

Two Electron Diatomic Molecules.

I. The James-Coolidge Method and Its Programs

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Computer programs which calculate energies and wave functions of two electron diatomic molecules by the James-Coolidge method are given. These programs can be applied to the singlet or the triplet Σ^+ states of two electron diatomic molecules of arbitrary nuclear charges.

§ 1. Introduction

To investigate various properties of molecules we need to know the electronic energies and the electronic wave functions of molecules in the adiabatic approximation scheme. Also to examine the atomic collision problems the knowledge on the energy correlation diagrams is very useful. For this purpose many methods, for example, Heitler-London method,¹⁾ molecular orbital method,²⁾ and configuration mixing method³⁾ etc., have been developed. Especially, for two electron diatomic molecules, the James-Coolidge method is the most powerful and by this method James-Coolidge,⁴⁾ Kołos-Roothaan,⁵⁾ and Kołos-Wolniewicz⁶⁾ have examined the hydrogen molecule and obtained the successful results. To extend their studies, we constructed the computer programs which can obtain the electronic energies and the electronic wave functions of the Σ^+ states of two electron diatomic molecules.

In § 2 the James-Coolidge method is explained, and in § 3 simple explanation of the computer programs and how to use them are shown. In Appendix A the matrix components of the unity and the Hamiltonian operator are expressed by auxiliary functions $Z'(m, n, j, k, p; 2\alpha)$ and in Appendix B the method of evaluating the functions $Z'(m, n, j, k, p; 2\alpha)$ is shown. Furthermore, we give the

lists of the computer programs in Appendix C.

§ 2. Method of calculation

In this paper we shall always use the atomic units. The non-relativistic Hamiltonian of two electron diatomic molecules in the adiabatic approximation is given by

$$\begin{aligned} H &= T + U, \\ T &= -\frac{1}{2}(\mathcal{A}_1 + \mathcal{A}_2), \\ U &= -\frac{Z_a}{r_{a1}} - \frac{Z_b}{r_{b1}} - \frac{Z_a}{r_{a2}} - \frac{Z_b}{r_{b2}} + \frac{1}{r_{12}} + \frac{Z_a Z_b}{R}, \end{aligned} \quad (1)$$

with the notation of Fig. 1, Z_a and Z_b being the nuclear charges.

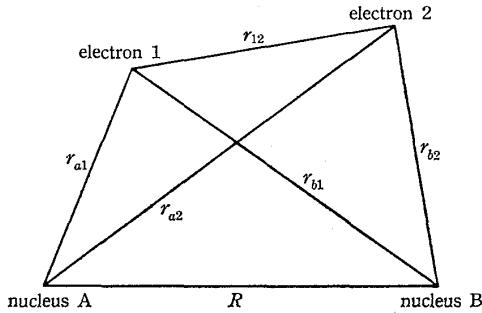


Fig. 1. Coordinates

Putting

$$\begin{aligned} \lambda_i &= (r_{ai} + r_{bi})/R, \\ \mu_i &= (r_{ai} - r_{bi})/R, \quad (i=1, 2), \end{aligned} \quad (2a)$$

and

$$\rho = 2r_{12}/R, \quad (2b)$$

the Hamiltonian (1) is expressed as follows,

$$\begin{aligned} H &= T + \left(\frac{Z_a + Z_b}{2}\right)U^{(1)} + \left(\frac{Z_a - Z_b}{2}\right)U^{(2)} + U^{(3)} + \frac{Z_a Z_b}{R} \\ &= R^{-2}T' + \left(\frac{Z_a + Z_b}{2}\right)R^{-1}U'^{(1)} + \left(\frac{Z_a - Z_b}{2}\right)R^{-1}U'^{(2)} + R^{-1}U'^{(3)} + R^{-1}Z_a Z_b, \end{aligned} \quad (3a)$$

where

$$T' = -\frac{1}{2}(\mathcal{A}_1 + \mathcal{A}_2)R^2, \quad (3b)$$

$$U'^{(1)} = -4\lambda_1/(\lambda_1^2 - \mu_1^2) - 4\lambda_2/(\lambda_2^2 - \mu_2^2), \quad (3c)$$

$$U'^{(2)} = 4\mu_1/(\lambda_1^2 - \mu_1^2) + 4\mu_2/(\lambda_2^2 - \mu_2^2), \quad (3d)$$

$$U'^{(3)} = \frac{2}{\rho}. \quad (3e)$$

For the Σ^+ state, the James-Coolidge wave function is

$$\Psi = \sum C_{mnjkp} [mnjkp], \quad (4)$$

where

$$[mnjkp] = N_{mnjkp} \exp [-\alpha(\lambda_1 + \lambda_2)] (\lambda_1^m \lambda_2^n \mu_1^j \mu_2^k \pm \lambda_1^n \lambda_2^m \mu_1^k \mu_2^j) \rho^p. \quad (5)$$

Here m, n, j, k , and p are a set of numbers each of which takes zero or positive integer, α is a variation parameter, and N_{mnjkp} is a normalization constant. The sign $+$ (or $-$) corresponds to the singlet state (or the triplet state). Furthermore, in the case of homonuclear molecules, the restriction $j+k=\text{even}$ (or odd) is added for the g state (or for the u state).

The electronic energy E and the coefficients C_{mnjkp} are determined by the following secular equation,

$$\det |H_{fg} - ES_{fg}| = 0, \quad (6)$$

where, f and g represent sets of m, n, j, k , and p . The S_{fg} and H_{fg} are the matrix components of the unity and the Hamiltonian operator,

$$S_{fg} = \int [m_f n_f j_f k_f p_f] [m_g n_g j_g k_g p_g] dV_1 dV_2, \quad (7a)$$

$$H_{fg} = R^{-2} T'_{fg} + R^{-1} \left\{ \left(\frac{Z_a + Z_b}{2} \right) U'_{fg}^{(1)} + \left(\frac{Z_a - Z_b}{2} \right) U'_{fg}^{(2)} + U'_{fg}^{(3)} + Z_a Z_b S_{fg} \right\}, \quad (7b)$$

$$T'_{fg} = \int [m_f n_f j_f k_f p_f] T' [m_g n_g j_g k_g p_g] dV_1 dV_2, \quad (7c)$$

$$U'_{fg}^{(1)} = \int [m_f n_f j_f k_f p_f] U'^{(1)} [m_g n_g j_g k_g p_g] dV_1 dV_2, \quad (7d)$$

$$U'_{fg}^{(2)} = \int [m_f n_f j_f k_f p_f] U'^{(2)} [m_g n_g j_g k_g p_g] dV_1 dV_2, \quad (7e)$$

and

$$U'_{fg}^{(3)} = \int [m_f n_f j_f k_f p_f] U'^{(3)} [m_g n_g j_g k_g p_g] dV_1 dV_2. \quad (7f)$$

The method of calculation of the matrix components will be given in Appendix A.

§ 3 Computer programs

We have constructed a set of programs which calculates the total energies and the wave functions of two electron diatomic molecules by the James-Coolidge method. The lists of programs are given in Appendix C. These programs are divided into seven parts. Each part forms one job and the relations among the jobs are shown in Fig. 2.

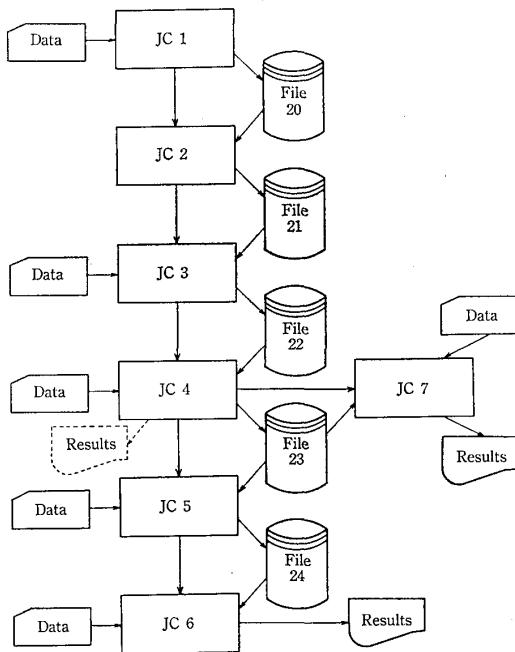


Fig. 2. Relations among the jobs.

1. Job JC1

This job calculates the auxiliary functions $Z^\nu(m, n, j, k, p; 2\alpha)$ for $p = -1$ and 0. The range of ν, m, n, j, k is

$$\begin{aligned} 0 \leq \nu &\leq 3, \\ 0 \leq n &\leq m \leq 20 - 2\nu, \\ 0 \leq k &\leq j \leq 20 - 2\nu. \end{aligned} \quad (8)$$

The quadruple precision calculation is used for the calculation of the auxiliary functions $W_\nu(m, n; 2\alpha)$ because of cancellation due to the recurrence formulas. For the remaining part, the double precision is used. As an input datum, the value of α is given. Then the values of the auxiliary functions $Z^\nu(m, n, j, k, p; 2\alpha)$ are written in the file (No. 20).

2. Job JC2

The values of $Z^0(m, n, j, k, p; 2\alpha)$ are evaluated from the results of the job JC1. The range of m, n, j, k, p is

$$\begin{aligned} 0 \leq n \leq m \leq 16, \\ 0 \leq k \leq j \leq 16, \quad \text{for } -1 \leq p \leq 4, \end{aligned} \quad (9a)$$

and

$$\begin{aligned} 0 \leq n \leq m \leq 14, \\ 0 \leq k \leq j \leq 14, \quad \text{for } p=5, 6. \end{aligned} \quad (9b)$$

The double precision calculation is used. There are no imput data. The results of this job are written in the file (No. 21).

3. Job JC3

This job calculates the matrix components S_{fg} , T_{fg} , and U_{fg} for the unnormalized bases. The imput data are the nuclear charges Z_a and Z_b , the multiplicity, the number of bases adopted, and the sets of parameters determining the bases. The nuclear charges Z_a and Z_b must be given in real type and the multiplicity means $2S+1$, namely 1 for the singlet state and 3 for the triplet state. Moreover, the number of bases can't exceed 160. Of course, one can relax this limitation on the number of bases, if available core memories are increased. Since, however, then the necessary CPU time increases extraordinary, the practical merit is not expected. The base is defined by m , n , j , k , and p . The sets of m , n , j , k , and p are put in one after another according to the order of bases. The range of m , n , j , k , and p is

$$\begin{aligned} 0 \leq m, n, j, k \leq 6, \\ 0 \leq p \leq 3. \end{aligned} \quad (10)$$

This program checks whether the base is allowed or not, evaluates the matrix components, and writes them in the file (No. 22).

4. Job JC4

The normalization of the bases and the rearrangement of the matrix components are very useful for the later calculation, and are performed by the use of the job JC4. The matrix components are written in the file (No. 23). Also they are printed, (or are not printed) in LP sheets if the input datum is not 0(or is 0).

5. Job JC5

In the calculation of the James-Coolidge method, it is desirable to select the important bases. But, the choice of the bases is very difficult and troublesome, because the nondiagonal matrix components of S are considerably large. If the orthonormalized bases are used, it seems that the bases which have a small coefficient in the wave function have small effect. Therefore, these bases can be dropped

out. It is desirable that the bases which are taken off have large value of $m+n+j+k+p$, since the matrix components for the bases with small $m+n+j+k+p$ can be obtained with small error. For such reasons, we adopt Schmidt's orthonormalization. In the job JC5 Schmidt's orthonormalization and the transformation of matrix components are performed. In the job JC5, the quadruple precision calculation is used. If the input datum is 0, the unnecessary bases are taken off in the later calculation, otherwise not. The results are written in the file (No. 24).

6. Job JC6

This job calculates the total energies and the wave functions by the use of the results of the job JC5. If the internuclear distance and the number of order of the considered state counted from the lowest of the same symmetry are given, the total energy and the wave function are obtained. The coefficients of the bases are not for the orthonormalized ones. We can, however, obtain, as the output, the coefficients for the orthonormalized bases by the control of the input datum. The secular equation is solved with the quadruple precision.

7. Job JC7

This job is the additional ones to the job JC5. Because of the large overlapping of the bases, appreciable amounts of errors may arise when Schmidt's orthonormalization is performed. Then, it is necessary to check the order of this error. We use the job JC7 for this purpose. If the values of the matrix components are required for selecting the important bases, we can put out the matrix components H_{fg} by specifying the control number in the input datum.

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Appendix A. The matrix components S_{fg} , T_{fg} , $U_{fg}^{(1)}$, $U_{fg}^{(2)}$, and $U_{fg}^{(3)}$.

$$\begin{aligned} S_{fg} &= N_f N_g \int \exp [-\alpha(\lambda_1 + \lambda_2)] (\lambda_1^{m_f} \lambda_2^{n_f} \mu_1^{j_f} \mu_2^{k_f} \rho^{p_f} \pm \lambda_1^{n_f} \lambda_2^{m_f} \mu_1^{k_f} \mu_2^{j_f} \rho^{p_f}) \\ &\quad \times \exp [-\alpha(\lambda_1 + \lambda_2)] (\lambda_1^{m_g} \lambda_2^{n_g} \mu_1^{j_g} \mu_2^{k_g} \rho^{p_g} \pm \lambda_1^{n_g} \lambda_2^{m_g} \mu_1^{k_g} \mu_2^{j_g} \rho^{p_g}) dV_1 dV_2 \\ &= 8\pi^2 N_f N_g \left(\frac{R}{2}\right)^6 \{s(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ &\quad \pm s(m_f n_f j_f k_f p_f, n_g m_g k_g j_g p_g; \alpha)\}, \end{aligned} \quad (\text{A1})$$

where

$$\begin{aligned} &s(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ &= \frac{1}{4\pi^2} \left(\frac{2}{R}\right)^6 \int \exp [-\alpha(\lambda_1 + \lambda_2)] \lambda_1^{m_f} \lambda_2^{n_f} \mu_1^{j_f} \mu_2^{k_f} \rho^{p_f} \\ &\quad \times \exp [-\alpha(\lambda_1 + \lambda_2)] \lambda_1^{m_g} \lambda_2^{n_g} \mu_1^{j_g} \mu_2^{k_g} \rho^{p_g} dV_1 dV_2. \end{aligned} \quad (\text{A2})$$

Using

$$dV = \left(\frac{R}{2}\right)^3 (\lambda^2 - \mu^2) d\lambda d\mu d\phi, \quad (\text{A3})$$

and the auxiliary functions

$$\begin{aligned} Z^\nu(m, n, j, k, p; 2\alpha) &= \frac{1}{4\pi^2} \int \exp [-2\alpha(\lambda_1 + \lambda_2)] \lambda_1^m \lambda_2^n \mu_1^j \mu_2^k \rho^p \\ &\quad \times [(\lambda_1^2 - 1)(\lambda_2^2 - 1)(1 - \mu_1^2)(1 - \mu_2^2)]^{\nu/2} \cos^\nu(\phi_1 - \phi_2) d\lambda_1 d\lambda_2 d\mu_1 d\mu_2 d\phi_1 d\phi_2, \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} &s(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ &= Z^0(m_f + m_g + 2, n_f + n_g + 2, j_f + j_g, k_f + k_g, p_f + p_g; 2\alpha) \\ &\quad - Z^0(m_f + m_g + 2, n_f + n_g, j_f + j_g, k_f + k_g + 2, p_f + p_g; 2\alpha) \\ &\quad - Z^0(m_f + m_g, n_f + n_g + 2, j_f + j_g + 2, k_f + k_g, p_f + p_g; 2\alpha) \\ &\quad + Z^0(m_f + m_g, n_f + n_g, j_f + j_g + 2, k_f + k_g + 2, p_f + p_g; 2\alpha). \end{aligned} \quad (\text{A5})$$

For this expression the following abbreviation is used

$$\begin{aligned} &s(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ &= Z(22000) - Z(20020) - Z(02200) + Z(00220). \end{aligned} \quad (\text{A6})$$

The method of calculation of the functions $Z^\nu(m, n, j, k, p; 2\alpha)$ will be given in Appendix B.

Similarly, the other matrix components are represented by using the same auxiliary functions $Z^\nu(m, n, j, k, p; 2\alpha)$. Namely,

$$\begin{aligned} T'_{fg} &= 8\pi^2 N_f N_g \left(\frac{R}{2}\right)^6 \{t(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ &\quad \pm t(m_f n_f j_f k_f p_f, n_g m_g k_g j_g p_g; \alpha)\}, \end{aligned} \quad (\text{A7a})$$

$$U'_{fg}^{(1)} = 8\pi^2 N_f N_g \left(\frac{R}{2}\right)^6 \{u^{(1)}(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ \pm u^{(1)}(m_f n_f j_f k_f p_f, n_g m_g j_g k_g p_g; \alpha)\}, \quad (\text{A7b})$$

$$U'_{fg}^{(2)} = 8\pi^2 N_f N_g \left(\frac{R}{2}\right)^6 \{u^{(2)}(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ \pm u^{(2)}(m_f n_f j_f k_f p_f, n_g m_g j_g k_g p_g; \alpha)\}, \quad (\text{A7c})$$

and

$$U'_{fg}^{(3)} = 8\pi^2 N_f N_g \left(\frac{R}{2}\right)^6 \{u^{(3)}(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ \pm u^{(3)}(m_f n_f j_f k_f p_f, n_g m_g j_g k_g p_g; \alpha)\}. \quad (\text{A7d})$$

Using the same abbreviation of Eq. (A6), the functions $t(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha)$ etc. are expressed as follows,

$$\begin{aligned} & t(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ &= -\frac{1}{2} [-4\alpha\{Z(12000)-Z(10020)+Z(21000)-Z(01200)\} \\ &+ \{(m_f-m_g)^2 + (m_f+m_g) - (j_f-j_g)^2 - (j_f+j_g) \\ &+ (p_f-p_g)(m_f-m_g-j_f+j_g)\}\{Z(02000)-Z(00020)\} \\ &+ \{(n_f-n_g)^2 + (n_f+n_g) - (k_f-k_g)^2 - (k_f+k_g) \\ &+ (p_f-p_g)(n_f-n_g-k_f+k_g)\}\{Z(20000)-Z(00200)\} \\ &- \{(m_f-m_g)^2 - (m_f+m_g)\}\{Z(-22000)-Z(-20020)\} \\ &- \{(n_f-n_g)^2 - (n_f+n_g)\}\{Z(2-2000)-Z(0-2200)\} \\ &+ \{(j_f-j_g)^2 - (j_f+j_g)\}\{Z(02-200)-Z(00-220)\} \\ &+ \{(k_f-k_g)^2 - (k_f+k_g)\}\{Z(200-20)-Z(002-20)\} \\ &+ [2\{(p_f-p_g)^2 + (p_f+p_g)\} + (p_f-p_g) \\ &\times (m_f-m_g+n_f-n_g+j_f-j_g+k_f-k_g)] \\ &\times \{Z(2200-2)-Z(2002-2)-Z(0220-2)+Z(0022-2)\} \\ &- (p_f-p_g)(m_f-m_g-j_f+j_g)\{Z(0400-2)-Z(0004-2)\} \\ &- (p_f-p_g)(n_f-n_g-k_f+k_g)\{Z(4000-2)-Z(0040-2)\} \\ &+ 2(p_f-p_g)(m_f-m_g)\{Z(-1311-2)-Z(-1113-2)\} \\ &+ 2(p_f-p_g)(n_f-n_g)\{Z(3-111-2)-Z(1-131-2)\} \\ &- 2(p_f-p_g)(j_f-j_g)\{Z(13-11-2)-Z(11-13-2)\} \\ &- 2(p_f-p_g)(k_f-k_g)\{Z(311-1-2)-Z(113-1-2)\}], \quad (\text{A8a}) \end{aligned}$$

$$\begin{aligned} & u^{(1)}(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ &= -4\{Z(12000)-Z(10020)+Z(21000)-Z(01200)\}, \quad (\text{A8b}) \end{aligned}$$

$$\begin{aligned} & u^{(2)}(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ &= 4\{Z(02100)-Z(00120)+Z(20010)-Z(00210)\}, \quad (\text{A8c}) \end{aligned}$$

and

$$\begin{aligned} u^{(3)}(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \\ = 2\{Z(2200-1) - Z(2002-1) - Z(0220-1) + Z(0022-1)\}. \quad (\text{A8d}) \end{aligned}$$

Appendix B. Auxiliary functions $Z^\nu(m, n, j, k, p; 2\alpha)$.

The auxiliary functions $Z^\nu(m, n, j, k, p; 2\alpha)$ are defined by Eq. (A4). By the relation

$$\begin{aligned} \rho^2 = \lambda_1^2 + \lambda_2^2 + \mu_1^2 + \mu_2^2 - 2 - 2\lambda_1\lambda_2\mu_1\mu_2 \\ - 2[(\lambda_1^2 - 1)(\lambda_2^2 - 1)(1 - \mu_1^2)(1 - \mu_2^2)]^{1/2} \cos(\phi_1 - \phi_2), \quad (\text{B1}) \end{aligned}$$

the following recurrence formula is obtained:

$$\begin{aligned} Z^\nu(m, n, j, k, p+2; 2\alpha) &= Z^\nu(m+2, n, j, k, p; 2\alpha) \\ &+ Z^\nu(m, n+2, j, k, p; 2\alpha) + Z^\nu(m, n, j+2, k, p; 2\alpha) \\ &+ Z^\nu(m, n, j, k+2, p; 2\alpha) - 2Z^\nu(m, n, j, k, p; 2\alpha) \\ &- 2Z^\nu(m+1, n+1, j+1, k+1, p; 2\alpha) - 2Z^{\nu+1}(m, n, j, k, p; 2\alpha). \quad (\text{B2}) \end{aligned}$$

Therefore, $Z^0(m, n, j, k, p; 2\alpha)$ with $p \geq 1$ can be obtained from $Z^\nu(m, n, j, k, -1; 2\alpha)$ and $Z^\nu(m, n, j, k, 0; 2\alpha)$.

For $p=0$, using the Eq. (A4),

$$Z^0(m, n, j, k, 0; 2\alpha) = 4A_m(2\alpha)A_n(2\alpha)/[(j+1)(k+1)], \quad (\text{B3a})$$

$$Z^1(m, n, j, k, 0, 2\alpha) = 0,$$

$$\begin{aligned} Z^2(m, n, j, k, 0; 2\alpha) &= 8[A_{m+2}(2\alpha) - A_m(2\alpha)] \\ &\times [A_{n+2}(2\alpha) - A_n(2\alpha)]/[(j+1)(j+3)(k+1)(k+3)] \quad (\text{B3c}) \end{aligned}$$

and

$$Z^3(m, n, j, k, 0; 2\alpha) = 0, \quad (\text{B3d})$$

when j and k are both even; otherwise the values of these functions are zero. Here, the function $A_n(x)^7$ is defined by

$$A_n(x) \equiv \int_1^\infty \lambda^n e^{-x\lambda} d\lambda, \quad (\text{B4})$$

and its value is calculated by the following recurrence formula,

$$A_n(x) = \frac{1}{x} \{e^{-x} + nA_{n-1}(x)\}, \quad (\text{B5a})$$

$$A_0(x) = e^{-x}/x. \quad (\text{B5b})$$

For $p=-1$, the Neumann expansion⁸⁾ of ρ^{-1} ,

$$\rho^{-1} = \sum_{\tau=0}^{\infty} \sum_{\nu=0}^{\tau} D_{\tau}^{\nu} P_{\tau}^{\nu} \binom{\lambda_1}{\lambda_2} Q_{\tau}^{\nu} \binom{\lambda_2}{\lambda_1} P_{\tau}^{\nu}(\mu_1) P_{\tau}^{\nu}(\mu_2) \cos \nu(\phi_1 - \phi_2), \quad \begin{cases} \lambda_1 < \lambda_2 \\ \lambda_2 < \lambda_1 \end{cases}, \quad (\text{B6a})$$

$$D_{\tau}^0 = 2\tau + 1, \quad (\text{B6b})$$

$$D_{\tau}^{\nu} = (-1)^{\nu} 2(2\tau+1)[(\tau-\nu)!/(\tau+\nu)!]^2, \quad \text{for } \nu > 0, \quad (\text{B6c})$$

is substituted into the Eq. (A4), and the following expressions are obtained.

$$Z^0(m, n, j, k, -1; 2\alpha) = \sum_{\tau=0}^{\infty} (2\tau+1) C_{\tau}^0(j) C_{\tau}^0(k) W_{\tau}^0(m, n; 2\alpha), \quad (\text{B7a})$$

$$Z^1(m, n, j, k, -1; 2\alpha) = - \sum_{\tau=1}^{\infty} [(2\tau+1)/\tau^2(\tau+1)^2] C_{\tau}^1(j) C_{\tau}^1(k) W_{\tau}^1(m, n; 2\alpha), \quad (\text{B7b})$$

$$\begin{aligned} Z^2(m, n, j, k, -1; 2\alpha) = & \frac{1}{2} \sum_{\tau=2}^{\infty} [(2\tau+1)/(\tau+2)^2(\tau+1)^2\tau^2(\tau-1)^2] \\ & \times C_{\tau}^2(j) C_{\tau}^2(k) W_{\tau}^2(m, n; 2\alpha) + \frac{1}{2} \sum_{\tau=0}^{\infty} (2\tau+1) \{C_{\tau}^0(j) - C_{\tau}^0(j+2)\} \\ & \times \{C_{\tau}^0(k) - C_{\tau}^0(k+2)\} \{W_{\tau}^0(m+2, n+2; 2\alpha) - W_{\tau}^0(m+2, n; 2\alpha) \\ & - W_{\tau}^0(m, n+2; 2\alpha) + W_{\tau}^0(m, n; 2\alpha)\}, \end{aligned} \quad (\text{B7c})$$

and

$$\begin{aligned} Z^3(m, n, j, k, -1; 2\alpha) = & - \frac{1}{4} \sum_{\tau=3}^{\infty} [(2\tau+1)/(\tau+3)^2(\tau+2)^2(\tau+1)^2\tau^2(\tau-1)^2(\tau-2)^2] \\ & \times C_{\tau}^3(j) C_{\tau}^3(k) W_{\tau}^3(m, n; 2\alpha) - \frac{3}{4} \sum_{\tau=1}^{\infty} [(2\tau+1)/\tau^2(\tau+1)^2] \{C_{\tau}^1(j) - C_{\tau}^1(j+2)\} \\ & \times \{C_{\tau}^1(k) - C_{\tau}^1(k+2)\} \{W_{\tau}^1(m+2, n+2; 2\alpha) - W_{\tau}^1(m+2, n; 2\alpha) \\ & - W_{\tau}^1(m, n+2; 2\alpha) + W_{\tau}^1(m, n; 2\alpha)\}, \end{aligned} \quad (\text{B7d})$$

where $C_{\tau}^{\nu}(k)$ ⁷ and $W_{\tau}^{\nu}(m, n; x)$ ⁷ are

$$C_{\tau}^{\nu}(k) \equiv \int_{-1}^1 d\mu (1-\mu^2)^{\nu/2} P_{\tau}^{\nu}(\mu) \mu^k, \quad (\text{B8a})$$

$$= \frac{2^{\tau+1} k! (\tau+\nu)! \left(\frac{k+\tau+\nu}{2}\right)!}{(\tau-\nu)! \left(\frac{k+\nu-\tau}{2}\right)! (k+\tau+\nu+1)!}, \quad \begin{cases} k+\tau+\nu = \text{even}, \\ \tau \geq \nu, \\ k \geq \tau-\nu, \end{cases} \quad (\text{B8b})$$

$$= 0, \quad \text{otherwise}, \quad (\text{B8c})$$

and

$$W_{\tau}^{\nu}(m, n; x) \equiv \int_1^{\infty} d\lambda_1 \int_1^{\infty} d\lambda_2 [(\lambda_1^2 - 1)(\lambda_2^2 - 1)]^{\nu/2} P_{\tau}^{\nu} \binom{\lambda_1}{\lambda_2} Q_{\tau}^{\nu} \binom{\lambda_2}{\lambda_1} \lambda_1^m \lambda_2^n e^{-x(\lambda_1 + \lambda_2)}. \quad (\text{B9})$$

The auxiliary functions $W_{\tau}^{\nu}(m, n; x)$ are familiar in the literatures of molecular integrals and the method of their calculation is given by Kotani, Amemiya, Ishiguro, and Kimura.⁷⁾

APPENDIX C LISTS OF PROGRAMS (1)

```

PROGRAM JC1
C*      PROGRAM JC1
C*      TWO ELECTRON SYSTEM IN DIATOMIC MOLECULES
C*      SIGMA PLUS STATE
C*      JAMES-COOLIDGE'S METHOD
C*      AUXILIARY FUNCTION Z(NU,M,N,J,K,P)
C*          0.LE.NU.LE.3
C*          0.LE.N.LE.M.LE.20-NU*2
C*          0.LE.K.LE.J.LE.20-NU*2
C*          P=-1 AND 0
C*      INPUT DATA
C*      ALPHA
C***** IMPLICIT REAL*8(A-H,O-Z)
REAL*16 QALPH2
DIMENSION Z(720)
COMMON /FACTOR/FC,FD
III=720
FC=1.D-60
FD=1.D0/DSQRT(FC)
C**** INPUT *****
READ(5,1000) ALPHA
WRITE(6,2000) ALPHA
ALPHA2=ALPHA+ALPHA
QAI.PH2=ALPHA2
CALL QW(17,3,14,QALPH2,QALPH2)
CALL DA(ALPHA2)
Z(1)=ALPHA
I=1
C**** Z(0,M,N,J,K,-1) *****
DO 40 JP1=1,21
J=JP1-1
L=J.AND.1
DO 40 KP1=1,JP1
K=KP1-1
IF(((J+K).AND.1).NE.0) GO TO 40
DO 30 MP1=1,21
M=MP1-1
DO 30 NP1=1,MP1
N=NP1-1
I=I+1
IF(I.LE.III) GO TO 10
WRITE(20) Z
I=1
10 ZZ=0.D0
DO 20 IT=L,K,2
ZZ=ZZ+DFLOAT(IT+IT+1)*C(0,IT,J)*C(0,IT,K)*W(IT,0,M,N)
20 CONTINUE
Z(I)=ZZ
30 CONTINUE
40 CONTINUE
C**** Z(1,M,N,J,K,-1) *****
DO 80 JP1=1,19
J=JP1-1
L=(J.AND.1)+1
DO 80 KP1=1,JP1
K=KP1-1
IF(((J+K).AND.1).NE.0) GO TO 80
MM=K+1
DO 70 MP1=1,19
M=MP1-1
DO 70 NP1=1,MP1
N=NP1-1
I=I+1
IF(I.LE.III) GO TO 50
WRITE(20) Z
I=1
50 ZZ=0.D0
DO 60 IT=L,MM,2
ZZ=ZZ-DFLOAT(IT+IT+1)*C(1,IT,J)*C(1,IT,K)*W(IT,1,M,N)
2    /DFLOAT((IT*(IT+1))**2)
60 CONTINUE
Z(I)=ZZ
70 CONTINUE

```

APPENDIX C LISTS OF PROGRAMS (2)

```

80 CONTINUE
***** Z(2,M,N,J,K,-1) *****
DO 130 JP1=1,17
J=JP1-1
L=J.AND.1
DO 130 KP1=1,JP1
K=KP1-1
IF(((J+K).AND.1).NE.0) GO TO 130
MM=K+2
DO 120 MP1=1,17
M=MP1-1
DO 120 NP1=1,MP1
N=NP1-1
I=I+1
IF(I.LE.III) GO TO 90
WRITE(20) Z
I=1
90 ZZ=0.D0
DO 100 IT=L,MM,2
ZZ=ZZ+DFLOAT(IT+IT+1)*(C(0,IT,J+2)-C(0,IT,J))*(C(0,IT,K+2)
2   -C(0,IT,K))*(W(IT,0,M+2,N+2)-W(IT,0,M+2,N)-W(IT,0,M,N+2)
3   +W(IT,0,M,N))
100 CONTINUE
DO 110 IT=L+2,MM,2
ZZ=ZZ+DFLOAT(IT+IT+1)*C(2,IT,J)*C(2,IT,K)*W(IT,2,M,N)
2   /DFLOAT(((IT+2)*(IT+1)*IT*(IT-1))**2)
110 CONTINUE
Z(I)=ZZ*0.5D0
120 CONTINUE
130 CONTINUE
***** Z(3,M,N,J,K,-1) *****
DO 180 JP1=1,15
J=JP1-1
L=(J.AND.1)+1
DO 180 KP1=1,JP1
K=KP1-1
IF(((J+K).AND.1).NE.0) GO TO 180
MM=K+3
DO 170 MP1=1,15
M=MP1-1
DO 170 NP1=1,MP1
N=NP1-1
I=I+1
IF(I.LE.III) GO TO 140
WRITE(20) Z
I=1
140 ZZ=0.D0
DO 150 IT=L,MM,2
ZZ=ZZ-DFLOAT(IT+IT+1)*(C(1,IT,J+2)-C(1,IT,J))*(C(1,IT,K+2)
2   -C(1,IT,K))*(W(IT,1,M+2,N+2)-W(IT,1,M+2,N)-W(IT,1,M,N+2)
3   +W(IT,1,M,N))/DFLOAT(((IT+1)*IT)**2)
150 CONTINUE
ZZ=ZZ*3.D0
DO 160 IT=L+2,MM,2
ZZ=ZZ-DFLOAT(IT+IT+1)*C(3,IT,J)*C(3,IT,K)*W(IT,3,M,N)
2   /DFLOAT(((IT+3)*(IT+2)*(IT+1)*IT*(IT-1)*(IT-2))**2)
160 CONTINUE
Z(I)=ZZ*0.25D0
170 CONTINUE
180 CONTINUE
***** Z(C,M,N,J,K,0) *****
DO 200 JP1=1,21,2
J=JP1-1
DO 200 KP1=1,JP1,2
K=KP1-1
DO 200 MP1=1,21
M=MP1-1
DO 200 NP1=1,MP1
N=NP1-1
I=I+1
IF(I.LE.III) GO TO 190
WRITE(20) Z
I=1
190 Z(I)=4.D0*A(M)*A(N)/DFLOAT((J+1)*(K+1))
200 CONTINUE

```

APPENDIX C LISTS OF PROGRAMS (3)

```

***** Z(2,M,N,J,K,0) *****
DO 220 JP1=1,17,2          *****10001510
J=JP1-1                   10001520
DO 220 KP1=1,JP1,2         10001530
K=KP1-1                   10001540
DO 220 MP1=1,17            10001550
M=MP1-1                   10001560
DO 220 NP1=1,MP1           10001570
N=NP1-1                   10001580
I=I+1                      10001590
IF(I.LE.III) GO TO 210    10001600
WRITE(20) Z                10001610
I=1                         10001620
210 Z(I)=8.D0*(A(M+2)-A(M))*(A(N+2)-A(N)) 10001630
2      /DFLOAT((J+3)*(J+1)*(K+3)*(K+1)) 10001640
220 CONTINUE                 10001650
      WRITE(20) Z             10001660
      STOP                     10001670
1000 FORMAT(D20.0)           10001680
2000 FORMAT(1H1,10X,'AUXILIARY FUNCTION Z(NU,M,N,J,K,P) P=-1,0', 10001690
2//16X,'ALPHA =',F10.5,/1H1) 10001700
      END                     10001710
      REAL FUNCTION A*8(N)     10001720
      IMPLICIT REAL*8(A-H,O-Z) 10001730
      COMMON /AD/AA(21)         10001740
      DIMENSION AAA(1)          10001750
      EQUIVALENCE (AAA(1),AA(2)) 10001760
      A=AAA(N)                 10001770
      RETURN                    10001780
      END                       10001790
      SUBROUTINE DA(ALPHA2)    10001800
      IMPLICIT REAL*8(A-H,O-Z) 10001810
      COMMON /AD/AA(21)         10001820
      ALI=1.D0/ALPHA2           10001830
      EXPMAL=DEXP(-ALPHA2)     10001840
      AA(1)=EXPMAL*ALI         10001850
      DO 10 N=1,20              10001860
      AA(N+1)=(EXPMAL+DFLOAT(N)*AA(N))*ALI 10001870
10   CONTINUE                  10001880
      RETURN                    10001890
      END                       10001900
      REAL FUNCTION C*8(NU,ITAU,M) 10001910
      IMPLICIT REAL*8(A-H,O-Z) 10001920
      COMMON /FACTOR/FC,FD       10001930
      COMMON /FCTRL/DFCT(57)    10001940
      DIMENSION DFCTRL(1)       10001950
      EQUIVALENCE(DFCTRL(1),DFCT(2)) 10001960
      I=NU+ITAU+M               10001970
      J=M+NU-ITAU               10001980
      IF(((I.AND.1).NE.0).OR.(J.LT.0)) GO TO 20 10001990
      C=DFLOAT(2**((ITAU+1))*DFCTRL(M)/DFCTRL(I+1) 10002000
      *DFCTRL((ITAU+NU))/DFCTRL(ITAU-NU)*DFCTRL(I/2)/DFCTRL(J/2)*FD 10002010
10   RETURN                    10002020
20   C=0.D0                   10002030
      GO TO 10                  10002040
      END                       10002050
      REAL FUNCTION W*8(/TAU/,/NU/,/M/,/N/) 10002060
*****MOLECULAR INTEGRAL(KAS) AUXILIARY FUNCTION W *****
C*      PICK OUT ROUTINE (W,DOUBLE PRECISION) *10002090
C* *****BY T.TAKEZAWA*****10002100
      REAL*16 WTN                10002110
      COMMON /WC/WTN(42350),IAD(72),NT(5),ITNM1 10002120
      INTEGER TAU                 10002130
      I=NT(NU+1)+TAU              10002140
      I=IAD(I)+(ITNM1-TAU-NU)*N+M 10002150
      W=WTN(I)                  10002160
      RETURN                     10002170
      END                       10002180
      SUBROUTINE GW(ITX,INX,IMNX,ALPHA,BETA) 10002190
*****MOLECULAR INTEGRAL(KAS) AUXILIARY FUNCTION W *****
C*      W TAU,NU(M,N,ALPHA,BETA) COVERING W0,0(0,0,ALPHA,BETA) *10002200
C*      TO W3,17(14,14,ALPHA,BETA) *10002210
C*      QUADRUPLE PRECISION *10002220
C*      MAX(TAU=20, MAX(NU)=3, MAX(M)=MAX(N)=34 *10002230
C*      MAX(TAU+NU)=20, MAX(TAU+NU+N)=34 *10002240
C*                                         *10002250

```

APPENDIX C LISTS OF PROGRAMS (4)

APPENDIX C LISTS OF PROGRAMS (5)

```

30 I=I+1                                10003010
    IF(NEZ .AND. ITX.EQ.1) GO TO 200      10003020
C ***** Z0(M,N,ALPHA,BETA), W2,0(M,N,ALPHA,BETA)*** 10003030
    I=IAD(3)                               10003040
    K=IAD(1)                               10003050
    L=IAD(2)+MEND                         10003060
    MEND=MEND-1                           10003070
    DO 45 N=1,MEND                         10003080
    NP1=N+1                                10003090
    NP2=NP1+1                             10003100
    DO 40 M=1,MEND                         10003110
    ZT(I)=S1(M,NP2)+S3(N,M+2)+S2(M+1,N)+S4(NP1,M)-THREE*WTN(L+1)
    WTN(I)=C1*WTN(K)-C2*ZT( I )          10003120
    I=I+1                                  10003130
    K=K+1                                  10003140
    40 L=L+1                               10003150
    K=K+2                                  10003160
    45 L=L+1                               10003170
    IF(NEZ .AND. ITX.EQ.2) GO TO 200      10003180
    MEND=MEND-1                           10003190
C ***** Z1(M,N,ALPHA,BETA),W3,0(M,N,ALPHA,BETA) *** 10003200
    IR2A=IAD(2)                            10003220
    IR1A=IR2A+(MEND+2)*2                  10003230
    IR3A=IAD(1)+MEND+3                  10003240
    IR4A=IAD(3)+MEND+1                  10003250
    IR5A=IAD(4)                            10003260
    DO 55 N=1,MEND                         10003270
    DO 50 M=1,MEND                         10003280
    ZT(IR5A)=THREE*(WTN(IR1A)+WTN(IR2A+2))-WTN(IR3A+1)-WTN(IR2A)
    ~ -FIVE*WTN(IR4A+1)                   10003290
    WTN(IR5A)=C3*WTN(IR2A)-C4*ZT(IR5A)   10003300
    IR1A=IR1A+1                           10003310
    IR2A=IR2A+1                           10003320
    IR3A=IR3A+1                           10003330
    IR4A=IR4A+1                           10003340
    50 IR5A=IR5A+1                           10003350
    IR1A=IR1A+2                           10003360
    IR2A=IR2A+2                           10003370
    IR3A=IR3A+3                           10003380
    55 IR4A=IR4A+1                           10003390
    IF(NEZ .AND. ITX.EQ.3) GO TO 200      10003400
C ***** W TAU,0 ,Z TAU ***               10003410
    TAU=THREE                            10003420
    DO 65 I=5,IWEND                      10003430
    MEND=MEND-1                           10003440
    TAU=TAU+ONE                           10003450
    IR1A=IAD(I)                           10003460
    IR2A=IAD(I-2)                          10003470
    IR3A=IR2A+MEND+MEND+4                10003480
    IR4A=IAD(I-3)+MEND+3                10003490
    IR5A=IAD(I-1)+MEND+1                10003500
    T2I=ONE/(TAU*TAU)                     10003510
    C01=TAU+TAU-THREE                    10003520
    C02=C01-TWO                          10003530
    C03=C01+TWO                          10003540
    C04=TAU-ONE                          10003550
    C04=C04*C04*T2I                      10003560
    C05=(C01+TWO)*T2I                   10003570
    DO 65 N=1,MEND                      10003580
    DO 60 M=1,MEND                      10003590
    ZT(IR1A)=ZT(IR2A)+C01*(WTN(IR2A+2)+WTN(IR3A))-C02*WTN(IR4A+1)
    1 -C03*WTN(IR5A+1)                   10003610
    WTN(IR1A)=C04*WTN(IR2A)-C05*ZT(IR1A) 10003620
    IR1A=IR1A+1                           10003630
    IR2A=IR2A+1                           10003640
    IR3A=IR3A+1                           10003650
    IR4A=IR4A+1                           10003660
    60 IR5A=IR5A+1                           10003670
    IR2A=IR2A+2                           10003680
    IR3A=IR3A+2                           10003690
    IR4A=IR4A+3                           10003700
    65 IR5A=IR5A+1                           10003710
    IF(NEZ) GO TO 200                     10003720
C ***** W TAU,NU ***                   10003730
    L1=IWEND-2                           10003740
                                            10003750

```

APPENDIX C LISTS OF PROGRAMS (6)

```

DO 85 JNU=1,INX          10003760
NU=JNU                   10003770
IWEND=IWEND-2            10003780
MEND=IWEND+IMNX          10003790
DO 80 JTAU=JNU,L1         10003800
TAU=JTAU                 10003810
IWI=NT(JNU+1)+JTAU       10003820
IWIL=NT(JNU)+JTAU        10003830
IR1A=IAD(IWI)             10003840
IR2A=IAD(IWIL)+MEND+1    10003850
IR3A=IAD(IWIL-1)          10003860
IR4A=IAD(IWIL+1)          10003870
C04=TAU+NU                10003880
H=TAU+ONE                 10003890
C05=H-NU                  10003900
C06=H+TAU                 10003910
C01=-C04*C05               10003920
C02=(C04-ONE)**2*C04/C06   10003930
C03=(C05+ONE)**2*C05/C06   10003940
DO 75 N=1,MEND            10003950
DO 70 M=1,MEND            10003960
WTN(IR1A)=C01*WTN(IR2A+1)+C02*WTN(IR3A)+C03*WTN(IR4A) 10003970
IR1A=IR1A+1                10003980
IR2A=IR2A+1                10003990
IR3A=IR3A+1                10004000
70 IR4A=IR4A+1              10004010
IR2A=IR2A+1                10004020
75 IR3A=IR3A+2              10004030
80 MEND=MEND-1              10004040
85 L1=L1-1                  10004050
200 RETURN                  10004060
300 DO 95 N=1,MEND          10004070
NM1=N-1                     10004080
DO 90 M=1,MEND              10004090
MN=M+NM1                    10004100
S1(M,N)=(H*S1(M,NM1)+EB*F0A(M)-F0AB(MN))*BJ           10004110
S2(M,N)=(H*S2(M,NM1)+EB*F1A(M)-F1AB(MN))*BI           10004120
S3(M,N)=S1(M,N)              10004130
90 S4(M,N)=S2(M,N)              10004140
95 H=ONE+H                   10004150
GO TO 100                   10004160
C ***** ERROR MESSAGE *****
500 WRITE(6,600) ITX,INX,IMNX          10004170
STOP                         10004180
501 WRITE(6,601) ALPHA,BETA          10004190
STOP                         10004200
10004210
600 FORMAT(1H0,15H(SUBR. QW) TAU=,I6,5X,3HNU=,I6,5X,2HM=,I6 /12X,60HTA10004220
1U AND NU AND M SHOULD BE SATISFY THE FOLLOWING INEQUALITIES /16X, 10004230
2 73H0.GE.TAU.LE.20, 0.GE.NU.LE.3, 0.GE.M.LE.34, TAU+NU.LE.20 10004240
3NU+M.LE.34, /)          10004250
601 FORMAT(1H0,17H(SUBR. QW) ALPHA=,1PE23.15,5X,5HBETA=,E23.15,5X, 10004260
1 25HARGUMENT OF W IS INVALID./) 10004270
END                          10004280
SUBROUTINE QF(M,ALPHA,F0,F1)      10004290
C*****MOLECULAR INTEGRAL(KAS) AUXILIARY FUNCTION F *****
C*          F 0(M,ALPHA), F 1(M,ALPHA)          *10004310
C*          QUADRUPLE PRECISION (36 DIGITS)      *10004320
C*          M.GE.1, ALPHA.GT.0                      *10004330
C*****BY T.TAKEZAWA*****10004340
IMPLICIT REAL*16(A-H,O-Z)        10004350
REAL*8 FC,FD                   10004360
DIMENSION F0(M),F1(M)          10004370
COMMON /FACTOR/FC,FD          10004380
DATA EULER/-.577215664901532860606512090082402431/ 10004390
EM=EXP(-ALPHA)*FC             10004400
X2=ALPHA+ALPHA                 10004410
EI2X=QEIE(-X2)                 10004420
EOGC=EULER+ LOG(X2)            10004430
FC(1)=EM*(EOGC+EI2X)/X2       10004440
XI=1.Q0/ALPHA                  10004450
H=2.Q0                         10004460
A0=EM*XI                        10004470
A1=(EM+A0)*XI                  10004480
A2=(EM+A1+A1)*XI                10004490
EEX=EI2X*EM*XI                  10004500

```

APPENDIX C LISTS OF PROGRAMS (7)

```

F1(1)=(E0GCA1-EEX+XI*EEX)/H-A0 10004510
F1(2)=(E0GCA2+EEX)/H-(EEX-XI*EEX+EM+HXXI*EM)*XI 10004520
F1(3)=F1(1)+(3.Q0*F1(2)-F0(1))*XI 10004530
F0(2)=F1(1)+A0 10004540
F0(3)=F1(2)+A1 10004550
DO 10 I=4,M 10004560
F0(I)=F1(I-1)+A2 10004570
H=1.Q0+H 10004580
A2=(EM+H*A2)*XI 10004590
10 F1(I)=F1(I-2)+(3.Q0*F1(I-1)-F0(I-2)-(2.Q0-H)*(F1(I-1)-F1(I-3)))*XI 10004600
RETURN 10004610
END 10004620
REAL FUNCTION GEIE*16(X) 10004630
C*****EXPONENTIAL INTEGRAL EI(X)*EXP(-X), -EI(-X)*EXP(X)*****10004640
C* QUADRUPLE PRECISION (36 DIGITS) *10004650
C*****BY T.TAKEZAWA*****10004660
IMPLICIT REAL*16(A-H,D-Z) 10004670
DIMENSION X0(18),TABLEP(18),TABLEM(18) 10004680
C *** ZERO POINTS *** 10004690
DATA X0/3.3Q+,4.Q0,4.8Q0,5.8Q0,7.1Q0,8.6Q0,10.4Q0,12.5Q0,15.2Q0,18.1Q0/ 10004700
1.4Q0,22.2Q0,26.9Q0,32.5Q0,39.4Q0,47.6Q0,57.6Q0,69.7Q0,83.Q0/, 10004710
2C100/100.Q0/,C1,C2/1.Q0,2.Q0/ 10004720
C *** MASTER VALUES OF EI(X)*EXP(-X) *** 10004730
DATA TABLEP 10004740
      /44.8537724756737459666837503688703855,35.9552007863620610004750
196177421675826607445,28.55548567959244356020188296843875,22.2830410004760
2130069319214.557583172208597,17.150837621207652885138170998453615910004770
3,13.5265041139175554681803929873875053,10.81282973538745844707760910004780
443306202,8.781902021178544408467802706076844297,7.084719123528884310004790
55210984346370704404, 10004800
6 5.76911530203858726665652398512543158,4.72874671023767410004810
183837309792258654404,3.86730060944143837783828361535021675,3.1780410004820
2035477284081938199607540047727,2.60603712949385051753123062834257610004830
317,2.1469579435134789629974881859707721,1.76735714626929724128145910004840
489927502125,1.4559220991807543601507263870521299,1.21969824417642010004850
543671159294416866409/ 10004860
C *** MASTER VALUES OF -EI(-X)*EXP(X) *** 10004870
DATA TABLEM 10004880
      /24.236103273851717984280290330013846,20.63456499010558310004890
1310204575876857809,17.655389992275490844225877258125266,14.9678910004900
27250602407607257532006592657,12.504018238713862459421003255044820810004910
3,10.5136538324982612526442436790694708,8.830924437781962276738399510004920
42840940368,7.44352751897750512563776275564418445,6.19408382644356810004930
523471326330680039114, 10004940
6 5.16718724165552396801215909735572161,4.31777404330991710004950
144765474643574252111,3.5885493954921341781086012050028467,2.98759410004960
241163658182489651049608223601,2.476696474779806275434329427614726410004970
36,2.05845148731713464081068544567428092,1.70696582852447115244268210004980
480473572445,1.4147u260005955216036937381007104502,1.1906410951618110004990
5287339459137226850272/ 10005000
C *** FULER CONSTANT *** 10005010
DATA EULER/.577215664901532860606512090082402431/ 10005020
ABSX=ABS(X)
IF( ABSX .GE. 90. ) GO TO 11 10005030
IF( ABSX .GE. 3. ) GO TO 3 10005040
10005050
C ***** POWER SERIES EXPANSION ***
IB=1 10005060
QEIE=X 10005080
TERM1=X 10005090
TERM2=X 10005100
H=C2 10005110
1 TERM2=TERM2*H 10005120
TERM1=TERM2/H 10005130
GO TO 16 10005140
2 QEIE= EXP(-X)*(QEIE+EULER+ LOG(ABSX)) 10005150
GO TO 14 10005160
C ***** INTERPOLATION (EXP(-X)*EI(X),EXP(X)*(-EI(-X))) ***
3 IB=2 10005170
DO 4 I=1,18 10005180
IF( .5*(X0(I+1)+X0(I))-ABSX ) 4,4,5 10005190
4 CONTINUE 10005200
I=18 10005210
5 IF(X)6,6,7 10005220
6 XX=-X0(I)-X 10005230
XXI=C1 +X/X0(I) 10005240
10005250

```

APPENDIX C LISTS OF PROGRAMS (8)

```

TERM1=TABLEM(I)/C100          10005260
GO TO 8                      10005270
7 XX=X0(I)-X                 10005280
XXI=XX/X0(I)                  10005290
TERM1=TABLEP(I)/C100          10005300
8 QEIE=TERM1                  10005310
XI=C1 /X0(I)                  10005320
H=C1                          10005330
TERM2=H                      10005340
9 TERM1=XXX*(TERM1-TERM2*XI)/H 10005350
GO TO 16                     10005360
10 TERM2=TERM2*XXI            10005370
GO TO 9                      10005380
C ***** ASYMPTOTIC EXPANSION ***
11 XI=C1/X                   10005390
IB=3                          10005400
QEIE=C1                      10005410
H=C1                          10005420
TERM1=C1                      10005430
12 TERM1=TERM1*H*XI          10005440
GO TO 16                     10005450
13 QEIE=QEIE/X               10005460
14 IF(X.LT.0.) QEIE=-QEIE    10005470
15 RETURN                      10005480
16 QEIN=QEIE+TERM1           10005490
IF(QEIE .EQ. QEIN) GO TO(2,15,13) , IB
QEIE=QEIN                     10005500
H=H+C1                        10005510
GO TO(1,10,12) , IB          10005520
RETURN                         10005530
10005540
END                           10005550
BLOCK DATA                     10005560
IMPLICIT REAL*8 (A-H,O-Z)     10005570
COMMON /FCTRL/DFCT1(57)       10005580
DATA DFCT1/                     10005590
1      Z4110000000000000, Z4110000000000000, Z4120000000000000, 10005610
1      Z4160000000000000, Z4218000000000000, Z4278000000000000, 10005620
1      Z432D000000000000, Z4413B0000000000, Z449D800000000000, 10005630
2      Z4558980000000000, Z46375F0000000000, Z4726115000000000, 10005640
2      Z481C8CFC00000000, Z4917328CC000000, Z4A144C3B28000000, 10005650
3      Z481307775800000, Z4C1307775800000, Z4D1437EECD80000, 10005660
3      Z4E16BECCA730000, Z4F1B02B930689000, Z5021C3677C82B400, 10005670
4      Z512C5077D36B8C40, Z523CEEAA4C2B3E0D8, Z5357970CD7E29336, 10005680
4      Z5483629343D3DCD1, Z55CD4A0619FB0906, Z5714D9849EA37EEA, 10005690
5      Z58232F0FCB83E62A, Z593D925BA47AD2C9, Z5A6F99461A1E9E0C, 10005700
5      Z5BD13F6370F96856, Z5D1956AD0AAE33A2, Z5E32AD5A155C6744, 10005710
6      Z5F688589CC0E94FC, Z60DE1BC4D19EFC97, Z621E5DCBE8A8BC88, 10005720
6      Z6344530ACB7BA832, Z649F0008F68DF4F3, Z661774015499125C, 10005730
7      Z67392AC33E351CC0, Z688EEAE81B84C7E0, Z6A16E39F2C684402, 10005740
7      Z6B3C1581D491B285, Z6CA179CCEB478FC5, Z6E1BC0EF38704CB5, 10005750
8      Z6F4E0EA0CEBB07BD, Z70E06A0E525C0C3F, Z72293378A11EE63F, 10005760
8      Z73789A69E35CB2BD, Z7517A88E4484BE36, Z7649EEBC961ED268, 10005770
9      Z77E8A6F91E823EA8, Z792FDE529A3274BA, Z7A9E90719EC722A8, 10005780
9      Z7C217277F77E014F, Z7U72F97C62C1247F, Z7F192693359A3FFB/10005790
END                           10005800

PROGRAM JC2                    20000010
C*****20000020
C* PROGRAM JC2                *20000030
C* TWO ELECTRON SYSTEM IN DIATOMIC MOLECULES *20000040
C* SIGMA PLUS STATE          *20000050
C* JAMES-COOLIDGE'S METHOD   *20000060
C* AUXILIARY FUNCTION Z(NU,M,N,J,K,P) *20000070
C* NU=0                      *20000080
C*   0.LE.N.LE.M.LE.16        FOR -1.LE.P.LE.4   *20000090
C*   0.LE.N.LE.M.LE.14        FOR P=5 OR 6      *20000100
C*   0.LE.K.LE.J.LE.16        FOR -1.LE.P.LE.4   *20000110
C*   0.LE.K.LE.J.LE.14        FOR P=5 OR 6      *20000120
C* INPUT DATA                 *20000130
C*   NONE                      *20000140
C*****20000150
IMPLICIT REAL*8(A-H,Q-Z)      20000160
IMPLICIT INTEGER(I-P)         20000170
COMMON /ZD/Z(89155)           20000180

```

APPENDIX C LISTS OF PROGRAMS (9)

```

DIMENSION Z0(720)                                                    20000190
III=720                                                                20000200
C**** INPUT FROM THE FILE 20                                        20000210
READ(20) Z0                                                            20000220
ALPHA=Z0(1)                                                            20000230
WRITE(6,1000) ALPHA                                                    20000240
J=1                                                                    20000250
DO 20 I=1,89155                                                    20000260
J=J+1                                                                    20000270
IF(J.LE.III) GO TO 10                                            20000280
READ(20) Z0                                                            20000290
J=1                                                                    20000300
10 Z(I)=Z0(J)                                                        20000310
20 CONTINUE                                                            20000320
Z0(1)=ALPHA                                                            20000330
I=1                                                                    20000340
DU 90 PP2=1,8                                                        20000350
P=PP2-2                                                                20000360
GO TO (60,60,30,60,30,60,30,60) ,PP2                        20000370
C**** Z(0,M,N,J,K,P)                                                20000380
30 II=0                                                                20000390
NUP1MX=3-P/2                                                        20000400
DO 50 PPP=1,2                                                        20000410
PP=P+PPP-1                                                            20000420
PPP2=PPP-2                                                            20000430
DO 50 NUP1=1,NUP1MX                                                20000440
NU=NUP1-1                                                            20000450
MP1MAX=20-P-NU*2                                                20000460
DO 50 JP1=1,MP1MAX                                                20000470
J=JP1-1                                                                20000480
DO 50 KP1=1,JP1                                                    20000490
K=KP1-1                                                                20000500
IF(((J+K).AND.1).NE.0) GO TO 50                                20000510
DO 40 MP1=1,MP1MAX                                                20000520
M=MP1-1                                                                20000530
DO 40 NP1=1,MP1                                                    20000540
N=NP1-1                                                                20000550
II=II+1                                                                20000560
Z(II)=ZZ(NU,M+2,N,J,K,PPM2)+ZZ(NU,M,N+2,J,K,PPM2)        20000570
2        +ZZ(NU,M,N,J+2,K,PPM2)+ZZ(NU,M,N,J,K+2,PPM2)        20000580
3        -2.D0*(ZZ(NU,M,N,J,K,PPM2)+ZZ(NU,M+1,N+1,J+1,K+1,PPM2) 20000590
4        +ZZ(NU+1,M,N,J,K,PPM2))                                20000600
40 CONTINUE                                                            20000610
50 CONTINUE                                                            20000620
C**** OUTPUT TO THE FILE 21                                        20000630
60 MP1MAX=17                                                        20000640
IF(P.GT.4) MP1MAX=15                                                20000650
DO 90 JP1=1,MP1MAX                                                20000660
J=JP1-1                                                                20000670
DO 90 KP1=1,JP1                                                    20000680
K=KP1-1                                                                20000690
IF(((J+K).AND.1).NE.0) GO TO 90                                20000700
DO 80 MP1=1,MP1MAX                                                20000710
M=MP1-1                                                                20000720
DO 80 NP1=1,MP1                                                    20000730
N=NP1-1                                                                20000740
I=I+1                                                                20000750
IF(I.LE.III) GO TO 70                                            20000760
WRITE(21) Z0                                                        20000770
I=1                                                                    20000780
70 Z0(I)=ZZ(0,M,N,J,K,P)                                        20000790
80 CONTINUE                                                            20000800
90 CONTINUE                                                            20000810
WRITE(21) Z0                                                        20000820
STOP                                                                    20000830
1000 FORMAT(1H1,10X,'AUXILIARY FUNCTION Z(0,M,N,J,K,P)', 20000840
2//16X,'ALPHA =',F10.5,/1H1)                                    20000850
END                                                                    20000860
REAL FUNCTION ZZ*8(NU,M,N,J,K,P)                                20000870
IMPLICIT REAL*8(A-H,Q-Z)                                        20000880
IMPLICIT INTEGER(I-P)                                                20000890
COMMON /ZD/Z(89155)                                                20000900
DIMENSION L(4,8),LL(4)                                            20000910
DATA L/1,27952,46952,59345,67025,0,82271,0, 20000920
2        1,19001,31394,0,39074,58074,70467,0, 20000930

```

APPENDIX C LISTS OF PROGRAMS (10)

```

3      1,12394,0,0,20074,32467,0,0,          20000940
4      1,0,0,0,7681,0,0,0,          20000950
DATA LL/231,190,153,120/          20000960
ZZ=0.D0          20000970
IF(M.GT.N) GO TO 10          20000980
MM=N          20000990
NN=M          20001000
GO TO 20          20001010
10 MM=M          20001020
NN=N          20001030
20 IF(J.GT.K) GO TO 30          20001040
JJ=K          20001050
KK=J          20001060
GO TO 40          20001070
30 JJ=J          20001080
KK=K          20001090
40 PP2=P+2          20001100
NUP1=NJ+1          20001110
IF(P.NE.0) GO TO 50          20001120
IF((NJ.AND.1).NE.0) GO TO 70          20001130
IF(((JJ.AND.1)+(KK.AND.1)).NE.0) GO TO 70          20001140
I=(JJ*(JJ+2)/8+KK/2)*LL(NUP1)+MM*(MM+1)/2+NN+L(NUP1,PP2) 20001150
GO TO 60          20001160
50 IF(((J+K).AND.1).NE.0) GO TO 70          20001170
I=((JJ*(JJ+2)+KK*2)/4)*LL(NUP1+(P+1)/2)+MM*(MM+1)/2+NN+L(NUP1,PP2) 20001180
60 ZZ=Z(I)          20001190
70 RETURN          20001200
END          20001210

```

```

PROGRAM JC3          30000010
*****30000020
C*      PROGRAM JC3          *30000030
C*      TWO ELECTRON SYSTEM IN DIATOMIC MOLECULES          *30000040
C*          SIGMA PLUS STATE          *30000050
C*          JAMES-COOLIDGE'S METHOD          *30000060
C*          CALCULATION OF MATRIX ELEMENTS          *30000070
C*          UNNORMALIZED BESES          *30000080
C*          INPUT DATA          *30000090
C*          NUCLEAR CHARGE ZA,ZB          *30000100
C*          MULTIPLICITY          *30000110
C*          NUMBER OF BASES          *30000120
C*          BASE (M,N,J,K,P)          *30000130
C*          0.LE.M,N,J,K.LE.6          *30000140
C*          0.LE.P.LE.3          *30000150
*****30000160
C*          IMPLICIT REAL*8(A-H,Q-Z)          30000170
C*          IMPLICIT INTEGER(I-P)          30000180
C*          LOGICAL HMPLR,TRPLT          30000190
C*          DIMENSION MM(160),NN(160),JJ(160),KK(160),PP(160),FF(720) 30000200
C*          COMMON /ZCD/ ZC(89718)          30000210
C*          COMMON /AZHT/ ALPHA,Z1,Z2,HMPLR,TRPLT          30000220
C*          III=720          30000230
C*          NBMAX=160          30000240
C*          MNMAX=6          30000250
C*          JKMAX=6          30000260
C*          PMAX=3          30000270
*****30000280
C***      INPUT          *****
READ(5,1000) ZA,ZB,MLTPLT,NBases,          30000290
2      (MM(I),NN(I),JJ(I),KK(I),PP(I),I=1,NBases)          30000300
Z1=(ZA+ZB)*0.5D0          30000310
Z2=(ZA-ZB)*0.5D0          30000320
HMPLR=Z2.EQ.0.D0          30000330
TRPLT=MLTPLT.EQ.3          30000340
IF(NBases.GT.NBMAX) GO TO 70          30000350
DO 20 I=1,NBases          30000360
IF(MM(I)-NN(I)) 3,1,5          30000370
1      IF(JJ(I)-KK(I)) 4,2,5          30000380
2      IF(TRPLT) GO TO 70          30000390
      GO TO 5          30000400
3      J=MM(I)          30000410
      MM(I)=NN(I)          30000420
      NN(I)=J          30000430
4      J=JJ(I)          30000440
      JJ(I)=KK(I)          30000450

```

APPENDIX C LISTS OF PROGRAMS (1i)

```

      KK(I)=J          30000460
  5 IF((NN(I).LT.0).OR.(MM(I).GT.MNMAX)) GO TO 70 30000470
  IF((KK(I).LT.0).OR.(JJ(I).GT.JKMAX)) GO TO 70 30000480
  IF((PP(I).LT.0).OR.(PP(I).GT.PMAX)) GO TO 70 30000490
  J=0          30000500
  10 J=J+1          30000510
  IF(J.EQ.1) GO TO 20 30000520
  IF((MM(I).EQ.MM(J)).AND.(NN(I).EQ.NN(J)).AND.(JJ(I).EQ.JJ(J))
  2 .AND.(KK(I).EQ.KK(J)).AND.(PP(I).EQ.PP(J))) GO TO 70 30000530
  GO TO 10          30000540
  20 CONTINUE          30000550
C***** INPUT FROM THE FILE 21 ****30000560
  READ(21) FF          30000570
  ALPHA=FF(1)
  WRITE(6,2000) ALPHA,ZA,ZB,MLTPLT,NBASES,
  2 (I,MM(I),NN(I),JJ(I),KK(I),PP(I),I=1,NBASES) 30000580
  J=1          30000590
  DO 40 I=1,89718 30000600
  J=J+1          30000610
  IF(J.LE.III) GO TO 30 30000620
  READ(21) FF          30000630
  J=1          30000640
  30 Z0(I)=FF(J)          30000650
  40 CONTINUE          30000660
C***** CALCULATION OF MATRIX ELEMENTS AND OUTPUT TO THE FILE 22. *30000700
  WRITE(22) ALPHA,ZA,ZB,MLTPLT,NBASES,MM,NN,JJ,KK,PP
  L=-2          30000710
  DO 60 J=1,NBASES 30000720
  MB=MM(J)          30000730
  NB=NN(J)          30000740
  JB=JJ(J)          30000750
  KB=KK(J)          30000760
  PB=PP(J)          30000770
  DO 60 I=1,J 30000780
  MA=MM(I)
  NA=NN(I)
  JA=JJ(I)
  KA=KK(I)
  PA=PP(I)
  L=L+3          30000790
  IF(L.LE.III) GO TO 50 30000800
  WRITE(22) FF          30000810
  L=1          30000820
  50 FF(L)=SSS(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB) 30000830
  FF(L+1)=TTT(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB) 30000840
  FF(L+2)=UUU(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB) 30000850
  60 CONTINUE          30000860
  WRITE(22) FF          30000870
  GO TO 80          30000880
  70 WRITE(6,3000) NBASES,(MM(I),NN(I),JJ(I),KK(I),PP(I),I=1,NBASES) 30000890
  80 WRITE(6,4000)          30000900
  STOP          30000910
  1000 FORMAT(2D10.0,I5,/I5,/(5I5))          30000920
  2000 FORMAT(1H1,10X,'CALCULATION OF MATRIX ELEMENTS', 30000930
  2 //16X,'ALPHA =',F10.5,          30000940
  3 //16X,'THE CHARGE OF THE NUCLEUS A',F10.2,          30000950
  4 //16X,'THE CHARGE OF THE NUCLEUS B',F10.2,          30000960
  5 //16X,'MULTIPLICITY',I10,          30000970
  6 //16X,'NUMBER OF BASES',I10,          30000980
  7 //21X,'NUMBER M N J K P',/(21X,I5,1X,5I4))          30000990
  3000 FORMAT(1H0,10X,'ERROR IN BASES',/11X,I5,/(11X,5I5)) 30001000
  4000 FORMAT(1H1)          30001010
  END          30001020
  REAL FUNCTION SSS*(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB) 30001030
  IMPLICIT REAL *8 (A-H,Q-Z)          30001040
  IMPLICIT INTEGER (I-P)          30001050
  LOGICAL HMPLR,TRPLT          30001060
  COMMON /AZHT/ALPHA,Z1,Z2,HMPLR,TRPLT          30001070
  SSS=SS(MA,NA,JA,KA,PA,NB,MB,KB,JB,PB)          30001080
  IF(TRPLT) SSS=-SSS          30001090
  SSS=SS(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)+SSS          30001100
  GO TO 10          30001110
  ENTRY TTT(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)          30001120
  SSS=TT(MA,NA,JA,KA,PA,NB,MB,KB,JB,PB)          30001130
  IF(TRPLT) SSS=-SSS          30001140
  30001150
  30001160
  30001170
  30001180
  30001190
  30001200

```

APPENDIX C LISTS OF PROGRAMS (12)

```

SSS=TT(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)+SSS      30001210
GO TO 10                                         30001220
ENTRY UUU(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)       30001230
SSS=U1(MA,NA,JA,KA,PA,NB,MB,KB,JB,PB)          30001240
IF(TRPLT) SSS=-SSS                               30001250
SSS=Z1*(U1(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)+SSS) 30001260
A=U3(MA,NA,JA,KA,PA,NB,MB,KB,JB,PB)           30001270
IF(TRPLT) A=-A                                 30001280
SSS=SSS+(U3(MA,NA,JA,KA,PA,MR,NB,JB,KB,PB)+A) 30001290
IF(HMPLR) GO TO 10                            30001300
A=U2(MA,NA,JA,KA,PA,NB,MB,KB,JB,PB)           30001310
IF(TRPLT) A=-A                                 30001320
SSS=SSS+Z2*(U2(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)+A) 30001330
10 RETURN                                         30001340
END                                              30001350
REAL FUNCTION SS*8(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB) 30001360
IMPLICIT REAL*8(A-H,Q-Z)                         30001370
IMPLICIT INTEGER(I-P)                           30001380
LOGICAL HMPLR,TRPLT                           30001390
COMMON /AZHT/ALPHA,Z1,Z2,HMPLR,TRPLT            30001400
I=1                                              30001410
GO TO 10                                         30001420
ENTRY TT(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)       30001430
I=2                                              30001440
GO TO 10                                         30001450
ENTRY U1(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)       30001460
I=3                                              30001470
GO TO 10                                         30001480
ENTRY U2(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)       30001490
I=4                                              30001500
GO TO 10                                         30001510
ENTRY U3(MA,NA,JA,KA,PA,MB,NB,JB,KB,PB)       30001520
I=5                                              30001530
10 MAB=MA+MB                                     30001540
NAB=NA+NAB                                     30001550
JAB=JA+JB                                      30001560
KAB=KA+KB                                      30001570
PAB=PA+PB                                      30001580
MABP2=MAB+2                                    30001590
NABP2=NAB+2                                    30001600
JABP2=JAB+2                                    30001610
KABP2=KAB+2                                    30001620
IF(I.GT.1) GO TO 20                           30001630
SS=      Z(MABP2,NABP2,JAB,KAB,PAB)-Z(MABP2,NAB,JAB,KABP2,PAB) 30001640
2      -Z(MAB,NABP2,JABP2,KAB,PAB)+Z(MAB,NAB,JABP2,KABP2,PAB) 30001650
GO TO 70                                         30001660
20 MABP1=MAB+1                                  30001670
NABP1=NAB+1                                  30001680
JABP1=JAB+1                                  30001690
KABP1=KAB+1                                  30001700
GO TO (70,30,40,50,60),I                      30001710
30 MABP4=MAB+4                                  30001720
NABP4=NAB+4                                  30001730
JABP4=JAB+4                                  30001740
KABP4=KAB+4                                  30001750
MABP3=MAB+3                                  30001760
NABP3=NAB+3                                  30001770
JABP3=JAB+3                                  30001780
KABP3=KAB+3                                  30001790
MABM1=MAB-1                                  30001800
NABM1=NAB-1                                  30001810
JABM1=JAB-1                                  30001820
KABM1=KAB-1                                  30001830
MABM2=MAB-2                                  30001840
NABM2=NAB-2                                  30001850
JABM2=JAB-2                                  30001860
KABM2=KAB-2                                  30001870
PABM2=PA2-2                                  30001880
MMAB=MA-MB                                     30001890
NNAB=NA-NB                                     30001900
JJAB=JA-JB                                     30001910
KKAB=KA-KB                                     30001920
PPAB=PA-PB                                     30001930
SS=-4.D0*ALPHA                                30001940
2      *(Z(MABP1,NABP2,JAB,KAB,PAB)-Z(MABP1,NAB,JAB,KABP2,PAB) 30001950

```

APPENDIX C LISTS OF PROGRAMS (13)

```

3      +Z(MABP2,NABP1,JAB,KAB,PAB)-Z(MAB,NABP1,JABP2,KAB,PAB)) 30001960
4      +DFLOAT(MMAB*MMAB+MAB-JJAB*JJAB-JAB+PPAB*(MMAB-JJAB)) 30001970
5      *(Z(MAB,NABP2,JAB,KAB,PAB)-Z(MAB,NAB,JAB,KABP2,PAB)) 30001980
6      +DFLOAT(NNAB*NNAB+NAB-KKAB*KKAB-KAB+PPAB*(NNAB-KKAB)) 30001990
7      *(Z(MABP2,NAB,JAB,KAB,PAB)-Z(MAB,NAB,JABP2,KAB,PAB)) 30002000
I=MMAB*MMAB-MAB
IF(I.NE.0) SS=SS-DFLOAT(I)
2      *(Z(MABM2,NABP2,JAB,KAB,PAB)-Z(MABM2,NAB,JAB,KABP2,PAB)) 30002030
I=NNAB*NNAB-NAB
IF(I.NE.0) SS=SS-DFLOAT(I)
2      *(Z(MABP2,NABM2,JAB,KAB,PAB)-Z(MAB,NABM2,JABP2,KAB,PAB)) 30002050
I=JJAB*JJAB-JAB
IF(I.NE.0) SS=SS+DFLOAT(I)
2      *(Z(MAB,NABP2,JABM2,KAB,PAB)-Z(MAB,NAB,JABM2,KABP2,PAB)) 30002070
I=KKAB*KKAB-KAB
IF(I.NE.0) SS=SS+DFLOAT(I)
2      *(Z(MABP2,NAB,JAB,KABM2,PAB)-Z(MAB,NAB,JABP2,KABM2,PAB)) 30002100
I=2*(PPAB*PPAB+PAB)+PPAB*(MMAB+NNAB+JJAB+KKAB)
IF(I.NE.0) SS=SS+DFLOAT(I)
2      *(Z(MABP2,NABP2,JAB,KAB,PABM2)-Z(MABP2,NAB,JAB,KABP2,PABM2)) 30002130
3      -Z(MAB,NABP2,JABP2,KAB,PABM2)+Z(MAB,NAB,JABP2,KABP2,PABM2)) 30002150
I=PPAB*(MMAB-JJAB)
IF(I.NE.0) SS=SS-DFLOAT(I)
2      *(Z(MAB,NABP4,JAB,KAB,PABM2)-Z(MAB,NAB,JABP4,KAB,PABM2)) 30002170
I=PPAB*(NNAB-KKAB)
IF(I.NE.0) SS=SS-DFLOAT(I)
2      *(Z(MABP4,NAB,JAB,KAB,PABM2)-Z(MAB,NAB,JABP4,KAB,PABM2)) 30002190
I=2*PPAB*MMAB
IF(I.NE.0) SS=SS+DFLOAT(I)
2      *(Z(MABM1,NABP3,JABP1,KABP1,PABM2)) 30002220
3      -Z(MABM1,NABP1,JABP1,KABP3,PABM2)) 30002240
I=2*PPAB*NNAB
IF(I.NE.0) SS=SS+DFLOAT(I)
2      *(Z(MABP3,NABM1,JABP1,KABP1,PABM2)) 30002250
3      -Z(MABP1,NABM1,JABP3,KABP1,PABM2)) 30002260
I=2*PPAB*JJAB
IF(I.NE.0) SS=SS-DFLOAT(I)
2      *(Z(MABP1,NABP3,JABM1,KABP1,PABM2)) 30002270
3      -Z(MABP1,NABP1,JABM1,KABP3,PABM2)) 30002280
I=2*PPAB*KKAB
IF(I.NE.0) SS=SS-DFLOAT(I)
2      *(Z(MABP3,NABP1,JABP1,KABM1,PABM2)) 30002300
3      -Z(MABP1,NABP1,JABP3,KABM1,PABM2)) 30002310
SS=-SS*0.5D0
GO TO 70
40 SS=-4.00
2      *(Z(MABP1,NABP2,JAB,KAB,PAB)-Z(MABP1,NAB,JAB,KABP2,PAB)) 30002320
3      +Z(MABP2,NABP1,JAB,KAB,PAB)-Z(MAB,NABP1,JABP2,KAB,PAB)) 30002330
GO TO 70
50 SS= 4.00
2      *(Z(MAB,NABP2,JABP1,KAB,PAB)-Z(MAB,NAB,JABP1,KABP2,PAB)) 30002340
3      +Z(MABP2,NAB,JAB,KABP1,PAB)-Z(MAB,NAB,JABP2,KABP1,PAB)) 30002350
GO TO 70
60 PABM1=PAB-1
SS=2.00
2      *(Z(MABP2,NABP2,JAB,KAB,PABM1)-Z(MABP2,NAB,JAB,KABP2,PABM1)) 30002360
3      -Z(MAB,NABP2,JABP2,KAB,PABM1)+Z(MAB,NAB,JABP2,KABP2,PABM1)) 30002370
70 RETURN
END
REAL FUNCTION Z*8(M,N,J,K,P)
IMPLICIT REAL*8(A-H,Q-Z)
IMPLICIT INTEGER(I-P)
COMMON /Z0D/Z0(89718)
DIMENSION L(8)
DATA L/1,12394,24787,37180,49573,61966,74359,82039/
IF((J+K).AND.1).NE.0) GO TO 60
IF(M.GT.N) GO TO 10
MM=N
NN=M
GO TO 20
10 MM=M
NN=N
20 IF(J.GT.K) GO TO 30
JJ=K
KK=J

```

APPENDIX C LISTS OF PROGRAMS (14)

```

GO TO 40                                30002710
30 JJ=J                                30002720
KK=K                                30002730
40 LL=153                                30002740
IF(P.GT.4) LL=120                      30002750
I=((JJ*(JJ+2)+KK*2)/4)*LL+MM*(MM+1)/2+NN+L(P+2) 30002760
Z=ZO(I)                                30002770
50 RETURN                                30002780
60 Z=0.00                                30002790
GO TO 50                                30002800
END                                     30002810

PROGRAM JC4                               40000010
C*****PROGRAM JC4                         40000020
C*      PROGRAM JC4                      *40000030
C*      TWO ELECTRON SYSTEM IN DIATOMIC MOLECULES  *40000040
C*      SIGMA PLUS STATE                  *40000050
C*      JAMES-COOLIDGE'S METHOD          *40000060
C*      NORMALIZATION AND REARRANGEMENT OF MATRIX ELEMENTS *40000070
C*      INPUT DATA                      *40000080
C*      PRINT                           *40000090
C*      PRINT OUT WHEN PRINT.NE.0       *40000100
C*****IMPLICIT REAL*8(A-H,Q-Z)           40000110
C*      IMPLICIT INTEGER(I-P)            40000120
C*      DIMENSION MM(160),NN(160),JJ(160),PP(160),FN(160), 40000130
2   S(12880),T(12880),U(12880),FF(720)    40000140
III=720                                 40000150
C*****INPUT                                40000160
READ(5,1000) PRINT                      40000170
C*****INPUT FROM THE FILE 22             40000180
READ(22) ALPHA,ZA,ZB,MLTPLT,NBASES,MM,NN,JJ,KK,PP 40000190
WRITE(6,2000) ALPHA,ZA,ZB,MLTPLT,NBASES, 40000200
2   (I,MM(I),NN(I),JJ(I),KK(I),PP(I),I=1,NBASES) 40000210
NMX=NBASES*(NBASES+1)/2                 40000220
J=III                                 40000230
DO 20 I=1,NMX                          40000240
J=J+3                                 40000250
IF(J.LE.III) GO TO 10                  40000260
READ(22) FF                           40000270
J=1                                 40000280
10 S(I)=FF(J)                         40000290
T(I)=FF(J+1)                         40000300
U(I)=FF(J+2)                         40000310
20 CONTINUE                            40000320
C*****NORMALIZATION                   40000330
DO 30 I=1,NBASES                      40000340
II=I*(I+1)/2                         40000350
FN(I)=1.00/DSQRT(S(II))              40000360
30 CONTINUE                            40000370
40000380
IJ=0                                 40000390
DO 40 J=1,NBASES                      40000400
DO 40 I=1,J                           40000410
IJ=IJ+1                             40000420
ANF=FN(I)*FN(J)                     40000430
S(IJ)=S(IJ)*ANF                      40000440
T(IJ)=T(IJ)*ANF                      40000450
U(IJ)=U(IJ)*ANF                      40000460
40 CONTINUE                            40000470
C*****OUTPUT TO THE FILE 23            40000480
WRITE(23) ALPHA,ZA,ZB,MLTPLT,NBASES,MM,NN,JJ,KK,PP 40000490
J=0                                 40000500
DO 60 I=1,NMX                          40000510
J=J+1                               40000520
IF(J.LE.III) GO TO 50                  40000530
WRITE(23) FF                           40000540
J=1                                 40000550
50 FF(J)=S(I)                         40000560
60 CONTINUE                            40000570
WRITE(23) FF                           40000580
J=0                                 40000590
DO 80 I=1,NMX                          40000600
J=J+1                               40000610
IF(J.LE.III) GO TO 70                  40000620

```

APPENDIX C LISTS OF PROGRAMS (15)

```

      WRITE(23) FF          40000630
      J=1                  40000640
  70  FF(J)=T(I)          40000650
  80  CONTINUE            40000660
      WRITE(23) FF          40000670
      J=0                  40000680
      DO 100 I=1,NMX       40000690
      J=J+1                40000700
      IF(J.LE.III) GO TO 90 40000710
      WRITE(23) FF          40000720
      J=1                  40000730
  90  FF(J)=U(I)          40000740
 100  CONTINUE            40000750
      WRITE(23) FF          40000760
      IF(PRINT.EQ.0) GO TO 120 40000770
      WRITE(6,3000)          40000780
      IJ=0                  40000790
      DO 110 J=1,NBases    40000800
      DO 110 I=1,J          40000810
      IJ=IJ+1                40000820
      WRITE(6,4000) I,J,S(IJ),T(IJ),U(IJ) 40000830
 110  CONTINUE            40000840
      WRITE(6,5000)          40000850
 120  STOP                40000860
 1000 FORMAT(I5)          40000870
 2000 FORMAT(1H1,10X,'NORMALIZATION AND REARRANGEMENT OF MATRIX ELEMENTS' 40000880
 2'',//16X,'ALPHA =',F10.5,          40000890
 3   '//16X,'THE CHARGE OF THE NUCLEUS A',F10.2,          40000900
 4   '//16X,'THE CHARGE OF THE NUCLEUS B',F10.2,          40000910
 5   '//16X,'MULTIPLICITY',I10,          40000920
 6   '//16X,'NUMBER OF BASES',I10,          40000930
 7   '//21X,'NUMBER M N J K P',(21X,15,1X,5I4))        40000940
 3000 FORMAT(1H1,15X,' I J',11X,'S(I,J)',14X,'T(I,J)',14X,'U(I,J)') 40000950
 4000 FORMAT(16X,214,3F20.10)          40000960
 5000 FORMAT(1H1)              40000970
      END                  40000980

      PROGRAM JC5          50000010
C*****PROGRAM JC5          50000020
C*      PROGRAM JC5          *50000030
C*      TWO ELECTRON SYSTEM IN DIATOMIC MOLECULES          *50000040
C*      SIGMA PLUS STATE          *50000050
C*      JAMES-COOLIDGE'S METHOD          *50000060
C*      SCHUMIDT'S ORTHONORMALIZATION          *50000070
C*      AND TRANSFORMATION OF MATRIX ELEMENTS          *50000080
C*      INPUT DATA          *50000090
C*      NBS(I)          *50000100
C*      TAKE IN THE BASE I WHEN NBS(I)=1          *50000110
C*****INPUT          50000120
      IMPLICIT REAL *16 (A-H,Q-Z)          50000130
      IMPLICIT INTEGER (I-P)          50000140
      DIMENSION MM(160),NN(160),JJ(160),KK(160),PP(160),NBS(160), 50000150
      2   A(12880),WW(160,160)          50000160
      REAL *8 S(12880),T(12880),U(12880),TA(12880),UA(12880),FF(720), 50000170
      2   ALPHA,ZA,ZB          50000180
      EQUIVALENCE (S(1),T(1),U(1)),(TA(1),UA(1),FF(1)) 50000190
      III=720          50000200
C***      INPUT          *****50000210
      READ(5,1000) NBS          50000220
C***      INPUT FROM THE FILE 23          *****50000230
      READ(23) ALPHA,ZA,ZB,MLTPLT,NBases,MM,NN,JJ,KK,PP 50000240
      NBSoLD=Nbases          50000250
      NMxOLD=Nbases*(nbases+1)/2          50000260
      I=0          50000270
      DO 10 J=1,NBSoLD          50000280
      IF(NBS(J).LE.0) GO TO 10          50000290
      I=I+1          50000300
      MM(I)=MM(J)          50000310
      NN(I)=NN(J)          50000320
      JJ(I)=JJ(J)          50000330
      KK(I)=KK(J)          50000340
      PP(I)=PP(J)          50000350
  10  CONTINUE            50000360
      NBases=I          50000370

```

APPENDIX C LISTS OF PROGRAMS (16)

```

NMX=NBASES*(NBASES+1)/2                                50000380
WRITE(6,2000) ALPHA,ZA,ZB,MLTPLT,NBASES,                50000390
2      (I,MM(I),NN(I),JJ(I),KK(I),PP(I),I=1,NBASES)    50000400
***** INPUT OF S ***** ***** ***** ***** ***** ***** 50000410
J=III                                                    50000420
DO 30 I=1,NMXOLD                                      50000430
J=J+1                                                    50000440
IF(J.LE.III) GO TO 20                                  50000450
READ(23) FF                                            50000460
J=1                                                    50000470
20 S(I)=FF(J)                                         50000480
30 CONTINUE                                              50000490
I=0                                                    50000500
J=0                                                    50000510
DO 40 L=1,NBSOLD                                      50000520
DO 40 K=1,L                                           50000530
J=J+1                                                    50000540
IF((NBS(K).LE.0).OR.(NBS(L).LE.0)) GO TO 40        50000550
I=I+1                                                    50000560
S(I)=S(J)                                              50000570
40 CONTINUE                                              50000580
***** SCHUMIDT'S ORTHONORMALIZATION ***** ***** ***** 50000590
DO 50 I=1,NMX                                         50000600
A(I)=0.Q0                                              50000610
50 CONTINUE                                              50000620
A(1)=1.Q0                                              50000630
DO 90 I=2,NBASES                                      50000640
IIM1=I*(I-1)/2                                         50000650
II=IIM1+I                                             50000660
A(II)=1.Q0                                              50000670
DO 70 J=1,I-1                                         50000680
JJM1=J*(J-1)/2                                         50000690
SS=0.Q0                                              50000700
DO 60 K=1,J                                           50000710
KI=IIM1+K                                             50000720
KJ=JJM1+K                                             50000730
SS=SS+A(KJ)*S(KI)                                     50000740
60 CONTINUE                                              50000750
DO 70 K=1,J                                           50000760
KI=IIM1+K                                             50000770
KJ=JJM1+K                                             50000780
A(KI)=A(KI)-SS*A(KJ)                                 50000790
70 CONTINUE                                              50000800
SS=0.Q0                                              50000810
KJ=0                                                    50000820
DO 80 J=1;I                                         50000830
JI=IIM1+J                                             50000840
DO 80 K=1,J                                           50000850
KJ=KJ+1                                              50000860
KI=IIM1+K                                             50000870
W=A(KI)*A(JI)*S(KJ)                                 50000880
IF(K.NE.J) W=W+W                                     50000890
SS=SS+*W                                              50000900
80 CONTINUE                                              50000910
W=1.Q0/WSQRT(SS)                                     50000920
DO 90 J=1,1                                         50000930
JI=IIM1+J                                             50000940
A(JI)=A(JI)*W                                     50000950
90 CONTINUE                                              50000960
***** OUTPUT TO THE FILE 24 ***** ***** ***** ***** 50000970
WRITE(24) ALPHA,ZA,ZB,MLTPLT,NBASES,MM,NN,JJ,KK,PP   50000980
J=0                                                    50000990
DO 110 I=1,NMX                                      50001000
J=J+1                                                    50001010
IF(J.LE.III) GO TO 100                               50001020
WRITE(24) FF                                            50001030
J=1                                                    50001040
100 FF(J)=A(I)                                         50001050
110 CONTINUE                                              50001060
WRITE(24) FF                                            50001070
***** INPUT OF T ***** ***** ***** ***** ***** ***** 50001080
J=III                                                    50001090
DO 130 I=1,NMXOLD                                      50001100
J=J+1                                                    50001110
IF(J.LE.III) GO TO 120                               50001120

```

APPENDIX C LISTS OF PROGRAMS (17)

```

READ(23) FF
J=1
120 T(I)=FF(J)
130 CONTINUE
I=0
J=0
DO 140 L=1,NBSOLD
DO 140 K=1,L
J=J+1
IF((NBS(K).LE.0).OR.(NBS(L).LE.0)) GO TO 140
I=I+1
T(I)=T(J)
140 CONTINUE
C***** TRANSFORMATION OF T *****
DO 180 I=1,NBASES
IIM1=I*(I-1)/2
DO 180 J=1,NBASES
W=0.Q0
DO 170 K=1,I
KI=IIM1+K
IF(K.GT.J) GO TO 150
KJ=JK*(J-1)/2+K
GO TO 160
150 KJ=K*(K-1)/2+J
160 W=W+A(KI)*T(KJ)
170 CONTINUE
WW(I,J)=W
180 CONTINUE
IJ=0
DO 200 J=1,NBASES
DO 200 I=1,J
IIM1=I*(I-1)/2
IJ=IJ+1
W=0.Q0
DO 190 K=1,I
KI=IIM1+K
W=W+A(KI)*WW(J,K)
190 CONTINUE
TA(IJ)=W
200 CONTINUE
C***** OUTPUT TO THE FILE 24 *****
J=0
DO 220 I=1,NMX
J=J+1
IF(J.LE.III) GO TO 210
WRITE(24) FF
J=1
210 FF(J)=TA(I)
220 CONTINUE
WRITE(24) FF
C***** INPUT OF U *****
J=III
DO 240 I=1,NMXOLD
J=J+1
IF(J.LE.III) GO TO 230
READ(23) FF
J=1
230 U(I)=FF(J)
240 CONTINUE
I=0
J=0
DO 250 L=1,NBSOLD
DO 250 K=1,L
J=J+1
IF((NBS(K).LE.0).OR.(NBS(L).LE.0)) GO TO 250
I=I+1
U(I)=U(J)
250 CONTINUE
C***** TRANSFORMATION OF U *****
DO 290 I=1,NBASES
IIM1=I*(I-1)/2
DO 290 J=1,NBASES
W=0.Q0
DO 280 K=1,I
KI=IIM1+K

```

50001130
50001140
50001150
50001160
50001170
50001180
50001190
50001200
50001210
50001220
50001230
50001240
50001250
50001260
50001270
50001280
50001290
50001300
50001310
50001320
50001330
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50001370
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50001390
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50001780
50001790
50001800
50001810
50001820
50001830
50001840
50001850
50001860
50001870

APPENDIX C LISTS OF PROGRAMS (18)

```

IF(K.GT.J) GO TO 260      50001880
KJ=J*(J-1)/2+K            50001890
GO TO 270                50001900
260 KJ=K*(K-1)/2+J        50001910
270 W=W+A(KJ)*U(KJ)       50001920
280 CONTINUE                50001930
WW(I,J)=W                50001940
290 CONTINUE                50001950
IJ=0                      50001960
DO 310 J=1,NBASES         50001970
DO 310 I=1,J              50001980
IIM1=I*(I-1)/2            50001990
IJ=IJ+1                  50002000
W=0.Q0                    50002010
DO 300 K=1,I              50002020
KI=IIM1*K                50002030
W=W+A(KI)*NW(J,K)        50002040
300 CONTINUE                50002050
UA(IJ)=W                50002060
310 CONTINUE                50002070
***** OUTPUT TO THE FILE 24 ***** 50002080
J=0                      50002090
DO 330 I=1,NMX            50002100
J=J+1                    50002110
IF(J.LE.III) GO TO 320    50002120
WRITE(24) FF              50002130
J=1                      50002140
320 FF(J)=UA(I)          50002150
330 CONTINUE                50002160
WRITE(24) FF              50002170
WRITE(6,3000)              50002180
STOP                      50002190
1000 FORMAT(80I1)          50002200
2000 FORMAT(1H1,10X,'SCHUMIDT''S ORTHONORMALIZATION AND TRANSFORMATION' 50002210
20F MATRIX ELEMENTS',//16X,'ALPHA =',F10.5,                         50002220
3 //16X,'THE CHARGE OF THE NUCLEUS A',F10.2,                         50002230
4 //16X,'THE CHARGE OF THE NUCLEUS B',F10.2,                         50002240
5 //16X,'MULTIPLICITY',I10,                                         50002250
6 //16X,'NUMBER OF BASES',I10,                                         50002260
7 //21X,'NUMBER M N J K P',(21X,I5,1X,5I4))                         50002270
3000 FORMAT(1H1)             50002280
END                      50002290

```

```

PROGRAM JC6               60000010
***** ***** ***** ***** ***** ***** 60000020
C* PROGRAM JC6             *60000030
C* TWO ELECTRON SYSTEM IN DIATOMIC MOLECULES *60000040
C* SIGMA PLUS STATE           *60000050
C* JAMES-COOLIDGE'S METHOD   *60000060
C* CALCULATION OF ENERGIES AND WAVE FUNCTIONS *60000070
C* INPUT DATA                 *60000080
C* PRINT                      *60000090
C* PRINT OUT THE COEFFICIENTS OF THE ORTHONORMALIZED *60000100
C* BASES WHEN PRINT.NE.0     *60000110
C* INTERNUCLEAR DISTANCE     *60000120
C* NUMBER OF THE STATE       *60000130
***** ***** ***** ***** ***** 60000140
IMPLICIT REAL *16 (A-H,Q-Z) 60000150
IMPLICIT INTEGER (I-P)      60000160
REAL *8 A(12880),TA(12880),UA(12880),FF(720), 60000170
2 ALPHA,ZA,ZB,R,RR          60000180
DIMENSION MM(160),NN(160),JJ(160),KK(160),PP(160),X(160),Y(160), 60000190
2 HH(160,160)                60000200
III=720                     60000210
***** INPUT ***** 60000220
READ(5,1000) PRINT          60000230
***** INPUT FROM THE FILE 24 ***** 60000240
READ(24) ALPHA,ZA,ZB,MLTPLT,NBASES,MM,NN,JJ,KK,PP 60000250
NMX=NBASES*(NBASES+1)/2      60000260
J=III                      60000270
DO 20 I=1,NMX                60000280
J=J+1                      60000290
IF(J.LE.III) GO TO 10        60000300
READ(24) FF                  60000310

```

APPENDIX C LISTS OF PROGRAMS (19)

```

J=1                               60000320
10 A(I)=FF(J)                   60000330
20 CONTINUE                      60000340
J=III                            60000350
DO 40 I=1,NMX                   60000360
J=J+1                            60000370
IF(J.LE.III) GO TO 30           60000380
READ(24) FF                      60000390
J=1                               60000400
30 TA(I)=FF(J)                  60000410
40 CONTINUE                      60000420
J=III                            60000430
DO 60 I=1,NMX                   60000440
J=J+1                            60000450
IF(J.LE.III) GO TO 50           60000460
READ(24) FF                      60000470
J=1                               60000480
50 UA(I)=FF(J)                  60000490
60 CONTINUE                      60000500
WRITE(6,2000) ALPHA,ZA,ZB,MLTPLT,NBASES,
2                                (I,MM(I),NN(I),JJ(I),KK(I),PP(I),I=1,NBASES) 60000510
IF(PRINT.EQ.0) GO TO 80          60000520
WRITE(6,3000)
L=0                               60000530
DO 70 I=1,NBASES                60000540
K=L+1                            60000550
L=L+1                            60000560
WRITE(6,4000) I,(A(J),J=K,L)    60000570
70 CONTINUE                      60000580
***** CALCULATION OF TOTAL ENERGY *****60000610
80 READ(5,5000,END=130) R,NSTATE
RR=R*R
K=0                               60000620
DO 90 J=1,NBASES                60000630
DO 90 I=1,J
K=K+1                            60000640
HH(I,J)=TA(K)/RR+UA(K)/R      60000650
HH(J,I)=HH(I,J)                 60000660
90 CONTINUE                      60000670
CALL SQEQ(NBASES,HH,NSTATE,ENERGY) 60000680
K=0                               60000690
DO 100 J=1,NBASES               60000700
DO 100 I=1,J
K=K+1                            60000710
HH(I,J)=TA(K)/RR+UA(K)/R      60000720
HH(J,I)=HH(I,J)                 60000730
100 CONTINUE                     60000740
CALL VECTOR(NBASES,HH,ENERGY,X) 60000750
TTLENR=ENERGY+ZA*ZB/R          60000760
IF(PRINT.NE.0) WRITE(6,6000) (I,X(I),I=1,NBASES) 60000770
DO 120 I=1,NBASES               60000780
W=0.Q0
DO 110 J=1,NBASES               60000790
K=J*(J-1)/2+I                  60000800
W=W+X(J)*A(K)                  60000810
110 CONTINUE                     60000820
Y(I)=W                          60000830
120 CONTINUE                     60000840
WRITE(6,7000) ALPHA,ZA,ZB,MLTPLT,R,NSTATE,NBASES,TTLENR,
2                                (I,MM(I),NN(I),JJ(I),KK(I),PP(I),Y(I),I=1,NBASES) 60000850
GO TO 80                         60000860
130 WRITE(6,8000)
STOP                            60000870
1000 FORMAT(I5)                  60000880
2000 FORMAT(1H1,10X,'CALCULATION OF ENERGIES AND WAVE FUNCTIONS',
2      //16X,'ALPHA =',F10.5,       60000890
3      //16X,'THE CHARGE OF THE NUCLEUS A ',F10.2,       60000900
4      //16X,'THE CHARGE OF THE NUCLEUS B ',F10.2,       60000910
5      //16X,'MULTIPLICITY',I10,        60000920
6      //16X,'NUMBER OF BASES',I10,        60000930
7      //21X,'NUMBER M N J K P',/(21X,I5,1X,5I4))        60000940
3000 FORMAT(1H1,10X,'ORTHONORMALIZED BASES BY SCHMITZ''S METHOD',
2      //11X,'NUMBER',10X,'COEFFICIENTS')                 60000950
4000 FORMAT(//11X,I5,6X,5D20.10,/(22X,5D20.10))        60000960
5000 FORMAT(D20.0,I5)             60000970

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APPENDIX C LISTS OF PROGRAMS (20)

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6000 FORMAT(1H1,10X,'THE WAVE FUNCTION',          60001070
2    //11X,'ORTHONORMALIZED BASES BY SCHUMIDT''S METHOD', 60001080
3    //11X,'NUMBER',10X,'COEFFICIENT',/(11X,I5,6X,D20.10)) 60001090
7000 FORMAT(1H1,10X,'ALPHA =',F10.5,           60001100
2    //11X,'THE CHARGE OF THE NUCLEUS A',F10.2,        60001110
3    //11X,'THE CHARGE OF THE NUCLEUS B',F10.2,        60001120
4    //11X,'MULTIPLICITY' I10,                      60001130
5    //11X,'INTERNUCLEAR DISTANCE',F10.5,          60001140
6    //11X,'THE',I3,'TH STATE',                   60001150
7    //11X,'NUMBER OF BASES',I10,                  60001160
8    //11X,'TOTAL ENERGY',F15.10,                 60001170
9    //11X,'THE WAVE FUNCTION',                   60001180
9    /11X,'NUMBER M N J K P ',10X,'COEFFICIENT',   60001190
9    /(11X,I5,4X,5I3,5X,D20.10))                60001200
8000 FORMAT(1H1)                                60001210
END
SUBROUTINE SSEQ(NN,A,NSTATE,EE)                 60001220
IMPLICIT REAL *16 (A-H,O-Z)                   60001230
DIMENSION A(160,160),P(160),U(160)            60001240
COMMON /QSQD/AA(160),BB(160),E,DET,N,ND      60001250
EQUIVALENCE (P(1),AA(1)),(U(1),BB(1))        60001260
N=NN
NM1=N-1
NM2=N-2
DO 90 K=1,NM2                               60001270
KP1=K+1
DO 10 I=KP1,N
U(I)=A(K,I)
10 CONTINUE
W=0.Q0
DO 20 I=KP1,N
W=W+U(I)*X2
20 CONTINUE
S=SQRT(W)
IF(U(KP1).GT.0.D0) S=-S
UUD2=W-U(KP1)*S
U(KP1)=U(KP1)-S
DO 50 I=KP1,N
W=0.Q0
DO 40 J=KP1,N
W=W+A(I,J)*U(J)
P(I)=W/UUD2
40 CONTINUE
50 CONTINUE
W=0.Q0
DO 60 I=KP1,N
W=W+U(I)*P(I)
60 CONTINUE
W=W/(UUD2+UUD2)
DO 70 I=KP1,N
P(I)=P(I)-W*U(I)
70 CONTINUE
DO 80 J=KP1,N
DO 80 I=KP1,J
A(I,J)=A(I,J)-U(I)*P(J)-P(I)*U(J)
A(J,I)=A(I,J)
80 CONTINUE
BB(KP1)=S
90 CONTINUE
DO 100 I=1,N
AA(I)=A(I,I)
100 CONTINUE
RB(N)=A(N-1,N)
EMIN=-(QABS(AA(1))+QABS(BB(2)))
DO 110 I=2,NM1
W=-(QABS(AA(I))+QABS(BB(I))+QABS(BB(I+1)))
IF(EMIN.LT.W) GO TO 110
EMIN=W
110 CONTINUE
W=-(QABS(AA(N))+QABS(BB(N)))
IF(EMIN.GT.W) EMIN=W
E=EMIN
CALL SQSUB
IF(DET.EQ.0.Q0) GO TO 170
NDS=ND-NSTATE
DELTA=QABS(EMIN)*0.3Q0

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APPENDIX C LISTS OF PROGRAMS (21)

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120 E=E+DELTA          60001820
CALL SQSUB             60001830
IF(DET.EQ.0.Q0) GO TO 170 60001840
IF(NDS-ND) 120,140,130 60001850
130 E=E-DELTA          60001860
DELTA=DELTA*0.5Q0       60001870
GO TO 120              60001880
140 ISND=ISN(DET)      60001890
150 EE=E                60001900
160 DELTA=DELTA*0.5Q0   60001910
E=EE-DELTA             60001920
IF(QABS(E-EE).LT.0.5Q-10) GO TO 170 60001930
CALL SQSUB             60001940
IF(ISN(DET)*ISND) 160,170,150 60001950
170 EE=E                60001960
RETURN                60001970
END                   60001980
SUBROUTINE SQSUB        60001990
IMPLICIT REAL *16 (A-H,O-Z) 60002000
COMMON /QSQD/AA(160),BB(160),E,DET,N,ND 60002010
ND=0                  60002020
IDFX=0                60002030
D2=1.Q0               60002040
DET=E-AA(1)            60002050
ISND=ISN(DET)          60002060
IF(ISND.LT.0) ND=1     60002070
DO 30 K=2,N             60002080
D1=D2                 60002090
D2=DET                60002100
IF(ISND.NE.0) ISN2=ISND 60002110
DET=(E-AA(K))*D2-BB(K)**2*D1 60002120
ISND=ISN(DET)          60002130
ADET=QABS(DET)         60002140
IF(ADET.LT.1.Q10) GO TO 10 60002150
D2=D2*1.Q-10           60002160
DET=DET*1.Q-10         60002170
IDFX=IDFX+10           60002180
GO TO 20               60002190
10 IF(ADET.GT.1.Q-10) GO TO 20 60002200
D2=D2*1.Q10             60002210
DET=DET*1.Q10           60002220
IDFX=IDFX-10           60002230
20 IF(ISND*ISN2.LT.0) ND=ND+1 60002240
30 CONTINUE              60002250
RETURN                60002260
END                   60002270
FUNCTION ISN(X)         60002280
IMPLICIT REAL *16 (A-H,O-Z) 60002290
IF(X) 10,20,30          60002300
10 ISN=-1               60002310
GO TO 40               60002320
20 ISN=0                60002330
GO TO 40               60002340
30 ISN=1                60002350
40 RETURN                60002360
END                   60002370
SUBROUTINE VECTOR(N,A,E,X) 60002380
IMPLICIT REAL *16 (A-H,O-Z) 60002390
DIMENSION A(160,160),X(160) 60002400
NM1=N-1                60002410
J=1                   60002420
A(1,1)=A(1,1)-E       60002430
W=QABS(A(1,1))         60002440
DO 10 I=2,N             60002450
A(I,I)=A(I,I)-E       60002460
Y=QABS(A(I,I))         60002470
IF(Y.GE.W) GO TO 10    60002480
J=I                   60002490
W=Y                   60002500
10 CONTINUE              60002510
DO 20 I=1,N             60002520
W=A(I,J)               60002530
A(I,J)=A(I,N)           60002540
A(I,N)=-W               60002550
20 CONTINUE              60002560

```

APPENDIX C LISTS OF PROGRAMS (22)

```

CALL CPLNEQ(NM1,N,A)          60002570
DO 30 I=1,NM1                60002580
X(I)=A(I,N)                  60002590
30 CONTINUE                   60002600
X(N)=X(J)                    60002610
X(J)=1.Q0                     60002620
W=0.Q0                       60002630
DO 40 I=1,N                  60002640
W=W+X(I)**2                  60002650
40 CONTINUE                   60002660
W=1.Q0/QSQRT(W)              60002670
DO 50 I=1,N                  60002680
X(I)=X(I)*W                  60002690
50 CONTINUE                   60002700
RETURN                        60002710
END                           60002720
SUBROUTINE CPLNEQ(M,N,A)      60002730
DIMENSION A(160,160)           60002740
IMPLICIT REAL *16 (A-H,O-Z)   60002750
DO 60 K=1,M                  60002760
L=0                           60002770
W=0.Q0                       60002780
DO 10 I=K,M                  60002790
Y=QABS(A(I,K))               60002800
IF(Y.LE.W) GO TO 10          60002810
L=I                           60002820
W=Y                           60002830
10 CONTINUE                   60002840
IF(L.EQ.K) GO TO 30          60002850
DO 20 J=K,N                  60002860
W=A(K,J)                     60002870
A(K,J)=A(L,J)                60002880
A(L,J)=W                     60002890
20 CONTINUE                   60002900
30 W=1.Q0*A(K,K)             60002910
DO 40 J=K,N                  60002920
A(K,J)=A(K,J)*W              60002930
40 CONTINUE                   60002940
DO 60 I=1,M                  60002950
IF(I.EQ.K) GO TO 60          60002960
W=A(I,K)                     60002970
DO 50 J=K,N                  60002980
A(I,J)=A(I,J)-A(K,J)*W     60002990
50 CONTINUE                   60003000
60 CONTINUE                   60003010
RETURN                        60003020
END                           60003030

```

```

PROGRAM JC7                      70000010
C*****PROGRAM JC7                70000020
C*      PROGRAM JC7                *70000030
C*      TWO ELECTRON SYSTEM IN DIATOMIC MOLECULES  *7.0000040
C*      SIGMA PLUS STATE          *70000050
C*      JAMES-COOLIDGE'S METHOD   *70000060
C*      SCHUMIDT'S ORTHONORMALIZATION AND PRINTING OUT *70000070
C*      THE MATRIX ELEMENTS      *70000080
C*      INPUT DATA               *70000090
C*      PRINT                     *70000100
C*      PRINT OUT THE MATRIX ELEMENTS WHEN P.NE.0    *70000110
C*      INTERNUCLEAR DISTANCE    *70000120
C*****                                70000130
C*      IMPLICIT REAL *16 (A-H,Q-Z)    70000140
C*      IMPLICIT INTEGER(I-P)        70000150
C*      DIMENSION MM(160),NN(160),JJ(160),KK(160),PP(160), 70000160
C*      2    A(12880),WW(160,160)       70000170
C*      REAL *8 S(12880),T(12880),U(12880),H(12880),HA(12880),FF(720), 70000180
C*      2    ALPHA,ZA,ZB,R            70000190
C*      EQUIVALENCE (S(1),H(1)),(T(1),HA(1)),(FF(1),A(1)) 70000200
C*      III=720                     70000210
C*      SERR=1.Q-6                  70000220
C*****      INPUT                 70000230
C*****      READ(5,1000) PRINT,R    70000240
C*****      INPUT FROM THE FILE 23 70000250
C*****      READ(23) ALPHA,ZA,ZB,MLTPLT,NBASES,MM,NN,JJ,KK,PP 70000260

```

APPENDIX C LISTS OF PROGRAMS (23)

```

NMX=NBASES*(NBASES+1)/2
J=III
DO 20 I=1,NMX
J=J+1
IF(J.LE.III) GO TO 10
READ(23) FF
J=1
10 S(I)=FF(J)
20 CONTINUE
J=III
DO 40 I=1,NMX
J=J+1
IF(J.LE.III) GO TO 30
READ(23) FF
J=1
30 T(I)=FF(J)
40 CONTINUE
J=III
DO 60 I=1,NMX
J=J+1
IF(J.LE.III) GO TO 50
READ(23) FF
J=1
50 U(I)=FF(J)
60 CONTINUE
C***** SCHMIDT'S ORTHONORMALIZATION *****
      WRITE(6,2000)
      DO 70 I=1,NMX
      A(I)=0.Q0
70 CONTINUE
      A(1)=1.Q0
      DO 130 I=2,NBASES
      IIM1=I*(I-1)/2
      II=IIM1+I
      A(II)=1.Q0
      SSS=1.Q0
      DO 90 J=1,I-1
      JJM1=J*(J-1)/2
      SS=0.Q0
      DO 80 K=1,J
      KI=IIM1+K
      KJ=JJM1+K
      SS=SS+A(KJ)*S(KI)
80 CONTINUE
      SSS=SSS-SS*SS
      DO 90 K=1,J
      KI=IIM1+K
      KJ=JJM1+K
      A(KI)=A(KI)-SS*A(KJ)
90 CONTINUE
      SS=0.Q0
      KJ=0
      DO 100 J=1,I
      JI=IIM1+J
      DO 100 K=1,J
      KJ=KJ+1
      KI=IIM1+K
      W=A(KI)*A(JI)*S(KJ)
      IF(K.NE.J) W=W+W
      SS=SS+W
100 CONTINUE
      W=QABS(SS/SSS-1.Q0)
      WRITE(6,3000) I,MM(I),NN(I),JJ(I),KK(I),PP(I),SS,SSS,W
      IF((SS.LT.0.D0).OR.(W.GT.SERR)) GO TO 110
      W=1.Q0/QSQRT(SS)
      GO TO 120
110 WRITE(6,4000)
      W=0.Q0
120 DO 130 J=1,I
      JI=IIM1+J
      A(JI)=A(JI)*W
130 CONTINUE
      IF(PRINT.EQ.0) GO TO 230
C***** TRANSFORMATION OF MATRIX ELEMENTS *****
      RR=R*R

```

APPENDIX C LISTS OF PROGRAMS (24)

```

DO 140 I=1,NMX          70001020
H(I)=T(I)/RR+U(I)/R    70001030
140 CONTINUE             70001040
DO 180 I=1,NBases        70001050
IIM1=I*(I-1)/2          70001060
DO 180 J=1,NBases        70001070
W=0.Q0                  70001080
DO 170 K=1,I             70001090
KI=IIM1+K               70001100
IF(K.GT.J) GO TO 150    70001110
KJ=J*(J-1)/2+K          70001120
GO TO 160                70001130
150 KJ=K*(K-1)/2+J      70001140
160 W=W+A(KI)*H(KJ)     70001150
170 CONTINUE              70001160
WW(I,J)=W                70001170
180 CONTINUE              70001180
IJ=0                     70001190
DO 200 J=1,NBases        70001200
DO 200 I=1,J             70001210
IIM1=I*(I-1)/2          70001220
IJ=IJ+1                  70001230
W=0.Q0                  70001240
DO 190 K=1,I             70001250
KI=IIM1+K               70001260
W=W+A(KI)*WW(J,K)       70001270
190 CONTINUE              70001280
HA(IJ)=W                 70001290
200 CONTINUE              70001300
WRITE(6,5000) ALPHA,ZA,ZB,MLTPLT,R,NBases,      70001310
2 (I,MM(I),NN(I),JJ(I),KK(I),PP(I),I=1,NBases) 70001320
WRITE(6,6000)             70001330
L=0                      70001340
DO 210 I=1,NBases        70001350
K=L+1                   70001360
L=L+1                   70001370
WRITE(6,7000) I,(A(J),J=K,L)      70001380
210 CONTINUE              70001390
WRITE(6,8000)             70001400
L=0                      70001410
K=0                     70001420
DO 220 J=1,NBases        70001430
DO 220 I=1,J             70001440
K=K+1                   70001450
L=L+1                   70001460
MM(L)=I                  70001470
NN(L)=J                  70001480
S(L)=HA(K)               70001490
IF(L.LT.5) GO TO 220    70001500
WRITE(6,9000) (MM(L),NN(L),S(L),L=1,5)      70001510
L=0                      70001520
220 CONTINUE              70001530
IF(L.NE.0) WRITE(6,9000) (MM(I),NN(I),S(I),I=1,L) 70001540
WRITE(6,1000)             70001550
230 STOP                  70001560
1000 FORMAT(I5,/D20.0)    70001570
2000 FORMAT(1H1,10X,'CHECK OF SCHUMIDT''S ORTHONORMALIZATION', 70001580
2 //11X,'BASE',5X,' M N J K P',16X,'(1/N)**2') 70001590
3000 FORMAT(11X,I4,5X,5I4,10X,2D20.10,D20.1)      70001600
4000 FORMAT(15X,'OMIT')   70001610
5000 FORMAT(1H1,15X,'ALPHA =',F10.5,      70001620
2 //16X,'THE CHARGE OF THE NUCLEUS A',F10.2, 70001630
3 //16X,'THE CHARGE OF THE NUCLEUS B',F10.2, 70001640
4 //16X,'MULTIPARTY' I10,    70001650
5 //16X,'INTERNUCLEAR DISTANCE',F10.5, 70001660
6 //16X,'NUMBER OF BASES',I10,    70001670
7 //21X,'NUMBER M N J K P',/(21X,I5,1X,5I4)) 70001680
6000 FORMAT(1H1,///11X,'ORTHONORMALIZED BASES', 70001690
2 //11X,'NUMBER',10X,'COEFFICIENTS') 70001700
7000 FORMAT(/11X,15,5X,5D20.10,/(21X,5D20.10)) 70001710
8000 FORMAT(1H1,///11X,'MATRIX ELEMENTS OF HAMILTONIAN OPERATOR', 70001720
2 //3X,5(3X,' I J H(I,J)',3X)) 70001730
9000 FORMAT(3X,5(3X,2I4,F15.8)) 70001740
10000 FORMAT(1H1)           70001750
END                      70001760

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