Delta r_3\right),$$

$$s_5 = \frac{1}{\sqrt{2}}\left(\Delta \alpha_2 - \Delta \alpha_3\right),$$

where Δr_i and $\Delta \alpha_i$ are the three N-H distances and H-N-H angles, respectively. h is the distance of the nitrogen atom from the plan spanned by the three hydrogen atoms, and all constants are given by

k_1 = -0.53741
k_2 = +2.08241
k_3 = -0.77902
k_4 = +0.3500
k'_1 = +1.0806
k'_2 = -5.7569

F_{11} = 6.8186
F_{12} = F_{44} = 6.8975
F_{33} = F_{55} = 0.6166

$F_{23} = F_{45} = 0.0028$
$F_{111} = -3.92836$
$F_{122} = F_{144} = -11.9988$
$F_{123} = F_{145} = -4.8718\times10^{-3}$
$F_{133} = F_{155} = -0.10989$
$F_{222} = -2.82914$
$F_{244} = 8.4874$
$F_{223} = -F_{344} = 5.9505\times10^{-6}$
$F_{245} = 1.1901\times10^{-5}$
$F_{233} = -F_{255} = -1.0983\times10^{-3}$
$F_{345} = 21.966\times10^{-3}$
$F_{333} = -0.06747$
$F_{355} = 0.2024$

$F_{1111} = 2.8351$
$F_{1122} = F_{1144} = 17.163$
$F_{1133} = F_{1155} = 0.08564$
$F_{1222} = 8.1277$
$F_{1244} = -24.3830$
$F_{1333} = 0.01625$
$F_{1355} = -0.04875$
$F_{2222} = F_{4444} = 4.3066$
$F_{2244} = 8.6133$
$F_{2233} = F_{2255} = F_{3344}$
$= F_{4455} = 0.04078$
$F_{3333} = F_{5555} = 0.08044$
$F_{3355} = 0.16087$

CURRICULUM VITAE

Police Captain Wiwat Sidhisoradej,
Inspector, Scientific Crime Detection Division,
Royal Thai Police.

1965	Born : Nov, 8th 1965 in Bangkok, THAILAND. Father : Thammanoon Sidhisoradej. Mother: Wijittra Sidhisoradej.
1971-1980	Elementary School Buranawit School, Bangkok.
1980-1981	High School, Wat Borwornniwed School, Bangkok.
1981-1985	Bachelor of Science (Physics), Chiangmai University, Chiangmai, THAILAND.
1985-1989	Master of Science (Physics), Chulalongkorn University, Bangkok, THAILAND.
1993-1998	Doctor of Philosophy (Physics), Chulalongkorn University, Bangkok, THAILAND.