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The Quantum Mechanics of Seven and Eight Electrons with Spin Degeneracy

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The eigenfunctions corresponding to the fourteen singlet states of a system of seven or eight electrons are given and the corresponding matrix elements tabulated in a form convenient for computation, neglecting multiple interchange integrals. Proof is given that the general method described in earlier work for writing bond eigenfunctions suffices to separate the multiplets. A method for calculating matrix components between bond eigenfunctions directly from the bond systems is also described.

IN a series of papers from this laboratory[1] the problem of five or six spherically symmetric atoms, each with one valence electron, has been solved to the first order of the perturbation theory of quantum mechanics and the results applied to the calculation of the activation energies of some typical chemical reactions. In the third paper of this series it was found to be necessary to extend the results to the case of eight atoms. In this paper we shall give the details of these calculations and at the same time supply proofs of certain theorems which were assumed in the earlier papers of this series.

The method of approach is an extension of a method used by Slater[2] for the problems of three and four atoms. Since the seven-electron problem is immediately obtained from the eight-electron problem by putting one electron at infinity, it need not be considered separately. Let the eigenfunctions (neglecting spin) of the eight atoms be $a(x, y, z)$, $b(x, y, z)$, $\cdots$, $h(x, y, z)$. Let the co-ordinates of the eight electrons be x_1, y_1, z_1, x_2, $\cdots$, z_8. We shall abbreviate such an expression as $a(x_1, y_1, z_1)$ to $a(1)$. Then an approximate solution of the problem of eight atoms is the eigenfunction $a(1)b(2)c(3)\cdots h(8)$. Any function which may be obtained from this by permuting the numbers 1 to 8 is an equally good solution.

If we now introduce the spin of the electron, we find that instead of the 8! solutions we have just obtained, we have $2^8 8!$ solutions since with

each space eigenfunction we may either associate the eigenfunction α representing the electron spin of $+1/2\ h/2\pi$ or the eigenfunction β representing a spin of $-1/2\ h/2\pi$. The Pauli exclusion principle, however, limits us to the 2^8 linear combinations of these eigenfunctions which are antisymmetric in the electrons. Following Slater, we shall take as these antisymmetric combinations the determinant

$$\frac{1}{(8!)^{\frac{1}{2}}} \begin{vmatrix} a\alpha(1) & b\alpha(1) & \cdots & h\alpha(1) \\ a\alpha(2) & b\alpha(2) & \cdots & h\alpha(2) \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ a\alpha(8) & b\alpha(8) & \cdots & h\alpha(8) \end{vmatrix} \quad (1)$$

and the 2^8-1 determinants which may be obtained from this by replacing any column or columns of α's by β's. We shall denote such an eigenfunction by a symbol such as

$$\begin{pmatrix} a & b & c & d & e & f & g & h \\ \alpha & \alpha & \beta & \alpha & \alpha & \beta & \alpha & \alpha \end{pmatrix},$$

this denoting that determinant in which the c and f columns contain β's and the rest α's.

Each of these eigenfunctions is an exact eigenfunction of S_z, the operator giving the total z-component of spin, since each term of the expansion of the determinant is an eigenfunction of S_z with the same eigenvalue. We may, therefore, classify these eigenfunctions according to their values of S_z, which are easily seen to be $(n_\alpha - n_\beta) \times h/4\pi$ where n_α is the number of columns of α's and n_β is the number of columns of β's. The number of eigenfunctions with each value of S_z is given in Table I. By a well-known theorem, if

[1] Sherman and Eyring, J. Am. Chem. Soc. **54**, 2661 (1932); Kimball and Eyring, J. Am. Chem. Soc. **54**, 3876 (1932); Taylor, Eyring and Sherman, J. Chem. Phys. **1**, 68 (1933).

[2] Slater, Phys. Rev. **38**, 1109 (1931).

spin interactions are neglected the matrix elements of the Hamiltonian operator H between eigenfunctions with different values of S_z all vanish, so that in the perturbation theory we can consider each group separately, instead of using all 256 eigenfunctions at once.

TABLE I.

S_z (in units $h/2\pi$)	4	3	2	1	0	−1	−2	−3	−4
No. eigenfunctions	1	8	28	56	70	56	28	8	1

Although these eigenfunctions are eigenfunctions of S_z, they are not in general eigenfunctions of S^2, the square of the total angular momentum. It is possible, however, to combine these eigenfunctions in such a way that the new eigenfunctions are eigenfunctions of S^2 as well. Consider, for example, the 70 eigenfunctions for which $S_z = 0$. We shall show that from this set we can form 70 linear combinations which are, of course, still eigenfunctions of S_z and in addition are now eigenfunctions of S^2. Of these new eigenfunctions, 1 will have the eigenvalue $20(h/2\pi)^2$, 7 the eigenvalue $12(h/2\pi)^2$, 20 the eigenvalue $6(h/2\pi)^2$, 28 the eigenvalue $2(h/2\pi)^2$ and 14 the eigenvalue 0. Moreover, these eigenfunctions will have no matrix elements of H between the various groups.

In order to find these combinations we define for each pair of atoms ab, ac, etc., a function $\delta_{ab}(k)$. This function $\delta_{ab}(k)$ has the value 1 if in the kth eigenfunction in the set of 70 the spin of a is α and the spin of b is β; it has the value −1 if the spin of a is β and the spin of b is α; and it has the value 0 if a and b have the same spin. By means of these functions we may construct an eigenfunction corresponding to any way of drawing bonds between the eight atoms. Suppose, for example, that we wish the eigenfunction corresponding to the bonds a–b c–d e–f g–h. The required eigenfunction is then

$$\sum_k \delta_{ab}(k)\delta_{cd}(k)\delta_{ef}(k)\delta_{gh}(k)\psi_k,$$

where ψ_k is the kth eigenfunction in the original set of 70. Although there are 105 ways of drawing

4 bonds between 8 atoms, only 14 of the resulting eigenfunctions are linearly independent.

We shall now show that these bond eigenfunctions are eigenfunctions of S^2. By definition

$$S^2 = S_x{}^2 + S_y{}^2 + S_z{}^2. \tag{2}$$

Remembering the commutation rules

$$S_x S_y - S_y S_x = ih/2\pi \quad S_z$$
$$S_y S_z - S_z S_y = ih/2\pi \quad S_x$$
$$S_z S_x - S_x S_z = ih/2\pi \quad S_y$$

we may write (2) in the form

$$S^2 = (S_x + iS_y)(S_x - iS_y) - h/2\pi S_z + S_z{}^2 \tag{3a}$$

or

$$S^2 = (S_x - iS_y)(S_x + iS_y) + h/2\pi S_z + S_z{}^2. \tag{3b}$$

It follows that if a function is an eigenfunction of S_z and S^2 it must also be an eigenfunction of $(S_x + iS_y)(S_x - iS_y)$ and of $(S_x - iS_y)(S_x + iS_y)$. Now the operator

$$S_x + iS_y = S_{x1} + iS_{y1} + S_{x2} + iS_{y2} + \cdots + S_{x8} + iS_{y8}$$

where S_{x1} and S_{y1} are the operators for the x and y components of the spin of electron 1. Since[3]

$$S_{x1}\alpha(1) = (h/4\pi)\beta(1); \qquad S_{x1}\beta(1) = (h/4\pi)\alpha(1)$$
$$S_{y1}\alpha(1) = (ih/4\pi)\beta(1); \qquad S_{y1}\beta(1) = (-ih/4\pi)\alpha(1)$$

we have $(S_{x1} + iS_{y1})\alpha(1) = 0$,

$$(S_{x1} + iS_{y1})\beta(1) = (h/2\pi)\alpha(1),$$

and also $(S_{x1} - iS_{y1})\alpha(1) = (h/2\pi)\beta(1)$,

$$(S_{x1} - iS_{y1})\beta(1) = 0.$$

Let us now consider the effect of the operator $S_x + iS_y$ on a typical Slater eigenfunction. Acting on

$$\begin{pmatrix} a & b & c & d & e & f & g & h \\ \alpha & \alpha & \alpha & \alpha & \alpha & \alpha & \alpha & \alpha \end{pmatrix}$$

the operator $S_x + iS_y$ obviously gives 0. Acting on any other eigenfunction of this type it is easily seen that the result is $h/2\pi$ times the sum of all the determinants which may be obtained by replacing one column of β's by α's. Thus

$$(S_x + iS_y)\begin{pmatrix} a & b & c & d & e & f & g & h \\ \beta & \beta & \alpha & \alpha & \alpha & \alpha & \alpha & \alpha \end{pmatrix} .$$

$$= \frac{h}{2\pi}\begin{pmatrix} a & b & c & d & e & f & g & h \\ \alpha & \beta & \alpha & \alpha & \alpha & \alpha & \alpha & \alpha \end{pmatrix} + \frac{h}{2\pi}\begin{pmatrix} a & b & c & d & e & f & g & h \\ \beta & \alpha & \alpha & \alpha & \alpha & \alpha & \alpha & \alpha \end{pmatrix}.$$

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[3] Pauli, Zeits. f. Physik **43**, 601 (1927).

Similarly the operator $S_x - iS_y$ gives 0 when it acts on

$$\begin{pmatrix} a & b & c & d & e & f & g & h \\ \beta & \beta & \beta & \beta & \beta & \beta & \beta & \beta \end{pmatrix}$$

and acting on any other Slater eigenfunction gives $h/2\pi$ times the sum of all the determinants which may be obtained by replacing one column of α's by β's.

It is now easily verified that the operator $S_x + iS_y$ acting on any bond eigenfunction corresponding to four bonds gives 0 as a result. Hence, the operator $(S_x - iS_y)(S_x + iS_y)$ also gives 0, and since S_z operating on any of the set of 70 original eigenfunctions gives 0, it follows that the operator S^2 acting on this eigenfunction also gives 0. The bond eigenfunctions corresponding to 4 bonds are, therefore, eigenfunctions of S^2 with the eigenvalue 0. A similar argument shows that those bond eigenfunctions corresponding to 3 bonds are eigenfunctions of S^2 with the eigenvalue $2(h/2\pi)^2$, those corresponding to 2 bonds have the eigenvalue $6(h/2\pi)^2$, those corresponding to 1 bond have the eigenvalue $12(h/2\pi)^2$, and that the single eigenfunction corresponding to no bonds has the eigenvalue $20(h/2\pi)^2$. It follows that the matrix components of H between bond eigenfunctions corresponding to different numbers of bonds all vanish.

Since in chemical problems it is almost always the state of lowest multiplicity which is of interest, we may from now on confine our attention to a set of fourteen linearly independent bond eigenfunctions with $S_z = 0$ and $S^2 = 0$. The actual set of fourteen used were those corresponding to the ways of drawing the bonds shown in Table II.

ψ_1	a–b c–d e–f g–h		ψ_8	a–c b–d e–g f–h
ψ_2	a–b c–e d–f g–h		ψ_9	a–c b–e d–g f–h
ψ_3	a–c b–d e–f g–h		ψ_{10}	a–d b–e c–g f–h
ψ_4	a–c b–e d–f g–h		ψ_{11}	a–h b–g c–d e–f
ψ_5	a–d b–e c–f g–h		ψ_{12}	a–h b–g c–e d–f
ψ_6	a–b c–d e–g f–h		ψ_{13}	a–h b–d c–e e–f
ψ_7	a–b c–e d–g f–h		ψ_{14}	a–b c–g d–h e–f

These eigenfunctions are independent, and since all other four-bond eigenfunctions can be expressed in terms of them they form a complete set.

By using these fourteen eigenfunctions as a basis for the usual perturbation theory, the energy is given to the first order by the secular equation

$$\begin{vmatrix} H_{1,1} - d_{1,1}E & H_{1,2} - d_{1,2}E & \cdots & H_{1,14} - d_{1,14}E \\ H_{2,1} - d_{2,1}E & H_{2,2} - d_{2,2}E & \cdots & H_{2,14} - d_{2,14}E \\ \cdot & \cdot & \cdots & \cdot \\ H_{14,1} - d_{14,1}E & H_{14,2} - d_{14,2}E & \cdots & H_{14,14} - d_{14,14}E \end{vmatrix} = 0, \qquad (4)$$

where

$$H_{ij} = \int \psi_i^* H \psi_j d\tau, \quad d_{ij} = \int \psi_i^* \psi_j d\tau.$$

We must, therefore, evaluate these integrals.

We shall suppose that the field due to all the electrons in each atom except the valence electron may be represented by a function $V(x, y, z)$, distinguishing the atoms by subscripts as $V_a(x, y, z)$. Then the Hamiltonian function takes the form

$$H = \sum_{i=1}^{8} -h^2/8\pi^2 m \nabla_i^2$$
$$+ \sum_{\nu=a, b, c \dots} \sum_{i=1}^{8} V_\nu(x_i, y_i, z_i) + \sum_{j>i} (e^2/r_{ij}).$$

Since the eigenfunction $a(i)$ is by hypothesis a solution of the equation

$$(-h^2/8\pi^2 m \nabla_i^2 + V_a(x_i, y_i, z_i))a(i) = E_a a(i),$$

where E_a is the lowest energy level of atom a, we may replace the operator $-(h^2/8\pi^2 m)\nabla_i^2$ by $E_a - V_a(i)$ whenever it operates on $a(i)$ and by similar expressions when it operates on the other atomic eigenfunctions. The matrix components of H between the Slater eigenfunctions have been discussed by Slater.[2] If we neglect the lack of orthogonality of the eigenfunctions $a(i)$, $b(i)$, $c(i) \cdots$, the multiple interchange integrals are all small and can be neglected. To this degree of ap-

proximation the matrix components are then given by the following rules:

(1) The matrix component between any Slater eigenfunction and itself is the coulombic integral

$$C = \int a(1)b(2)\cdots h(8)IIa(1)b(2)\cdots h(8)d\tau$$

minus the sum of all the interchange integrals between atoms having the same spin. The interchange integral between two atoms, say a and b, is the integral

$$(ab) = \int a(1)b(2)\cdots h(8)Hb(1)a(2)\cdots h(8)d\tau.$$

(2) The matrix element between two different Slater eigenfunctions is zero unless the two eigenfunctions differ only by a single interchange of spins on two atoms, in which case the matrix component is the negative of the interchange integral between these two atoms. For example, the diagonal matrix element for the eigenfunction

$$\begin{pmatrix} a & b & c & d & e & f & g & h \\ \alpha & \alpha & \alpha & \alpha & \beta & \beta & \beta & \beta \end{pmatrix}$$

is $C - (ab) - (ac) - (ad) - (bc) - (bd) - (cd) - (ef) - (eg) - (eh) - (fg) - (fh) - (gh)$, while the matrix element between this and

$$\begin{pmatrix} a & b & c & d & e & f & g & h \\ \beta & \alpha & \alpha & \alpha & \alpha & \beta & \beta & \beta \end{pmatrix}$$

is $-(ae)$.

These rules enable us to find the matrix elements between the various bond eigenfunctions. Suppose, for example, that we wished to find the matrix element between the eigenfunction representing the bond system a–b c–d e–f g–h and that representing the bonds a–c b–d e–g f–h. We could, of course, actually write out these eigenfunctions in terms of the Slater eigenfunctions and, knowing the matrix components of H between these, find the required matrix element. It is, however, possible to set up rules for finding the matrix element directly. It is evident that the matrix element we seek will be the sum of some multiple of C and certain multiples of the various interchange integrals. We shall now show how the coefficients of the various integrals in the matrix element may be simply determined. Let us first consider C. The only way C can occur in the re-

sult is from the presence of the same Slater eigenfunction as a part of both bond eigenfunctions. The coefficient of C is, therefore, equal to the number of Slater eigenfunctions which occur once in each of the two bond eigenfunctions, taken with $a+$ or $-$ sign according to whether they occur with the same or opposite signs in the two bond eigenfunctions. In order to find this number we write the two bond systems above one another, thus:

$$a\text{–}b \quad c\text{–}d \quad e\text{–}f \quad g\text{–}h$$
$$a\text{–}c \quad b\text{–}d \quad e\text{–}g \quad f\text{–}h.$$

We now start assigning spins to the various atoms. Taking a arbitrarily to have the spin α, we must have the spin β on b in order to have the bond a–b. We, therefore, write α on the a's and β on the b's. In the same way we see that the spin of c must be β and that of d must be α. We now have the following picture:

$$\alpha \quad \beta \quad \beta \quad \alpha$$
$$a\text{–}b \quad c\text{–}d \quad e\text{–}f \quad g\text{–}h$$
$$a\text{–}c \quad b\text{–}d \quad e\text{–}g \quad f\text{–}h$$
$$\alpha \quad \beta \quad \beta \quad \alpha.$$

We may now choose the spin of e arbitrarily, but then all the spins are determined, thus:

$$\alpha \quad \beta \quad \beta \quad \alpha \quad \alpha \quad \beta \quad \beta \quad \alpha$$
$$a\text{–}b \quad c\text{–}d \quad e\text{–}f \quad g\text{–}h$$
$$a\text{–}c \quad b\text{–}d \quad e\text{–}g \quad f\text{–}h$$
$$\alpha \quad \beta \quad \beta \quad \alpha \quad \alpha \quad \beta \quad \beta \quad \alpha.$$

Since we could have chosen a to be either α or β, and likewise e to be either α or β, there are four Slater eigenfunctions common to the two bond eigenfunctions. It is easily seen that these eigenfunctions all enter both bond eigenfunctions with the same sign, so that the coefficient of C in the matrix element is $+4$.

In order to find the coefficient of an interchange integral such as (ab) we proceed in a similar way. We note first that such an integral can arise in two ways: it may arise from the presence of a Slater eigenfunction common to both eigenfunctions in which a and b have the same spin; or it may arise from the presence of two Slater eigenfunctions differing only in the interchange of the spins of a and b. The two cases are considered

separately. To obtain the contribution of the first case we again put down our two bond systems and now write α's on the a's and also on the b's. We then proceed to fix the other spins by the requirement that wherever there is a bond between two atoms the spins must be opposite. The process is continued until every spin is fixed or an inconsistency is reached. For example, taking the same bond system as before the result for (ab) is immediately inconsistent because of the bond a–b in the first eigenfunction. If we take the integral (ae), however, we find

$$
\begin{array}{cccc}
\alpha\ \beta & \beta\ \alpha & \alpha\ \beta & \beta\ \alpha \\
a\text{–}b & c\text{–}d & e\text{–}f & g\text{–}h \\
a\text{–}c & b\text{–}d & e\text{–}g & f\text{–}h \\
\alpha\ \beta & \beta\ \alpha & \alpha\ \beta & \beta\ \alpha.
\end{array}
$$

There are, therefore, only two Slater eigenfunctions giving rise to the integral (ae) (one with α's, the other with β's on a and e). Each has a positive sign, so that the contribution to the coefficient of (ae) is -2 (the negative sign arising from the original rules for matrix elements between Slater eigenfunctions). Taking the integral (ad) as a further example we find

$$
\begin{array}{cccc}
\alpha\ \beta & \beta\ \alpha & \alpha\ \beta & \beta\ \alpha \\
a\text{–}b & c\text{–}d & e\text{–}f & g\text{–}h \\
a\text{–}c & b\text{–}d & e\text{–}g & f\text{–}h \\
\alpha\ \beta & \beta\ \alpha & \alpha\ \beta & \beta\ \alpha.
\end{array}
$$

In this case, when the spins of a, b, c and d were assigned we were left free to choose either spin for e, so that there are four eigenfunctions giving the integral (ad). The contribution to the coefficient of (ad) is, therefore, -4.

In order to find the other part of the coefficient of (ab) we write α on a and β on b in the first bond system and β on a and α on β in the second, continuing the process as before. Thus we find

$$
\begin{array}{cccc}
\alpha\ \beta & \alpha\ \beta & \alpha\ \beta & \beta\ \alpha \\
a\text{–}b & c\text{–}d & e\text{–}f & g\text{–}h \\
a\text{–}c & b\text{–}d & e\text{–}g & f\text{–}h \\
\beta\ \alpha & \alpha\ \beta & \alpha\ \beta & \beta\ \alpha.
\end{array}
$$

The sign of the first is negative and the second positive, and we could have chosen α or β on a and also on e. The contribution is, therefore, $+4$. The total coefficient of (ab) is, therefore, $+4$. The diagrams for (ae) and (ad) and their contributions are

$$
(ae)\quad
\begin{array}{cccc}
\alpha\ \beta & \beta\ \alpha & \beta & \\
a\text{–}b & c\text{–}d & e\text{–}f & g\text{–}h \\
a\text{–}c & b\text{–}d & e\text{–}g & f\text{–}h \\
\beta\ \beta & \alpha\ \alpha & &
\end{array}
\quad\text{(inconsistent)}
$$

$$
(ad)\quad
\begin{array}{cccc}
\alpha\ \beta & \alpha\ \beta & \alpha\ \beta & \beta\ \alpha \\
a\text{–}b & c\text{–}d & e\text{–}f & g\text{–}h \\
a\text{–}c & b\text{–}d & e\text{–}g & f\text{–}h \\
\beta\ \alpha & \beta\ \alpha & \alpha\ \beta & \beta\ \alpha.
\end{array}
\quad(-4)
$$

The total coefficient of (ae) is, therefore, -2 and that of (ad), -8.

TABLE III.

$$\chi_1 = \psi_1$$
$$\chi_2 = \psi_2 - \tfrac{1}{2}\psi_1$$
$$\chi_3 = \psi_3 - \tfrac{1}{2}\psi_1$$
$$\chi_4 = \psi_4 - \tfrac{1}{2}\psi_3 - \tfrac{1}{2}\psi_2 + \tfrac{1}{4}\psi_1$$
$$\chi_5 = \psi_5 - \tfrac{1}{3}\psi_4 - \tfrac{1}{3}\psi_3 - \tfrac{1}{3}\psi_2 + \tfrac{2}{3}\psi_1$$
$$\chi_6 = \psi_6 - \tfrac{1}{2}\psi_1$$
$$\chi_7 = \psi_7 - \tfrac{1}{2}\psi_6 - \tfrac{1}{2}\psi_2 + \tfrac{1}{4}\psi_1$$
$$\chi_8 = \psi_8 - \tfrac{1}{2}\psi_6 - \tfrac{1}{2}\psi_3 + \tfrac{1}{4}\psi_1$$
$$\chi_9 = \psi_9 - \tfrac{1}{2}\psi_8 - \tfrac{1}{2}\psi_7 + \tfrac{1}{4}\psi_6 - \tfrac{1}{2}\psi_4 + \tfrac{1}{4}\psi_3 + \tfrac{1}{4}\psi_2 - \tfrac{1}{8}\psi_1$$
$$\chi_{10} = \psi_{10} - \tfrac{1}{3}\psi_9 - \tfrac{1}{3}\psi_8 - \tfrac{1}{3}\psi_7 + \tfrac{2}{3}\psi_6 - \tfrac{1}{2}\psi_5 + \tfrac{1}{6}\psi_4 + \tfrac{1}{6}\psi_3 + \tfrac{1}{6}\psi_2 - \tfrac{1}{3}\psi_1$$
$$\chi_{11} = \psi_{11} - \tfrac{2}{3}\psi_{10} + \tfrac{2}{3}\psi_9 - \tfrac{1}{3}\psi_6 + \tfrac{1}{3}\psi_5 - \tfrac{1}{3}\psi_4 - \tfrac{1}{3}\psi_1$$
$$\chi_{12} = \psi_{12} - \tfrac{1}{2}\psi_{11} - \tfrac{1}{3}\psi_{10} - \tfrac{1}{3}\psi_9 + \tfrac{2}{3}\psi_8 + \tfrac{1}{3}\psi_7 - \tfrac{1}{2}\psi_6 + \tfrac{1}{6}\psi_5 + \tfrac{1}{6}\psi_4 - \tfrac{1}{3}\psi_3 - \tfrac{1}{3}\psi_2 + \tfrac{1}{2}\psi_1$$
$$\chi_{13} = \psi_{13} + \tfrac{1}{9}\psi_{12} - \tfrac{2}{9}\psi_{11} - \tfrac{4}{9}\psi_{10} - \tfrac{4}{9}\psi_9 + \tfrac{5}{9}\psi_8 + \tfrac{7}{9}\psi_7 - \tfrac{2}{9}\psi_6 + \tfrac{2}{9}\psi_5 + \tfrac{2}{9}\psi_4 - \tfrac{7}{9}\psi_3 - \tfrac{5}{9}\psi_2 + \tfrac{2}{9}\psi_1$$
$$\chi_{14} = \psi_{14} - \tfrac{3}{4}\psi_{13} - \tfrac{1}{4}\psi_{12} + \tfrac{1}{2}\psi_{11} + \tfrac{1}{3}\psi_{10} + \tfrac{1}{3}\psi_9 - \tfrac{5}{12}\psi_8 + \tfrac{1}{12}\psi_7 + \tfrac{1}{6}\psi_6 - \tfrac{1}{6}\psi_5 - \tfrac{1}{6}\psi_4 + \tfrac{7}{12}\psi_3 + \tfrac{1}{12}\psi_2 - \tfrac{5}{6}\psi_1$$

TABLE IV.

	$H_{1,1}$	$H_{1,2}$	$H_{1,3}$	$H_{1,4}$	$H_{1,5}$	$H_{1,6}$	$H_{1,7}$	$H_{1,8}$	$H_{1,9}$	$H_{1,10}$	$H_{1,11}$	$H_{1,12}$	$H_{1,13}$	$H_{1,14}$	$H_{2,2}$	$H_{2,3}$	$H_{2,4}$	$H_{2,5}$	$H_{2,6}$	$H_{2,7}$	$H_{2,8}$	$H_{2,9}$	$H_{2,10}$	$H_{2,11}$	$H_{2,12}$	$H_{2,13}$	$H_{2,14}$	$H_{3,3}$
C	8	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	6
ab	8	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	-6
ac	-4	0	6	0	0	0	0	0	0	0	0	0	0	0	-3	0	9/2	0	0	0	0	0	0	0	0	0	0	3
ad	-4	0	-6	0	0	0	0	0	0	0	0	0	0	0	-3	0	3/2	0	0	0	0	0	0	0	0	0	0	3
ae	-4	0	0	-3	4	0	0	0	0	0	0	0	0	0	-3	-3	-3	2	0	0	0	0	0	0	0	0	0	-3
af	-4	0	0	3	-4	0	0	0	0	0	0	0	0	0	-3	3	-3	-2	0	0	0	0	0	0	0	0	0	-3
ag	-4	0	0	0	0	0	0	0	3/2	-2	-4	0	0	0	-3	0	0	0	0	0	3/2	-3/2	-1	0	-3	0	0	-3
ah	-4	0	0	0	0	0	0	0	-3/2	2	4	0	0	0	-3	0	0	0	0	0	-3/2	3/2	1	0	3	0	0	-3
bc	-4	0	-6	0	0	0	0	0	0	0	0	0	0	0	-3	0	-9/2	0	0	0	0	0	0	0	0	0	0	3
bd	-4	0	6	0	0	0	0	0	0	0	0	0	0	0	-3	0	-3/2	0	0	0	0	0	0	0	0	0	0	3
be	-4	0	0	3	-4	0	0	0	0	0	0	0	0	0	-3	3	3	2	0	0	0	0	0	0	0	0	0	-3
bf	-4	0	0	-3	4	0	0	0	0	0	0	0	0	0	-3	3	3	-2	0	0	0	0	0	0	0	0	0	-3
bg	-4	0	0	0	0	0	0	0	-3/2	2	4	0	0	0	-3	0	0	0	0	0	-3/2	3/2	1	0	3	0	0	-3
bh	-4	0	0	0	0	0	0	0	3/2	-2	-4	0	0	0	-3	0	0	0	0	0	3/2	-3/2	-1	0	-3	0	0	-3
cd	8	0	0	0	0	0	0	0	0	0	0	0	0	0	-6	0	0	0	0	0	0	0	0	0	0	0	0	-6
ce	-4	6	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	-4	0	0	0	0	0	0	0	0	0	-3
cf	-4	-6	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	4	0	0	0	0	0	0	0	0	0	-3
cg	-4	0	0	0	0	0	-3	0	0	0	0	0	2	5/2	-3	0	0	0	-3	3	0	0	0	0	0	1	5/4	-3
ch	-4	0	0	0	0	0	3	0	0	0	0	0	-2	-5/2	-3	0	0	0	3	-3	0	0	0	0	0	-1	-5/4	-3
de	-4	-6	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	-3
df	-4	6	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	-3
dg	-4	0	0	0	0	0	3	0	0	0	0	0	-2	-5/2	-3	0	0	0	3	3	0	0	0	0	0	1	5/4	-3
dh	-4	0	0	0	0	0	-3	0	0	0	0	0	2	5/2	-3	0	0	0	-3	-3	0	0	0	0	0	-1	-5/4	-3
ef	8	0	0	0	0	0	0	0	0	0	0	0	0	0	-6	0	0	0	0	0	0	0	0	0	0	0	0	6
eg	-4	0	0	0	0	6	0	0	0	0	0	0	0	0	-3	0	0	0	0	0	-3/2	0	0	0	0	-2	-5/2	-3
eh	-4	0	0	0	0	-6	0	0	0	0	0	0	0	0	-3	0	0	0	0	0	3/2	0	0	0	0	2	5/2	-3
fg	-4	0	0	0	0	-6	0	0	0	0	0	0	0	0	-3	0	0	0	0	0	-9/2	0	0	0	0	0	0	-3
fh	-4	0	0	0	0	6	0	0	0	0	0	0	0	0	-3	0	0	0	0	0	9/2	0	0	0	0	0	0	-3
gh	8	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	6

	$H_{3,4}$	$H_{3,5}$	$H_{3,6}$	$H_{3,7}$	$H_{3,8}$	$H_{3,9}$	$H_{3,10}$	$H_{3,11}$	$H_{3,12}$	$H_{3,13}$	$H_{3,14}$	$H_{4,4}$	$H_{4,5}$	$H_{4,6}$	$H_{4,7}$	$H_{4,8}$	$H_{4,9}$	$H_{4,10}$	$H_{4,11}$	$H_{4,12}$	$H_{4,13}$	$H_{4,14}$	$H_{5,5}$	$H_{5,6}$	$H_{5,7}$	$H_{5,8}$	$H_{5,9}$	$H_{5,10}$
C	0	0	0	0	0	0	0	0	0	0	0	9/2	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0
ab	0	0	0	0	0	0	0	0	0	0	0	-9/2	0	0	0	0	0	0	0	0	0	0	-4	0	0	0	0	0
ac	0	0	0	0	0	0	0	0	0	0	0	9/4	0	0	0	0	0	0	0	0	0	0	-4	0	0	0	0	0
ad	0	0	0	0	0	0	0	0	0	0	0	-15/4	2	0	0	0	0	0	0	0	0	0	4/3	0	0	0	0	0
ae	3	2	0	0	0	0	0	0	0	0	0	3/4	-1	0	0	0	0	0	0	0	0	0	4/3	0	0	0	0	0
af	-3	-2	0	0	0	0	0	0	0	0	0	3/4	-1	0	0	0	0	0	0	0	0	0	4/3	0	0	0	0	0
ag	0	0	0	0	3/2	0	-3/2	-1	0	1	-8/3	-9/4	0	3/2	-3/2	-3/2	3/2	-1/2	1	-1	-4/3	-2	-2	-2	-1	-1	-1/2	5/3
ah	0	0	0	0	-3/2	0	3/2	1	0	-1	8/3	-9/4	0	-3/2	3/2	3/2	-3/2	1/2	-1	1	4/3	-2	-2	2	1	1	1/2	-5/3
bc	0	0	0	0	0	0	0	0	0	0	0	9/4	0	0	0	0	0	0	0	0	0	0	-4	0	0	0	0	0
bd	0	0	0	0	0	0	0	0	0	0	0	-15/4	2	0	0	0	0	0	0	0	0	0	4/3	0	0	0	0	0
be	3	2	0	0	0	0	0	0	0	0	0	3/4	-1	0	0	0	0	0	0	0	0	0	4/3	0	0	0	0	0
bf	-3	-2	0	0	0	0	0	0	0	0	0	3/4	-1	0	0	0	0	0	0	0	0	0	4/3	0	0	0	0	0
bg	0	0	0	-3/2	0	-3/2	-1	0	1	-2/3	5/2	-9/4	0	-3/2	3/2	-3/2	3/2	-1/2	1	-1	-1/3	5/4	-2	2	1	-1	-1/2	5/3
bh	0	0	0	3/2	0	3/2	1	0	-1	2/3	-5/2	-9/4	0	3/2	-3/2	3/2	-3/2	1/2	-1	1	1/3	-5/4	-2	-2	-1	1	1/2	-5/3
cd	0	0	0	0	0	0	0	0	0	0	0	-3/2	-4	0	0	0	0	0	0	0	0	0	4/3	0	0	0	0	0
ce	-3/2	-4	0	0	0	0	0	0	0	0	0	-15/4	2	0	0	0	0	0	0	0	0	0	4/3	0	0	0	0	0
cf	3/2	4	0	0	0	0	0	0	0	0	0	-15/4	2	0	0	0	0	0	0	0	0	0	4/3	0	0	0	0	0
cg	0	0	0	0	0	3/4	2	2	-1	5/3	-5/4	-9/4	0	0	0	3/4	-3/4	1	-1	5/2	5/6	-5/8	-2	0	0	2	1	5/3
ch	0	0	0	0	0	-3/4	-2	-2	1	-5/3	5/4	-9/4	0	0	0	-3/4	3/4	-1	1	-5/2	-5/6	5/8	-2	0	0	-2	-1	-5/3
de	-9/2	0	0	0	0	0	0	0	0	0	0	9/4	0	0	0	0	0	0	0	0	0	0	-4	0	0	0	0	0
df	9/2	0	0	0	0	0	0	0	0	0	0	9/4	0	0	0	0	0	0	0	0	0	0	-4	0	0	0	0	0
dg	0	0	0	0	0	9/4	0	-2	-1	5/3	-5/4	-9/4	0	0	0	9/4	9/4	0	1	1/2	-5/6	5/8	-2	0	0	0	0	-1
dh	0	0	0	0	0	-9/4	0	2	1	-5/3	5/4	-9/4	0	0	0	-9/4	-9/4	0	-1	-1/2	5/6	-5/8	-2	0	0	0	0	1
ef	0	0	0	0	9/2	0	0	0	0	0	0	-9/2	0	0	0	0	0	0	0	0	0	0	-4	0	0	0	0	0
eg	0	0	0	0	-9/2	0	0	0	0	0	0	-9/4	0	0	0	0	-9/8	0	-2	-1	5/3	-5/4	-2	0	0	0	0	-1
eh	0	0	0	0	9/2	0	0	0	0	0	0	-9/4	0	0	0	0	9/8	0	2	1	-5/3	5/4	-2	0	0	0	0	1
fg	0	0	0	0	-9/2	0	0	0	0	0	0	-9/4	0	0	0	0	-27/8	0	0	0	0	0	-2	0	0	0	0	-3
fh	0	0	0	0	9/2	0	0	0	0	0	0	-9/4	0	0	0	0	27/8	0	0	0	0	0	-2	0	0	0	0	3
gh	0	0	0	0	0	0	0	0	0	0	0	9/2	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0

TABLE IV. (*Continued*).

	$H_{5,11}$	$H_{5,12}$	$H_{5,13}$	$H_{5,14}$	$H_{6,6}$	$H_{6,7}$	$H_{6,8}$	$H_{6,9}$	$H_{6,10}$	$H_{6,11}$	$H_{6,12}$	$H_{6,13}$	$H_{6,14}$	$H_{7,7}$	$H_{7,8}$	$H_{7,9}$	$H_{7,10}$	$H_{7,11}$	$H_{7,12}$	$H_{7,13}$	$H_{7,14}$	$H_{8,8}$	$H_{8,9}$	$H_{8,10}$	$H_{8,11}$
C	0	0	0	0	6	0	0	0	0	0	0	0	0	9/2	0	0	0	0	0	0	0	9/2	0	0	0
ab	0	0	0	0	6	0	0	0	0	0	0	0	0	9/2	0	0	0	0	0	0	0	-9/2	0	0	0
ac	0	0	0	0	-3	0	9/2	0	0	0	0	0	0	-9/4	0	27/8	0	0	0	0	0	9/4	0	0	0
ad	0	0	0	0	-3	0	-9/2	0	0	0	0	0	0	-9/4	0	9/8	3	0	0	0	0	9/4	0	0	0
ae	0	0	0	0	-3	0	0	-9/4	3	0	0	0	0	-9/4	-9/4	-9/4	-3/2	0	0	0	0	-9/4	9/4	3/2	0
af	0	0	0	0	-3	0	0	-3/4	1	-4	0	0	0	-9/4	-3/4	3/4	1/2	0	-3	0	0	9/4	3/4	1/2	0
ag	-4/3	-2/3	-8/9	0	-3	0	0	3/2	-2	2	0	0	0	-9/4	3/2	-3/2	-1	0	3/2	0	0	9/4	-3/2	-1	0
ah	4/3	2/3	8/9	0	-3	0	0	3/2	-2	2	0	0	0	-9/4	3/2	-3/2	-1	0	3/2	0	0	-9/4	-3/2	-1	0
bc	0	0	0	0	-3	0	-9/2	0	0	0	0	0	0	-9/4	0	-27/8	0	0	0	0	0	9/4	0	0	0
bd	0	0	0	0	-3	0	9/2	0	0	0	0	0	0	-9/4	0	-9/8	-3	0	0	0	0	9/4	0	0	0
be	0	0	0	0	-3	0	0	9/4	-3	0	0	0	0	-9/4	9/4	9/4	3/2	0	0	0	0	-9/4	9/4	3/2	0
bf	0	0	0	0	-3	0	0	3/4	-1	4	0	0	0	-9/4	3/4	-3/4	-1/2	0	3	0	0	-9/4	3/4	1/2	0
bg	-4/3	-2/3	-2/9	5/6	-3	0	0	-3/2	2	-2	0	0	0	-9/4	-3/2	3/2	1	0	-3/2	0	0	-9/4	-3/2	-1	0
bh	4/3	2/3	2/9	-5/6	-3	0	0	-3/2	2	-2	0	0	0	-9/4	-3/2	3/2	1	0	-3/2	0	0	-9/4	-3/2	-1	0
cd	0	0	0	0	6	0	0	0	0	0	0	0	0	-9/2	0	0	0	0	0	0	0	-9/2	0	0	0
ce	0	0	0	0	-3	9/2	0	0	0	0	0	0	0	9/4	0	0	0	0	0	0	0	-9/4	-9/8	-3	0
cf	0	0	0	0	-3	3/2	0	0	0	0	0	2	5/2	-15/4	0	0	0	0	0	1	5/4	-9/4	-3/8	-1	2
cg	-2/3	-1/3	-10/9	5/6	-3	-3	0	0	0	0	0	-1	-5/4	3/4	0	0	0	0	0	-1/2	-5/8	-9/4	3/4	2	-1
ch	2/3	1/3	10/9	-5/6	-3	-3	0	0	0	0	0	-1	-5/4	3/4	0	0	0	0	0	-1/2	-5/8	-9/4	3/4	2	-1
de	0	0	0	0	-3	-9/2	0	0	0	0	0	0	0	9/4	0	0	0	0	0	0	0	-9/4	-27/8	0	0
df	0	0	0	0	-3	-3/2	0	0	0	0	0	-2	-5/2	-15/4	0	0	0	0	0	1	5/4	-9/4	-9/8	0	-2
dg	2/3	7/3	10/9	-5/6	-3	3	0	0	0	0	0	1	5/4	3/4	0	0	0	0	0	-1/2	-5/8	-9/4	9/4	0	1
dh	-2/3	-7/3	-10/9	5/6	-3	3	0	0	0	0	0	1	5/4	3/4	0	0	0	0	0	-1/2	-5/8	-9/4	9/4	0	1
ef	0	0	0	0	-6	0	0	0	0	0	0	0	0	-3/2	0	0	0	0	0	-2	-5/2	-9/2	0	0	0
eg	8/3	-2/3	10/9	-5/6	3	0	0	0	0	0	0	0	0	-15/4	0	0	0	0	0	1	5/4	9/4	0	0	0
eh	-8/3	2/3	-10/9	5/6	3	0	0	0	0	0	0	0	0	-15/4	0	0	0	0	0	1	5/4	9/4	0	0	0
fg	0	0	0	0	3	0	0	0	0	0	0	0	0	9/4	0	0	0	0	0	0	0	9/4	0	0	0
fh	0	0	0	0	3	0	0	0	0	0	0	0	0	9/4	0	0	0	0	0	0	0	9/4	0	0	0
gh	0	0	0	0	-6	0	0	0	0	0	0	0	0	-9/2	0	0	0	0	0	0	0	-9/2	0	0	0

	$H_{8,12}$	$H_{8,13}$	$H_{8,14}$	$H_{9,9}$	$H_{9,10}$	$H_{9,11}$	$H_{9,12}$	$H_{9,13}$	$H_{9,14}$	$H_{10,10}$	$H_{10,11}$	$H_{10,12}$	$H_{10,13}$	$H_{10,14}$	$H_{11,11}$	$H_{11,12}$	$H_{11,13}$	$H_{11,14}$	$H_{12,12}$	$H_{12,13}$	$H_{12,14}$	$H_{13,13}$	$H_{13,14}$	$H_{14,14}$
C	0	0	0	27/8	0	0	0	0	0	3	0	0	0	0	4	0	0	0	3	0	0	8/3	0	5/4
ab	0	0	0	-27/8	0	0	0	0	0	-3	0	0	0	0	-4	0	0	0	-3	0	0	-2/3	5/2	5/8
ac	0	0	0	27/16	0	0	0	0	0	-3	0	0	0	0	-2	1	-2/3	5/2	-5/2	-1/3	5/4	-22/9	-5/6	5/8
ad	0	0	0	-45/16	3/2	0	0	0	0	1	0	0	0	0	-2	-1	2/3	-5/2	-5/2	-1/3	5/4	-22/9	-5/6	5/8
ae	0	0	0	9/16	-3/4	0	0	0	0	1	0	0	0	0	-4	0	0	-1	2/3	-5/2		-22/9	-5/6	5/8
af	1	-8/3	0	-39/16	1/4	1	-1	-4/3	0	-7/3	-4/3	-2/3	-8/9	0	4/3	0	0	0	1	0	0	8/9	0	-5/2
ag	-1/2	4/3	0	-3/16	-1/2	-1/2	1/2	2/3	0	1/6	2/3	1/3	4/9	0	4/3	0	0	0	1	0	0	8/9	0	-5/2
ah	-1/2	4/3	0	-3/16	-1/2	-1/2	1/2	2/3	0	1/6	2/3	1/3	4/9	0	4/3	0	0	0	1	0	0	8/9	0	-5/2
bc	0	0	0	27/16	0	0	0	0	0	-3	0	0	0	0	-2	1	-8/3	0	-5/2	-4/3	0	8/9	0	-5/2
bd	0	0	0	-45/16	3/2	0	0	0	0	1	0	0	0	0	-2	-1	8/3	0	-5/2	-4/3	0	8/9	0	-5/2
be	0	0	0	9/16	-3/4	0	0	0	0	1	0	0	0	0	-4	0	0	-1	8/3	0	0	8/9	0	-5/2
bf	1	-2/3	5/2	-39/16	1/4	1	-1	-1/3	5/4	-7/3	-4/3	-2/3	-2/9	5/6	4/3	0	0	0	1	0	0	-22/9	-5/6	5/8
bg	-1/2	1/3	-5/4	-3/16	-1/2	-1/2	1/2	1/6	-5/8	1/6	2/3	1/3	1/9	1/9	4/3	0	0	0	1	0	0	-22/9	-5/6	5/8
bh	-1/2	1/3	-5/4	-3/16	-1/2	-1/2	1/2	1/6	-5/8	1/6	2/3	1/3	1/9	1/9	4/3	0	0	0	1	0	0	-22/9	-5/6	5/8
cd	0	0	0	-9/8	-3	0	0	0	0	1	0	0	0	0	-2	4	0	0	-3	0	0	-8/3	0	-5/2
ce	0	0	0	-45/16	3/2	0	0	0	0	1	0	0	0	0	-2	3	0	0	3/2	0	0	-8/3	0	-5/2
cf	-1	5/3	-5/4	-21/16	-1/2	-1	5/2	5/6	-5/8	-7/3	-2/3	-1/3	-10/9	5/6	-2	-5/3	10/9	-5/6	1/6	5/9	-5/12	14/27	5/18	5/8
cg	1/2	-5/6	5/8	-39/16	1	1/2	-5/4	-5/12	5/16	1/6	1/3	1/6	5/9	-5/12	-2	-5/3	10/9	-5/6	1/6	5/9	-5/12	14/27	5/18	5/8
ch	1/2	-5/6	5/8	-39/16	1	1/2	-5/4	-5/12	5/16	1/6	1/3	1/6	5/9	-5/12	-2	-5/3	10/9	-5/6	1/6	5/9	-5/12	14/27	5/18	5/8
de	0	0	0	27/16	0	0	0	0	0	-3	0	0	0	0	-2	-3	0	0	3/2	0	0	-8/3	0	-5/2
df	-1	5/3	-5/4	-45/16	0	1	1/2	-5/6	5/8	-1	2/3	7/3	10/9	-5/6	-2	5/3	-10/9	5/6	1/6	5/9	-5/12	14/27	5/18	5/8
dg	1/2	-5/6	5/8	9/16	0	-1/2	-1/4	1/2	-5/6	-5/2	-1/3	-7/6	-5/9	5/12	-2	5/3	-10/9	5/6	1/6	5/9	-5/12	14/27	5/18	5/8
dh	1/2	-5/6	5/8	9/16	0	-1/2	-1/4	5/12	-5/16	-5/2	-1/3	-7/6	-5/9	5/12	-2	5/3	-10/9	5/6	1/6	5/9	-5/12	14/27	5/18	5/8
ef	0	0	0	-9/8	0	-2	-1	5/3	-5/4	-1	8/3	-2/3	10/9	-5/6	4/3	0	0	0	-7/3	-10/9	5/6	14/27	5/18	5/8
eg	0	0	0	-45/16	0	1	1/2	-5/6	5/8	-5/2	-4/3	1/3	-5/9	5/12	4/3	0	0	0	-7/3	-10/9	5/6	14/27	5/18	5/8
eh	0	0	0	-45/16	0	1	1/2	-5/6	5/8	-5/2	-4/3	1/3	-5/9	5/12	4/3	0	0	0	-7/3	-10/9	5/6	14/27	5/18	5/8
fg	0	0	0	27/16	0	0	0	0	0	3/2	0	0	0	0	-4	0	0	0	-3	0	0	-8/3	0	-5/2
fh	0	0	0	27/16	0	0	0	0	0	3/2	0	0	0	0	-4	0	0	0	-3	0	0	-8/3	0	-5/2
gh	0	0	0	-27/8	0	0	0	0	0	-3	0	0	0	0	-4	0	0	0	-3	0	0	-8/3	0	-5/2

Having found the matrix of H in this way it is a simple matter to find the matrix of unity, for if we neglect the integrals arising from the lack of orthogonality of the eigenfunctions, d_{ij} is just the coefficient of C in H_{ij}. If the various interchange integrals and the coulombic integral can be found, we can, therefore, set up the secular equation and complete the first order perturbation theory.

Since the bond eigenfunctions are not orthogonal, the secular equation contains E in every element. It is more convenient for numerical work to orthogonalize the fourteen bond eigenfunctions. The set of orthogonalized eigenfunctions is shown in Table III. The first eigenfunction in this table is just the first of the set of bond eigenfunctions of Table II. Each succeeding one is obtained by orthogonalizing the corresponding bond eigenfunction to the eigenfunctions occurring earlier in the table.

It is not as simple to compute the matrix components between these eigenfunctions as it was for the bond eigenfunctions themselves. It was found best to express these eigenfunctions in terms of the Slater eigenfunctions and compute the matrix elements from the rules for forming matrix components between the Slater eigenfunctions. The results are shown in Table IV. In the calculation of these matrix elements each eigenfunction was multiplied by the arbitrary factor $1/(2)^{\frac{1}{2}}$.

The greatest advantage gained by the orthogonalization comes from the fact that in symmetrical configurations and also some configurations in which some of the interchange integrals can be neglected a proper assignment of letters to

the atoms will give a secular equation which may immediately be factored into smaller determinants. A brief inspection of the various possibilities is usually sufficient to determine the correct assignment of the letters in these cases. It is, of course, always convenient to make as many matrix components zero as possible and important that the maximum number of these fall in a particular row or column. Having done this, three evaluations of the determinant for proper choices of E ordinarily suffice to estimate the lowest root of the equation.

Not every choice of fourteen independent bond eigenfunctions would lead to orthogonal eigenfunctions which have as simple matrix components as the set chosen here. To secure simplicity each bond eigenfunction should differ from the others as little as possible without losing independence.

The seven electron problem is, of course, simply a special case of the eight-electron problem in which one of the electrons is at infinity. This amounts simply to setting equal to zero all the integrals containing one particular letter, say h.

The problem still remains: to what systems do these simplified calculations apply? At present this question seems best answered by a detailed application to a variety of cases. One of these cases we have already referred to and others are being investigated. In any case it seems logical to consider first the approximations given here, since the results may readily be extended to include the neglected multiple interchange integrals and orthogonality integrals should this be found desirable.