**A SEMICLASSICAL, DYNAMICAL MODEL
OF THE WATER MOLECULE**

Donald Greenspan

Mathematics Department
University of Texas at Arlington

Technical Report #303

A SEMICLASSICAL, DYNAMICAL MODEL OF THE WATER MOLECULE

Donald Greenspan

Mathematics Department
University of Texas at Arlington

Technical Report #303

ABSTRACT

A model of the ground state water molecule is formulated dynamically and studied by computer simulations. Excellent approximations of NMR determined bond angles and bond lengths are achieved through electron pairing and simulation of ice *I*.

1. Introduction. The past 75 years has seen an immense amount of research directed at the most fundamental molecule in living matter, the water molecule ⁽¹⁻³⁾. And yet, from both the classical and quantum mechanical points of view, many fundamental questions remain unanswered ⁽¹⁻⁴⁾. For a single water molecule, only static models are available, and these include those of Bader; Bernal; Duncan and Pople; Ellison and Shull; Gillespie; Heath and Linnett; Rowlinson; and Vernay ^(1,5,6). Since a dynamical simulation of the water molecule quantum mechanically would require the exact or approximate solution of Schrodinger's equation for a wave function in 39 space dimensions and one time dimension, we will begin more simply in this paper by studying a semiclassical model. The keys to our excellent results will be the introduction of electron pairing and the use of a crystalline state.

2. General Model Formulation. Consider a ground state water molecule M_1 whose oxygen nucleus is denoted by O_1 . Let M_2, M_3, M_4, M_5 , with respective oxygen nuclei O_2, O_3, O_4, O_5 , be four neighboring molecules of M_1 . Assume that $M_1 - M_5$ are water molecules in ice *I*, thus allowing us to avoid the complex motions of the liquid state and allowing the introduction of available experimental results into the model ^(1,3,7).

For the crystal structure of ice *I*, we assume that $O_2 - O_5$ are at the vertices of a regular tetrahedron with O_1 at the centroid, as shown in Figure 2.1. In each M_i , let the two hydrogen nuclei be H_{ij} , $i = 1, 2, 3, 4, 5$; $j = 1, 2$. Experimentally ^(1,2,3,7), then, the distance from O_1 to each of O_2, O_3, O_4, O_5 is $2.76 \text{ \AA}$ and on each line joining O_1 to O_2, O_3, O_4, O_5 there is exactly one H_{ij} , one possible such arrangement being that shown in Figure 2.1.

It will be important to recall that the ground state energy E of M_1 is ^(8,9,10)

$$E = - (3333.04) 10^{-12} \text{ erg.}$$

We now concentrate primarily on M_1 , whose vibrational motions will be simulated.

Figure 2.1

First, let us approximate the Coulombic effect of $M_2 - M_5$ on M_1 . For this purpose, consider then the effect of M_2 on M_1 . Let M_2 be a static Duncan and Pople molecule, as shown in Figure 2.2. (Other possible static models will be discussed in Section 6.) Let Q_1 be the oxygen nucleus; Q_2, Q_3 the protons; and $Q_4 - Q_7$ negative charges. In terms of $e = (4.8028)10^{-10}$ esu, the Duncan and Pople model assigns charges $C(Q_i)$ by

$$C(Q_1) = 6e, \quad C(Q_2) = C(Q_3) = e,$$

$$C(Q_4) = C(Q_5) = C(Q_6) = C(Q_7) = -2e.$$

Now set a hypothetical particle of unit charge e at $Q_8 = (2.18, 0, 1.69)$, in the coordinate system of Figure 2.2, so that the distance from Q_1 to Q_8 is $2.76 \text{ \AA}$. Then, the effective Coulombic force of $Q_1 - Q_7$ on Q_8 is, approximately, $0.06e^2(10)^{16}$. Thus, we replace M_2 by a single fixed point charge at O_2 of $C_1 = 0.45e$. Similarly, M_3 is replaced by a single point charge at O_3 whose charge is $0.45e$. Analogous calculations allow us to replace M_4 and M_5 by point charges at O_4 and O_5 whose charges are $C_2 = -0.23e$.

As shown in Figure 2.3, the oxygen nucleus O_1 and the four fixed charges which replace $M_2 - M_5$ are taken to be a motionless, rigid skeletal structure, into which the protons and electrons of M_1 will be inserted and allowed to move freely, constrained only by conservation of system energy. The coordinates of the $0.45e$ and $-0.23e$ charges will be taken to be $(0, 2.25, -1.59)$, $(0, -2.25, -1.59)$, $(2.25, 0, 1.59)$, $(-2.25, 0, 1.59)$, which are the vertices of a regular tetrahedron with edge length 4.5 whose circumscribed sphere has radius 2.76.

3. Computer Model Formulation. Using the results of Section 2, we proceed now to formulate equations of motion for our water molecule model. We proceed in a new notation which is most convenient for digital computer simulation. In addition, we will introduce changes of variables which simplify the numerical simulation of related initial value problems.

Consider the particles $P_1 - P_{17}$ shown in Figure 3.1. P_1 is an oxygen nucleus, P_2 and P_3 are protons, $P_4 - P_{11}$ are electrons, P_{12} and P_{13} are the two first ring electrons of P_1 , and $P_{14} - P_{17}$ are the point charges which are replacing $M_2 - M_5$. In cgs units, for $i = 1, 2, \dots, 17$ and at any time t , let P_i be located at $\vec{r}_i = (x_i, y_i, z_i)$, have velocity $\vec{v}_i = (\dot{x}_i, \dot{y}_i, \dot{z}_i)$ and have acceleration $\vec{a}_i = (\ddot{x}_i, \ddot{y}_i, \ddot{z}_i)$.

Quantum mechanically, the Ehrenfest equations, which are Newtonian dynamical equations for expectation values, are always valid ⁽¹¹⁾. Moreover, when the wave function is narrow, Newton's equations themselves provide valid dynamical approximations over short time periods ⁽¹¹⁻¹³⁾. We proceed then under assumptions which allow us to employ Newton's equations for short time periods. Since P_1 and $P_{14} - P_{17}$ are fixed for all time, the classical equations of motion for the moving particles P_i , $i = 2, 3, \dots, 13$, are

$$(3.1) \quad m_i \vec{a}_i = \sum_{\substack{j=1 \\ j \neq i}}^{17} \frac{e_i e_j}{r_{ij}^2} \frac{\vec{r}_{ji}}{r_{ij}}, \quad i = 2, 3, \dots, 13,$$

Figure 2.2

Figure 2.3

in which $\vec{r}_{ji}$ is the vector from P_j to P_i , $r_{ij} = r_{ji} = \|\vec{r}_{ji}\|$, the mass m_i and the charge e_i of each P_i , $i = 1, 2, \dots, 13$, are

$$(3.2) \quad m_1 = 16(16724)10^{-28} \text{ gr}$$

$$(3.3) \quad m_2 = m_3 = (16724)10^{-28} \text{ gr}$$

$$(3.4) \quad m_4 = m_5 = \dots = m_{13} = (9.1085)10^{-28} \text{ gr}$$

$$(3.5) \quad e_1 = 8(4.8028)10^{-10} \text{ esu}$$

$$(3.6) \quad e_2 = e_3 = (4.8028)10^{-10} \text{ esu}$$

$$(3.7) \quad e_4 = e_5 = \dots = e_{13} = - (4.8028)10^{-10} \text{ esu},$$

and,

$$(3.8) \quad e_{14} = e_{15} = .45(4.8028)10^{-10} \text{ esu}$$

$$(3.9) \quad e_{16} = e_{17} = - .23(4.8028)10^{-10} \text{ esu}.$$

From given initial data, the time invariant ground state energy must always satisfy

$$(3.10) \quad - (3333.04)10^{-12} = \frac{1}{2} \sum_{i=2}^{13} m_i v_i^2 + \sum_{j=i+1}^{17} \sum_{i=1}^{16} \frac{e_i e_j}{r_{ij}}.$$

We now make some convenient changes of variables. First set

$$(3.11) \quad T = 10^{22} t, \quad \vec{R}_i = 10^{12} \vec{r}_i,$$

in which $\vec{R}_i = (X_i, Y_i, Z_i)$. Then,

$$\vec{V}_i = \frac{d\vec{R}_i}{dT} = \left(\frac{dX_i}{dT}, \frac{dY_i}{dT}, \frac{dZ_i}{dT} \right) = 10^{-10} \vec{v}_i$$

$$\vec{A}_i = \frac{d\vec{V}_i}{dT} = 10^{-32} \vec{a}_i.$$

If, in addition, we set

$$M_i = m_i 10^{28}, \quad E_i = e_i 10^{10} (4.8028)^{-1},$$

then system (3.1) simplifies to

(3.12)

$$M_i \frac{d^2 \vec{R}_i}{dT^2} = (23.06689) \sum_{\substack{j=1 \\ j \neq i}}^{17} \frac{E_i E_j}{R_{ij}^2} \frac{\vec{R}_{ji}}{R_{ij}}, i = 2, 3, \dots, 13$$

in which

$$\begin{aligned} M_1 &= 16(16724) \\ M_2 &= M_3 = 16724 \\ M_4 &= M_5 = \dots = M_{12} = M_{13} = 9.1085 \\ E_1 &= 8 \\ E_2 &= E_3 = 1 \\ E_4 &= E_5 = \dots = E_{13} = -1 \\ E_{14} &= E_{15} = 0.45 \\ E_{16} &= E_{17} = -0.23 \end{aligned}$$

Further, energy equation (3.10) reduces to

$$(3.13) \quad - (3333.04)10^{-4} = \frac{1}{2} \sum_{i=2}^{13} M_i V_i^2 + 23.06689 \sum_{j=i+1}^{17} \sum_{i=1}^{16} \frac{E_i E_j}{R_{ij}}$$

Unless otherwise specified, further discussion is in terms of the R and T variables.

At this point we introduce electron pairing by means of a new model of bonding which has thus far yielded the correct bond lengths and bond angles for dynamical simulations of all the diatomic molecules through oxygen ⁽¹⁴⁾. We assume that the hydrogen electrons bond with two oxygen electrons through electron attraction.

Observe that electron attraction is, of course, not unknown. For example, Nobelists Bardeen, Cooper, and Schrieffer showed that the quantum mechanical theory of superconductivity requires electron attraction ⁽¹⁵⁾. In addition, it must be noted that the behavior of electrons and protons within atoms and molecules has not been determined experimentally. Pauling and Wilson point out that "We do not know that the electron and proton attract each other in the same way that two macroscopic electrically charged bodies do, inasmuch as the force between two particles in a hydrogen atom has never been directly measured" ⁽¹⁶⁾.

For consistency with previous studies we choose the paired electrons to be separated maximally, so the pairs (P_4, P_8) , (P_6, P_{10}) will be chosen. We must then replace the terms $E_4 E_8$ and $E_6 E_{10}$ in both (3.12) and (3.13) by $-E_4 E_8$, $-E_6 E_{10}$, respectively. The new equations will be called the semiclassical equations.

Once initial data are assigned, it will be incumbent upon us to solve semiclassical system (3.12) in such a fashion that the energy at each time step is invariant, that is, that

4. Assignment of Initial Data. As shown in Figure 3.1, the initial positions of $P_1 - P_{17}$, in (X, Y, Z) coordinates, will be set as follows. The arrangement will assure a degree of symmetry which will decrease the required computer time.

P_1 is fixed for all time at $(0,0,0)$. In terms of positive parameters X_2 and Z_2 , P_2 and P_3 are set at $(X_2, 0, Z_2)$, $(-X_2, 0, Z_2)$, respectively, with initial velocities $\vec{0}$. For positive parameter R_1 , $P_4 - P_{11}$ are set, respectively, at (R_1, R_1, R_1) , $(R_1, -R_1, R_1)$, $(-R_1, -R_1, R_1)$, $(-R_1, R_1, R_1)$, $(-R_1, -R_1, -R_1)$, $(-R_1, R_1, -R_1)$, $(R_1, R_1, -R_1)$, $(R_1, -R_1, -R_1)$. In terms of a positive velocity parameter V_1 , the initial velocities of $P_4 - P_{11}$ are taken, respectively, to be $(0, -V_1, 0)$, $(-V_1, 0, 0)$, $(0, V_1, 0)$, $(V_1, 0, 0)$, $(V_1, 0, 0)$, $(0, -V_1, 0)$, $(-V_1, 0, 0)$, $(0, V_1, 0)$. The two first ring electrons P_{12} and P_{13} are set at $(0, 0, 680)$, $(0, 0, -680)$, and since the ground state energy $^{(10)}$ of O^{6+} is $(-1952.9758)10^{-12}$ erg, their velocities are approximated to be $(0, 0.171453, 0)$, $(0, -0.171453, 0)$, respectively. $P_{14} - P_{17}$ are fixed for all time at $(0, 22500, -15900)$, $(0, -22500, -15900)$, $(22500, 0, 15900)$, $(-22500, 0, 15900)$, respectively.

Once the parameters X_2 , Z_2 , and R_1 are selected, the value V_1 follows directly from semiclassical (3.13), and all initial data will be determined. Thus, for example, for $X_2 = 7570$, $Z_2 = 5860$, $R_1 = 4500$, one finds $V_1 = 0.02420179732$.

5. Examples. Observe next that, whereas water vapor spectra $^{(1)}$ imply that the average bond length of a water molecule is $0.96 \text{ \AA}$ with an average bond angle of 104.5° , one might expect variations in ice *I* due to the expansion of water at 4° C . Indeed, experimental NMR results $^{(1)}$ which relate allowable bond angles and bond lengths for ice are those which lie in the shaded region of Figure 5.1. Thus, for example, for an angle of 104.5° , a bond length of $0.99 \text{ \AA}$ would be consistent with NMR measurements, while a bond length of $0.96 \text{ \AA}$ would not.

Figures 5.1 and 2.3 now lead to the following surmises. Initial data which lie in the stable shaded region of Figure 5.1 should yield dynamical results which also lie in the stable region, since the effects of C_1 and C_2 on the protons should be in relative balance. Initial data which lie below the stable region should, in time, yield dynamical results which also lie in the stable region, because the repulsive effects of C_1 on the protons should dominate. Initial data which lie above the stable region should yield dynamical results which do not lie in the stable region because the attractive effects of C_2 on the protons should dominate. We will see next through several extensive examples that these surmises are correct. Calculations will be described in terms of the R and T variables discussed in Sections 3 and 4. Each example was run on an Alpha 150 or an Alpha 275 using a 64 bit word. The energy conserving method $^{(17)}$ incorporates iteration tolerances of $4(10)^{-9}$ for position components and $4(10)^{-12}$ for velocity components. A variable time step procedure is incorporated as follows. At each time step, let $R^* = \min R_{ij}; i = 1, 2, \dots, 13; j = 1, 2, \dots, 13; i \neq j$. Then

if $1500 \leq R^*$, set $\Delta T = 2.0$,
 if $1000 \leq R^* < 1500$, set $\Delta T = 1.0$,
 if $750 \leq R^* < 1000$, set $\Delta T = 0.2$,
 if $500 \leq R^* < 750$, set $\Delta T = 0.02$,
 if $250 \leq R^* < 500$, set $\Delta T = 0.002$,
 if $R^* < 250$, set $\Delta T = 0.0002$.

Ionization, which does occur rarely ⁽¹⁾, is neglected by assuming that, on the average, each water molecule has ten electrons. To implement this conservatively, we assume that if $|P_1 P_2|$, $j = 4, 5, 6, \dots, 13$ exceeds 13800 units (i.e., $\frac{1}{2}(2.76) \text{ \AA}$), then P_j is reflected simply by resetting its velocity $\vec{V}_j$ to $-\vec{V}_j$.

A typical FORTRAN program is available in Appendix A of Greenspan ⁽¹⁸⁾. A program to generate initial data is available in Appendix B of the same reference.

Consider now the choices $X_2 = 7933.5334$, $Z_2 = 6087.6143$, $R_1 = 4500$, for which $V_1 = 0.02423441038$. For these data the HOH angle is 105° and the OH length is 10000, which are shown at the point A in Figure 5.2. The variation of the bond length with the bond angle is shown in the figure through three billion time steps and terminates at A'. The real time of the system's motion is $(5.18)10^{-16}$ sec. Though two electrons were always core electrons, these were not always the same two, which is consistent with recent quantum Monte Carlo simulations ⁽¹⁹⁾.

Figure 5.1. Ice I equilibrium dimensions derived from NMR measurements and shown as a shaded strip.

Consider second the choices $X_2 = 7570$, $Z_2 = 5860$, $R_1 = 4500$, so that $V_1 = 0.02420179732$. For these data, the angle HOH is 104.5125° and the OH length is 9573.1134, which are shown as the point B in Figure 5.2. The variation of bond length with bond angle is shown in the figure through four billion time steps and terminates at B' . The related real time is $(4.99)10^{-16}$ sec. The initial point B is outside and below the allowable NMR region, but the terminal point B' is inside.

Figure 5.2

For the third example, consider $X_2 = 7797.4115$, $Z_2 = 5769.7810$, $R_1 = 4500$, so that $V_1 = 0.02419214137$. For these data, the angle HOH is 107° and the length OH is 9700, which are shown as the point C in Figure 5.2. The point C is relatively high in the shaded area of Figure 5.1. The variation of bond length with bond angle is shown in Figure 5.2 through three billion time steps and terminates at C' . The real time of the system's motion is $(3.83)10^{-16}$ sec. The results are entirely within the acceptable NMR region.

Consider next $X_2 = 8038.5686$, $Z_2 = 5948.2279$, $R_1 = 4500$, so that $V_1 = 0.02421523072$. For these data, the angle HOH is 107° and the length OH is 10000, which are shown as the point D in Figure 5.2. The point D is above the allowable NMR region. The variation of bond length with bond angle is shown in Figure 5.2 through 2.1 billion time steps and terminates at D' . The related real time is $(3.94)10^{-16}$ sec. The motion is clearly away from the stable NMR region and is characterized in particular by rapidly increasing values of OH.

For $R_1 = 4500$, additional examples with initial data E_1, E_2, E_3 below the allowable NMR region (consult Figure 5.2) and with initial data F_1, F_2 above the NMR region were also run, but only until their larger motions were apparent. For the cases E_1, E_2, E_3 the motion was toward the NMR region while for F_1, F_2 the motion was away from the stable region.

All the examples in this section confirm the surmises made at the very beginning of this section.

6. Remarks. Some additional important points must now be made.

It was shown previously that pairing is essential for a semiclassical, dynamical simulation of H_2 ⁽²⁰⁾. To test the importance of pairing in the present study, we ran the second example of Section 5 but without pairing for two billion time steps. Whereas with pairing the bond length varied with the bond angle from B to B' in Figure 5.2, without pairing there was no such variation at all. Indeed, while the angle remained at 104.5° throughout the simulation, the bond length decreased from 9573 to 9570.

Replacement of the Duncan and Pople constants $0.45e, -0.23e$ by the Bjerrum ⁽⁷⁾ constants $0.53e, -0.23e$ or by the Rowlinson ⁽⁶⁾ constants $0.38e, -0.23e$ had only minor effects on dynamical results.

Finally, replacement of the reflection from a sphere to reflection from a cube with edge length 27600 and P_1 at its center also had only a minor effect on dynamical results.

REFERENCES

1. D. Eisenberg and W. Kauzmann, *The Structure and Properties of Water*, Oxford Univ. Press, Oxford, 1969.
2. R. A. Horne (Ed.), *Water and Aqueous Solutions: Structure, Thermodynamics, and*

- Transport Processes*, Wiley, N.Y., 1972.
3. R. A. Horne, *Encyclopedia Britannica*, 15th Ed., Vol 15, 1993, p. 759.
 4. I. Ohmine, *J. Chem. Phys.*, 99, 1995, p. 6767.
 5. R. J. Gillespie, *J. Chem. Ed.*, 40, 1963, p. 295.
 6. J. Hirschfelder, D. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids*, Wiley, N. Y., 1967.
 7. N. Bjerrum, *Science*, 115, 1952, p. 385.
 8. L. Pauling, *The Nature of the Chemical Bond*, Cornell Univ. Press, 3rd Ed., Ithaca, 1973.
 9. B. H. Mahan, *University Chemistry*, Addison-Wesley, Reading, MA, 1966.
 10. D. R. Lide (Ed.), *CRC Handbook of Chemistry and Physics*, CRC Press, Boca Raton, FL, 1990-1991.
 11. D. Park, *Introduction to Quantum Theory*, McGraw-Hill, N.Y., 1964.
 12. M. Gell-Mann and J. B. Hartle, *UCSBTH - 91 - 15*, UC Santa Barbara (no date).
 13. M. Nauenberg, C. Stroud and J. Yeazell, *Scientific American*, June, 1994, p. 44.
 14. D. Greenspan, *Physica Scripta*, 52, 1995, p. 267.
 15. J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Phys. Rev.*, 108, 1957, p. 1175.
 16. L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, Dover, N.Y., 1963.
 17. D. Greenspan, *Comp. Math. Applic.*, 29, 1995, p. 37.
 18. D. Greenspan, *TR #303*, Math Dept., UT Arlington, Arlington, TX USA 76019.
 19. Z. Sun, M. M. Soto, and W. A. Lester, *J. Chem. Phys.*, 100, 1994, p. 1278.
 20. D. Greenspan, *Comp. Math. Applic.*, 22, 1991, p. 73.

APPENDIX A

```

C IT IS IMPORTANT TO NOTE THAT THE IMPLICIT METHOD TO
C BE USED CONSERVES energy, LINEAR MOMENTUM, AND ANGULAR
c MOMENTUM. It is most important also to
c note that initial data r and v in cgs units and energy
c in ergs are to be transformed through R=r(10**12),T=t(10**22),
c U=v(10**10), A=a(10**32). The initial data for
c this program are then R and v.
c In this program, P1 and bonding elements 14 -17 are fixed.
  double precision XO(17),YO(17),UXO(17),UYO(17),
  IX(17,17),Y(17,17),UX(17,17),UY(17,17),
  Ixx(17),yy(17),vxx(17),vyy(17)
  I,zo(17),vzo(17),z(17,17),vz(17,17),zz(17),vzz(17)
  I,r(17,17),rn(17,17),rr(17,17),xxx(17,17),yyy(17,17),zzz(17,17)
  I,xm(17),e(17),v(17)
  I,xtime,energy1,energy2,energy
  open (unit=85,file='zz10.dat',status='old')
  open (unit=86,file='zz10.out',status='new')
  open (unit=87,file='zz10.xke',status='new')
  kprint=5000000
  xtime=0.0
  K=1
  kref=1
  x(1,2)=0.0
  x(1,1)=0.0
  x(1,3)=0.0
  y(1,2)=0.0
  y(1,1)=0.0
  y(1,3)=0.0
  z(1,2)=-0.
  z(1,1)=-0.
  z(1,3)=-0.
  x(14,2)=22500.
  x(14,1)=22500.
  x(14,3)=22500.
  y(14,2)=0.
  y(14,1)=0.
  y(14,3)=0.
  z(14,2)=15900.
  z(14,1)=15900.
  z(14,3)=15900.
  x(15,1)=-22500.
  x(15,2)=-22500.
  x(15,3)=-22500.
  y(15,2)=0.
  y(15,1)=0.
  y(15,3)=0.
  z(15,2)=15900.
  z(15,1)=15900.
  z(15,3)=15900.
  x(16,1)=0.
  x(16,2)=0.
  x(16,3)=0.
  y(16,1)=22500
  y(16,2)=22500

```

```
g(16,3)=22500
z(16,1)=-15900.
z(16,2)=-15900.
z(16,3)=-15900.
x(17,1)=0.
x(17,2)=0.
x(17,3)=0.
g(17,1)=-22500.
g(17,2)=-22500.
g(17,3)=-22500.
z(17,1)=-15900.
z(17,2)=-15900.
z(17,3)=-15900.
vx(1,2)=0.0
vx(1,1)=0.0
vx(1,3)=0.0
vg(1,2)=0.
vg(1,1)=0.
vg(1,3)=0.
vz(1,2)=-0.
vz(1,1)=-0.
vz(1,3)=-0.
vx(14,1)=0.0
vx(14,2)=0.0
vx(14,3)=0.0
vg(14,2)=-0.
vg(14,1)=-0.
vg(14,3)=-0.
vz(14,2)=-0.
vz(14,1)=-0.
vz(14,3)=-0.
vx(15,1)=0.0
vx(15,2)=0.0
vx(15,3)=0.0
vg(15,2)=-0.
vg(15,1)=-0.
vg(15,3)=-0.
vz(15,2)=-0.
vz(15,1)=-0.
vz(15,3)=-0.
vx(16,2)=0.0
vx(16,1)=0.0
vx(16,3)=0.0
vg(16,2)=0.
vg(16,1)=0.
vg(16,3)=0.
vz(16,2)=-0.
vz(16,1)=-0.
vz(16,3)=-0.
vx(17,1)=0.0
vx(17,2)=0.0
vx(17,3)=0.0
vg(17,2)=-0.
vg(17,1)=-0.
vg(17,3)=-0.
vz(17,2)=-0.
vz(17,1)=-0.
vz(17,3)=-0.
```



```

C READ IN THE INITIAL DATA.
  READ (85,10) (X0(I),y0(I),z0(I),VX0(I),VY0(I),Vz0(I),
  11=1,13)
10   FORMAT(3f16.8,f16.11,2f16.11)
C WE NOW SOLVE FOR THE NEW POSITIONS AND VELOCITIES WITH
C FORMULAS WHICH REQUIRE ITERATION. WE WILL USE THE
C IDEAS OF THE GENERALIZED NEWTON'S METHOD without
c updating each iterate.
c
C SET THE INPUT DATA.
  DO 30 i=2,13
    X(I,1)=X0(I)
    Y(I,1)=Y0(I)
    z(I,1)=z0(I)
    VX(I,1)=VX0(I)
    VY(I,1)=VY0(I)
    Vz(I,1)=Vz0(I)
30   CONTINUE
  GO TO 100
65   DO 70 i=2,13
    X(I,1)=X(I,2)
    Y(I,1)=Y(I,2)
    z(I,1)=z(I,2)
    VX(I,1)=VX(I,2)
    VY(I,1)=VY(I,2)
    Vz(I,1)=Vz(I,2)
70   CONTINUE
C FIX THE FIRST GUESS X(I,2) OF THE ITERATION.
100  DO 1633 i=2,13
    X(I,2)=X(I,1)
    Y(I,2)=Y(I,1)
    z(I,2)=z(I,1)
    VX(I,2)=VX(I,1)
    VY(I,2)=VY(I,1)
    Vz(I,2)=Vz(I,1)
1633 CONTINUE
    do 103 i=1,17
      do 102 J=1,17
        r(i,J)=(x(i,1)-x(J,1))**2+(y(i,1)-y(J,1))**2
        1+(z(i,1)-z(J,1))**2
        r(i,J)=dsqrt(r(i,J))
102   continue
103   continue
    delt=2.0
    min=100000.
    do 1111 i=1,12
      kkk=i+1
      do 1112 J=kkk,13
        if (r(i,J).lt.min) min=r(i,J)
1112  continue
1111  continue

```

```

if (min.lt.1500.) delt=1.0
if (min.lt.1000.) delt=0.1
if (min.lt.750.) delt=0.02
if (min.lt.500.) delt=0.002
if (min.lt.250.) delt=0.0002
KK=1
GO TO 110
105 DO 108 JJ=2,13
X(JJ,2)=X(JJ,3)
Y(JJ,2)=Y(JJ,3)
Z(JJ,2)=Z(JJ,3)
VX(JJ,2)=VX(JJ,3)
VY(JJ,2)=VY(JJ,3)
VZ(JJ,2)=VZ(JJ,3)
108 CONTINUE
110 DO 203 I=1,17
DO 202 J=1,17
RN(I,J)=(X(I,2)-X(J,2))**2+(Y(I,2)-Y(J,2))**2
1+(Z(I,2)-Z(J,2))**2
RN(I,J)=DSQRT(RN(I,J))
202 CONTINUE
203 CONTINUE
DO 109 I=2,13
X(I,3)=X(I,1)+0.5*delt*(VX(I,2)+VX(I,1))
Y(I,3)=Y(I,1)+0.5*delt*(VY(I,2)+VY(I,1))
Z(I,3)=Z(I,1)+0.5*delt*(VZ(I,2)+VZ(I,1))
109 CONTINUE
X(3,3)=-X(2,3)
Y(3,3)=-Y(2,3)
Z(3,3)=Z(2,3)
X(6,3)=-X(4,3)
Y(6,3)=-Y(4,3)
Z(6,3)=Z(4,3)
X(7,3)=-X(5,3)
Y(7,3)=-Y(5,3)
Z(7,3)=Z(5,3)
X(10,3)=-X(8,3)
Y(10,3)=-Y(8,3)
Z(10,3)=Z(8,3)
X(11,3)=-X(9,3)
Y(11,3)=-Y(9,3)
Z(11,3)=Z(9,3)
X(13,3)=-X(12,3)
Y(13,3)=-Y(12,3)
Z(13,3)=Z(12,3)

```

```

do 300 i=1,17
do 299 j=1,17
xxx(i,j)=x(i,2)+x(i,1)-x(j,2)-x(j,1)
yyy(i,j)=y(i,2)+y(i,1)-y(j,2)-y(j,1)
zzz(i,j)=z(i,2)+z(i,1)-z(j,2)-z(j,1)
299 continue
300 continue
do 400 i=1,17
do 399 j=1,17
rr(i,j)=r(i,j)*rn(i,j)*(r(i,j)+rn(i,j))
399 continue
400 continue
vx(2,3)=vx(2,1)+.0013792687*delt*(8.0*xxx(2,1)/rr(2,1)
1+xxx(2,3)/rr(2,3)-xxx(2,4)/rr(2,4)
1-xxx(2,5)/rr(2,5)-xxx(2,6)/rr(2,6)
1-xxx(2,7)/rr(2,7)-xxx(2,8)/rr(2,8)
1-xxx(2,9)/rr(2,9)-xxx(2,10)/rr(2,10)
1-xxx(2,11)/rr(2,11)-xxx(2,12)/rr(2,12)
1-xxx(2,13)/rr(2,13)-.23*xxx(2,14)/rr(2,14)
1-.23*xxx(2,15)/rr(2,15)+.45*xxx(2,16)/rr(2,16)
1+.45*xxx(2,17)/rr(2,17))
vy(2,3)=vy(2,1)+.0013792687*delt*(8.0*yyy(2,1)/rr(2,1)
1+yyy(2,3)/rr(2,3)-yyy(2,4)/rr(2,4)
1-yyy(2,5)/rr(2,5)-yyy(2,6)/rr(2,6)
1-yyy(2,7)/rr(2,7)-yyy(2,8)/rr(2,8)
1-yyy(2,9)/rr(2,9)-yyy(2,10)/rr(2,10)
1-yyy(2,11)/rr(2,11)-yyy(2,12)/rr(2,12)
1-yyy(2,13)/rr(2,13)-.23*yyy(2,14)/rr(2,14)
1-.23*yyy(2,15)/rr(2,15)+.45*yyy(2,16)/rr(2,16)
1+.45*yyy(2,17)/rr(2,17))
vz(2,3)=vz(2,1)+.0013792687*delt*(8.0*zzz(2,1)/rr(2,1)
1+zzz(2,3)/rr(2,3)-zzz(2,4)/rr(2,4)
1-zzz(2,5)/rr(2,5)-zzz(2,6)/rr(2,6)
1-zzz(2,7)/rr(2,7)-zzz(2,8)/rr(2,8)
1-zzz(2,9)/rr(2,9)-zzz(2,10)/rr(2,10)
1-zzz(2,11)/rr(2,11)-zzz(2,12)/rr(2,12)
1-zzz(2,13)/rr(2,13)-.23*zzz(2,14)/rr(2,14)
1-.23*zzz(2,15)/rr(2,15)+.45*zzz(2,16)/rr(2,16)
1+.45*zzz(2,17)/rr(2,17))
vx(4,3)=vx(4,1)+2.532457594*delt*(-8.0*xxx(4,1)/rr(4,1)
1-xxx(4,2)/rr(4,2)-xxx(4,3)/rr(4,3)
1+xxx(4,5)/rr(4,5)+xxx(4,6)/rr(4,6)
1+xxx(4,7)/rr(4,7)-xxx(4,8)/rr(4,8)
1+xxx(4,9)/rr(4,9)+xxx(4,10)/rr(4,10)
1+xxx(4,11)/rr(4,11)+xxx(4,12)/rr(4,12)
1+xxx(4,13)/rr(4,13)+.23*xxx(4,14)/rr(4,14)
1+.23*xxx(4,15)/rr(4,15)-.45*xxx(4,16)/rr(4,16)
1-.45*xxx(4,17)/rr(4,17))
vy(4,3)=vy(4,1)+2.532457594*delt*(-8.0*yyy(4,1)/rr(4,1)
1-yyy(4,2)/rr(4,2)-yyy(4,3)/rr(4,3)
1+yyy(4,5)/rr(4,5)+yyy(4,6)/rr(4,6)
1+yyy(4,7)/rr(4,7)-yyy(4,8)/rr(4,8)
1+yyy(4,9)/rr(4,9)+yyy(4,10)/rr(4,10)
1+yyy(4,11)/rr(4,11)+yyy(4,12)/rr(4,12)
1+yyy(4,13)/rr(4,13)+.23*yyy(4,14)/rr(4,14)
1+.23*yyy(4,15)/rr(4,15)-.45*yyy(4,16)/rr(4,16)
1-.45*yyy(4,17)/rr(4,17))

```

```

    vz(4,3)=vz(4,1)+2.532457594*delt*(-8.0*zzz(4,1)/rr(4,1)
1-zzz(4,2)/rr(4,2)-zzz(4,3)/rr(4,3)
1+zzz(4,5)/rr(4,5)+zzz(4,6)/rr(4,6)
1+zzz(4,7)/rr(4,7)-zzz(4,8)/rr(4,8)
1+zzz(4,9)/rr(4,9)+zzz(4,10)/rr(4,10)
1+zzz(4,11)/rr(4,11)+zzz(4,12)/rr(4,12)
1+zzz(4,13)/rr(4,13)+.23*zzz(4,14)/rr(4,14)
1+.23*zzz(4,15)/rr(4,15)-.45*zzz(4,16)/rr(4,16)
1-.45*zzz(4,17)/rr(4,17))
    vx(5,3)=vx(5,1)+2.532457594*delt*(-8.0*xxx(5,1)/rr(5,1)
1-xxx(5,2)/rr(5,2)-xxx(5,3)/rr(5,3)
1+xxx(5,4)/rr(5,4)+xxx(5,6)/rr(5,6)
1+xxx(5,7)/rr(5,7)+xxx(5,8)/rr(5,8)
1+xxx(5,9)/rr(5,9)+xxx(5,10)/rr(5,10)
1+xxx(5,11)/rr(5,11)+xxx(5,12)/rr(5,12)
1+xxx(5,13)/rr(5,13)+.23*xxx(5,14)/rr(5,14)
1+.23*xxx(5,15)/rr(5,15)-.45*xxx(5,16)/rr(5,16)
1-.45*xxx(5,17)/rr(5,17))
    vy(5,3)=vy(5,1)+2.532457594*delt*(-8.0*yyy(5,1)/rr(5,1)
1-yyy(5,2)/rr(5,2)-yyy(5,3)/rr(5,3)
1+yyy(5,4)/rr(5,4)+yyy(5,6)/rr(5,6)
1+yyy(5,7)/rr(5,7)+yyy(5,8)/rr(5,8)
1+yyy(5,9)/rr(5,9)+yyy(5,10)/rr(5,10)
1+yyy(5,11)/rr(5,11)+yyy(5,12)/rr(5,12)
1+yyy(5,13)/rr(5,13)+.23*yyy(5,14)/rr(5,14)
1+.23*yyy(5,15)/rr(5,15)-.45*yyy(5,16)/rr(5,16)
1-.45*yyy(5,17)/rr(5,17))
    vz(5,3)=vz(5,1)+2.532457594*delt*(-8.0*zzz(5,1)/rr(5,1)
1-zzz(5,2)/rr(5,2)-zzz(5,3)/rr(5,3)
1+zzz(5,4)/rr(5,4)+zzz(5,6)/rr(5,6)
1+zzz(5,7)/rr(5,7)+zzz(5,8)/rr(5,8)
1+zzz(5,9)/rr(5,9)+zzz(5,10)/rr(5,10)
1+zzz(5,11)/rr(5,11)+zzz(5,12)/rr(5,12)
1+zzz(5,13)/rr(5,13)+.23*zzz(5,14)/rr(5,14)
1+.23*zzz(5,15)/rr(5,15)-.45*zzz(5,16)/rr(5,16)
1-.45*zzz(5,17)/rr(5,17))
    vx(8,3)=vx(8,1)+2.532457594*delt*(-8.0*xxx(8,1)/rr(8,1)
1-xxx(8,2)/rr(8,2)-xxx(8,3)/rr(8,3)
1-xxx(8,4)/rr(8,4)+xxx(8,5)/rr(8,5)
1+xxx(8,6)/rr(8,6)+xxx(8,7)/rr(8,7)
1+xxx(8,9)/rr(8,9)+xxx(8,10)/rr(8,10)
1+xxx(8,11)/rr(8,11)+xxx(8,12)/rr(8,12)
1+xxx(8,13)/rr(8,13)+.23*xxx(8,14)/rr(8,14)
1+.23*xxx(8,15)/rr(8,15)-.45*xxx(8,16)/rr(8,16)
1-.45*xxx(8,17)/rr(8,17))
    vy(8,3)=vy(8,1)+2.532457594*delt*(-8.0*yyy(8,1)/rr(8,1)
1-yyy(8,2)/rr(8,2)-yyy(8,3)/rr(8,3)
1-yyy(8,4)/rr(8,4)+yyy(8,5)/rr(8,5)
1+yyy(8,6)/rr(8,6)+yyy(8,7)/rr(8,7)
1+yyy(8,9)/rr(8,9)+yyy(8,10)/rr(8,10)
1+yyy(8,11)/rr(8,11)+yyy(8,12)/rr(8,12)
1+yyy(8,13)/rr(8,13)+.23*yyy(8,14)/rr(8,14)
1+.23*yyy(8,15)/rr(8,15)-.45*yyy(8,16)/rr(8,16)
1-.45*yyy(8,17)/rr(8,17))

```

```

    vz(8,3)=vz(8,1)+2.532457594*delat*(-8.0*zzz(8,1)/rr(8,1)
1-zzz(8,2)/rr(8,2)-zzz(8,3)/rr(8,3)
1-zzz(8,4)/rr(8,4)+zzz(8,5)/rr(8,5)
1+zzz(8,6)/rr(8,6)+zzz(8,7)/rr(8,7)
1+zzz(8,9)/rr(8,9)+zzz(8,10)/rr(8,10)
1+zzz(8,11)/rr(8,11)+zzz(8,12)/rr(8,12)
1+zzz(8,13)/rr(8,13)+.23*zzz(8,14)/rr(8,14)
1+0.23*zzz(8,15)/rr(8,15)-.45*zzz(8,16)/rr(8,16)
1-.45*zzz(8,17)/rr(8,17))
    vx(9,3)=vx(9,1)+2.532457594*delat*(-8.0*xxx(9,1)/rr(9,1)
1-xxx(9,2)/rr(9,2)-xxx(9,3)/rr(9,3)
1+xxx(9,4)/rr(9,4)+xxx(9,5)/rr(9,5)
1+xxx(9,6)/rr(9,6)+xxx(9,7)/rr(9,7)
1+xxx(9,8)/rr(9,8)+xxx(9,10)/rr(9,10)
1+xxx(9,11)/rr(9,11)+xxx(9,12)/rr(9,12)
1+xxx(9,13)/rr(9,13)+.23*xxx(9,14)/rr(9,14)
1+0.23*xxx(9,15)/rr(9,15)-.45*xxx(9,16)/rr(9,16)
1-.45*xxx(9,17)/rr(9,17))
    vy(9,3)=vy(9,1)+2.532457594*delat*(-8.0*yyy(9,1)/rr(9,1)
1-yyy(9,2)/rr(9,2)-yyy(9,3)/rr(9,3)
1+yyy(9,4)/rr(9,4)+yyy(9,5)/rr(9,5)
1+yyy(9,6)/rr(9,6)+yyy(9,7)/rr(9,7)
1+yyy(9,8)/rr(9,8)+yyy(9,10)/rr(9,10)
1+yyy(9,11)/rr(9,11)+yyy(9,12)/rr(9,12)
1+yyy(9,13)/rr(9,13)+.23*yyy(9,14)/rr(9,14)
1+0.23*yyy(9,15)/rr(9,15)-.45*yyy(9,16)/rr(9,16)
1-.45*yyy(9,17)/rr(9,17))
    vz(9,3)=vz(9,1)+2.532457594*delat*(-8.0*zzz(9,1)/rr(9,1)
1-zzz(9,2)/rr(9,2)-zzz(9,3)/rr(9,3)
1+zzz(9,4)/rr(9,4)+zzz(9,5)/rr(9,5)
1+zzz(9,6)/rr(9,6)+zzz(9,7)/rr(9,7)
1+zzz(9,8)/rr(9,8)+zzz(9,10)/rr(9,10)
1+zzz(9,11)/rr(9,11)+zzz(9,12)/rr(9,12)
1+zzz(9,13)/rr(9,13)+.23*zzz(9,14)/rr(9,14)
1+0.23*zzz(9,15)/rr(9,15)-.45*zzz(9,16)/rr(9,16)
1-.45*zzz(9,17)/rr(9,17))
    vx(12,3)=vx(12,1)+2.532457594*delat*(-8.0*xxx(12,1)/rr(12,1)
1-xxx(12,2)/rr(12,2)-xxx(12,3)/rr(12,3)
1+xxx(12,4)/rr(12,4)+xxx(12,5)/rr(12,5)
1+xxx(12,6)/rr(12,6)+xxx(12,7)/rr(12,7)
1+xxx(12,8)/rr(12,8)+xxx(12,9)/rr(12,9)
1+xxx(12,10)/rr(12,10)+xxx(12,11)/rr(12,11)
1+xxx(12,13)/rr(12,13)+.23*xxx(12,14)/rr(12,14)
1+0.23*xxx(12,15)/rr(12,15)-.45*xxx(12,16)/rr(12,16)
1-.45*xxx(12,17)/rr(12,17))
    vy(12,3)=vy(12,1)+2.532457594*delat*(-8.0*yyy(12,1)/rr(12,1)
1-yyy(12,2)/rr(12,2)-yyy(12,3)/rr(12,3)
1+yyy(12,4)/rr(12,4)+yyy(12,5)/rr(12,5)
1+yyy(12,6)/rr(12,6)+yyy(12,7)/rr(12,7)
1+yyy(12,8)/rr(12,8)+yyy(12,9)/rr(12,9)
1+yyy(12,10)/rr(12,10)+yyy(12,11)/rr(12,11)
1+yyy(12,13)/rr(12,13)+.23*yyy(12,14)/rr(12,14)
1+0.23*yyy(12,15)/rr(12,15)-.45*yyy(12,16)/rr(12,16)
1-.45*yyy(12,17)/rr(12,17))

```

```

      vz(12,3)=vz(12,1)+2.532457594*delat*(-8.0*zzz(12,1)/rr(12,1)
1-zzz(12,2)/rr(12,2)-zzz(12,3)/rr(12,3)
1+zzz(12,4)/rr(12,4)+zzz(12,5)/rr(12,5)
1+zzz(12,6)/rr(12,6)+zzz(12,7)/rr(12,7)
1+zzz(12,8)/rr(12,8)+zzz(12,9)/rr(12,9)
1+zzz(12,10)/rr(12,10)+zzz(12,11)/rr(12,11)
1+zzz(12,13)/rr(12,13)+.23*zzz(12,14)/rr(12,14)
1+.23*zzz(12,15)/rr(12,15)-.45*zzz(12,16)/rr(12,16)
1-.45*zzz(12,17)/rr(12,17))
      vx(3,3)=-vx(2,3)
      vy(3,3)=-vy(2,3)
      vz(3,3)=vz(2,3)
      vx(6,3)=-vx(4,3)
      vy(6,3)=-vy(4,3)
      vz(6,3)=vz(4,3)
      vx(7,3)=-vx(5,3)
      vy(7,3)=-vy(5,3)
      vz(7,3)=vz(5,3)
      vx(10,3)=-vx(8,3)
      vy(10,3)=-vy(8,3)
      vz(10,3)=vz(8,3)
      vx(11,3)=-vx(9,3)
      vy(11,3)=-vy(9,3)
      vz(11,3)=vz(9,3)
      vx(13,3)=-vx(12,3)
      vy(13,3)=-vy(12,3)
      vz(13,3)=vz(12,3)
      KK=KK+1
      IF (KK.GT.50000) GO TO 83
      do 9875 i=1,17
      xx(i)=abs(x(i,3)-x(i,2))
      yy(i)=abs(y(i,3)-y(i,2))
      zz(i)=abs(z(i,3)-z(i,2))
      vxx(i)=abs(vx(i,3)-vx(i,2))
      vyy(i)=abs(vy(i,3)-vy(i,2))
      vzz(i)=abs(vz(i,3)-vz(i,2))
9875      CONTINUE
      index=-1
      do 600 i=1,17
      if (xx(i).st.0.000000004) index=+1
      if (yy(i).st.0.000000004) index=+1
      if (zz(i).st.0.000000004) index=+1
      if (vxx(i).st.0.000000000004) index=+1
      if (vyy(i).st.0.000000000004) index =+1
      if (vzz(i).st.0.000000000004) index=+1
600      continue

```

```

      if (index.eq.+1) go to 105
      DO 1008 JJ=2,13
      X(JJ,2)=X(JJ,3)
      Y(JJ,2)=Y(JJ,3)
      Z(JJ,2)=Z(JJ,3)
      VX(JJ,2)=VX(JJ,3)
      VY(JJ,2)=VY(JJ,3)
      VZ(JJ,2)=VZ(JJ,3)
1008   CONTINUE
      K=K+1
      xtime=xtime+delt
c We now reflect to simulate the molecular interchange of
c electrons. This is done every kref1 steps.
c This is done at half the distance between water molecules.
      if (rn(1,4).lt.13800.) go to 2001
      do 3759 i=2,13
      x(i,2)=x(i,1)
      y(i,2)=y(i,1)
      z(i,2)=z(i,1)
      vx(i,2)=vx(i,1)
      vy(i,2)=vy(i,1)
      vz(i,2)=vz(i,1)
3759   continue
      vx(4,2)=-vx(4,2)
      vy(4,2)=-vy(4,2)
      vz(4,2)=-vz(4,2)
      kref=kref+1
2001   if (rn(1,5).lt.13800.) go to 2002
      do 3758 i=2,13
      x(i,2)=x(i,1)
      y(i,2)=y(i,1)
      z(i,2)=z(i,1)
      vx(i,2)=vx(i,1)
      vy(i,2)=vy(i,1)
      vz(i,2)=vz(i,1)
3758   continue
      vx(5,2)=-vx(5,2)
      vy(5,2)=-vy(5,2)
      vz(5,2)=-vz(5,2)
      kref=kref+1
2002   if (rn(1,8).lt.13800.) go to 2003
      do 3757 i=2,13
      x(i,2)=x(i,1)
      y(i,2)=y(i,1)
      z(i,2)=z(i,1)
      vx(i,2)=vx(i,1)
      vy(i,2)=vy(i,1)
      vz(i,2)=vz(i,1)
3757   continue
      vx(8,2)=-vx(8,2)
      vy(8,2)=-vy(8,2)
      vz(8,2)=-vz(8,2)
      kref=kref+1

```

```

2003   if (rn(1,9).lt.13800.) go to 2004
      do 3756 i=2,13
        x(i,2)=x(i,1)
        y(i,2)=y(i,1)
        z(i,2)=z(i,1)
        vx(i,2)=vx(i,1)
        vy(i,2)=vy(i,1)
        vz(i,2)=vz(i,1)
3756   continue
      vx(9,2)=-vx(9,2)
      vy(9,2)=-vy(9,2)
      vz(9,2)=-vz(9,2)
      kref=kref+1
2004   if (rn(1,12).lt.13800.) go to 2010
      do 6421 i=2,13
        x(i,2)=x(i,1)
        y(i,2)=y(i,1)
        z(i,2)=z(i,1)
        vx(i,2)=vx(i,1)
        vy(i,2)=vy(i,1)
        vz(i,2)=vz(i,1)
6421   continue
      vx(12,2)=-vx(12,2)
      vy(12,2)=-vy(12,2)
      vz(12,2)=-vz(12,2)
      kref=kref+1
2010   if (MOD(K,KPRINT).GT.0) GO TO 82
c calculate and print energy
      do 8808 i=1,17
c We use v(i) for v(i)*v(i).
      v(i)=vx(i,2)**2+vy(i,2)**2+vz(i,2)**2
8808   continue
      xm(1)=16.*16724.
      e(1)=8.
      do 8810 i=2,3
        xm(i)=16724.
        e(i)=1.
8810   continue
      do 9738 i=16,17
        xm(i)=16724.
        e(i)=.45
9738   continue
      do 8811 i=4,13
        xm(i)=9.1085
        e(i)=-1.
8811   continue
      do 7767 i=14,15
        xm(i)=16724.
        e(i)=-.23
7767   continue
      energyl=0.0
      do 8813 i=1,16
        kkk=i+1
        do 8814 j=kkk,17
          energyl=energyl+e(i)*e(j)/rn(i,j)
8814   continue
8813   continue

```



```

energy1=energy1-2.*e(4)*e(8)/rn(4,8)-2.*e(6)*e(10)/rn(6,10)
energy1=23.06689*energy1
energy2=0.0
do 8815 i=1,17
energy2=energy2+.5*xm(i)*v(i)
8815 continue
energy=energy1+energy2
energy=10000.*energy
xcos=rn(1,3)**2+rn(1,2)**2-rn(3,2)**2
xcos=xcos/(2.*rn(1,2)*rn(1,3))
c energy must be multiplied by 10**(-12) .
write (87,8000) k,kref,energy,rn(1,2),rn(1,4),rn(1,5),rn(1,8)
1,rn(1,9),rn(1,12),xcos,delt
8000 format (i11,i6,f11.4,6f8.0,f11.7,f8.5)
82 if (K.le.75000000) GO TO 65
83 write (86,10) (X(I,2),Y(I,2),z(i,2),vx(I,2),VY(I,2),vz(i,2)
1,i=1,17)
write (86,7717) xtime
7717 format (f15.5)
STOP
END

```

APPENDIX B

```

      double precision x(17),y(17),z(17),v(17),r(17,17),
      vx(17),vy(17),vz(17),
      lm(17),e(17),vsg(17),c1,c2,c3,c4,c5,c6,energy,
      lee,c10,c11,c12,c13,c14,c15,c16
      OPEN (UNIT=22,file='szz10.out',status='new')
      OPEN (UNIT=23,file='szz10.xke',status='new')
      x(1)=0.
      y(1)=0.0
      z(1)=-0.
      z(2)=5748.9593
      y(2)=-0.
      x(2)=8059.7436
      x(3)=-x(2)
      y(3)=0.
      z(3)=z(2)
      x(4)=4500.
      y(4)=4500.
      z(4)=4500.
      x(5)=4500.
      y(5)=-4500.
      z(5)=4500.
      x(6)=-4500.
      y(6)=-4500.
      z(6)=4500.
      x(7)=-4500.
      y(7)=4500.
      z(7)=4500.
      x(8)=-4500.
      y(8)=-4500.
      z(8)=-4500.
      x(9)=-4500.
      y(9)=4500.
      z(9)=-4500.
      x(10)=4500.
      y(10)=4500.
      z(10)=-4500.
      x(11)=4500.
      y(11)=-4500.
      z(11)=-4500.
      x(12)=680.
      x(13)=-680.
      vy(12)=.171453
      vy(13)=-.171453
      x(14)=22500.
      y(14)=0.0
      z(14)=15900.
      x(15)=-22500.
      y(15)=0.0
      z(15)=15900.
      x(16)=0.
      y(16)=22500.
      z(16)=-15900.
      x(17)=0.
      y(17)=-22500.
      z(17)=-15900.
      do 101 i=1,17
      do 102 j=1,17

```

```

      r(i,j)=(x(i)-x(j))**2+(y(i)-y(j))**2+(z(i)-z(j))**2
      r(i,j)=dsqrt(r(i,j))
102      continue
101      continue
8838      format (3f20.12)
9999      format (f15.10)
      ee=-.333304
      m(1)=16.*16724.
      e(1)=8.
      do 1234 i=2,3
      m(i)=16724.
      e(i)=1.
1234      continue
      do 1235 i=4,13
      m(i)=9.1085
      e(i)=-1.
1235      continue
      do 1236 i=14,15
      m(i)=16724.
      e(i)=-.23
1236      continue
      do 9472 i=16,17
      m(i)=16724.
      e(i)=.45
9472      continue
      c13=0.0
      do 1238 i=1,16
      kkk=i+1
      do 1239 j=kkk,17
      c13=c13+e(i)*e(j)/r(i,j)
1239      continue
1238      continue
      c13=c13-2./r(4,8)-2./r(6,10)
      c13=23.06689*c13
      do 1562 i=1,17
      vsa(i)=vx(i)**2+vy(i)**2+vz(i)**2
1562      continue
      c14=ee-c13-.5*2.*m(12)*vsa(12)
      c15=c14/(8.*.5*m(4))
      c8=dsqrt(c15)
      vy(4)=-c8
      vx(5)=-c8
      vy(6)=c8
      vx(7)=c8
      vx(8)=c8
      vy(9)=-c8
      vx(10)=-c8
      vy(11)=c8
      write (22,10) (x(i),y(i),z(i),vx(i),vy(i),vz(i),
1i=1,17)
10      format (3f16.8,3f16.11)
      energy=c13
      do 9876 i=1,17
      vsa(i)=vx(i)**2+vy(i)**2+vz(i)**2
9876      continue
      do 9875 i=1,17
      energy = energy+.5*m(i)*vsa(i)
9875      continue
      write (23,9809) ee,energy,vy(4),vx(5),vy(6),vx(7)
9809      format(2f13.8,4f14.10)
      STOP
      END

```