

Hybridization in ML_k ($k > 2$) Systems

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This paper describes a generalized and extended treatment of the preceding papers in which the maximum overlap method was employed but the results were limited by the condition that the number of ligands surrounding the central atom should be two, that is, $k = 2$ in molecule ML_k . Based on the special assumption that the angles $\angle L_pML_q = \alpha$ between any two $M-L_j$ bonds in molecule ML_k are equal, many general formulas related to the diagonal matrix $D(\lambda)$, unitary matrix U^T , overlap matrix S_1 and the bond strength F are derived. The properties of matrix SS^T are also discussed.

1. A SHORT REVIEW

In the preceding papers of this series^{1,2}, we began with the maximum overlap method proposed by Murrell³ and simplified and developed by Golebiewski⁴, Lykos and Schmeising⁵, and Maksić *et al.*^{6,7}, according to the concept of bond strength pointed out by Mulliken⁸. The bond strength, bond angle and the composition of a given orbital with orbital angular momentum quantum number l of a hybrid atomic orbital (HAO) were discussed for molecule ML_k where k equals two. In the present case, the treatment will be extended to $k > 2$.

The same notation is used as in the preceding papers. For the type of molecule ML_k which is constructed by simple σ bond $M-L_j$, the atomic orbitals (AO) of the central atom are represented by χ_i , its HAO by ψ_i . Both of them are real and orthonormal wave functions and are denoted by row matrices $X = (\chi_1 \dots \chi_n)$ and $\bar{\Psi} = (\psi_1 \dots \psi_n)$, respectively. We have

$$\bar{\Psi} = XA^T \quad (1)$$

where A is a coefficient matrix of order n which is self-adjoint ($AA^T = I$), T means a transpose and I is the unit matrix. The AOs of k ligands L_1, \dots, L_k are denoted by $\omega_1 \dots \omega_k$, respectively, and may also be represented by a row matrix $\Omega = (\omega_1 \dots \omega_k \ 0 \dots 0)$ in which $k \leq n$.

In the practical procedure of using the maximum overlap method, the first step is to find a $k \times n$ overlap matrix between the AOs of ligands and AOs of the central atom, as shown below:

$$S = \begin{vmatrix} \langle \omega_1 \chi_1 \rangle & \dots & \langle \omega_1 \chi_n \rangle \\ \vdots & & \vdots \\ \langle \omega_k \chi_1 \rangle & \dots & \langle \omega_k \chi_n \rangle \end{vmatrix} \quad (2)$$

Then, a symmetric matrix SS^T of order k is obtained, which can be diagonalized by a similarity transformation yielding a diagonal matrix $D(\lambda)$ with elements of $\lambda_1, \dots, \lambda_k$. Taking the positive values of the square root of these diagonal elements, an overlap matrix between the AOs of ligands and the HAOs of the central atom

$$S_1 = U^T D(\sqrt{\lambda}) U \quad (3)$$

can then be obtained where S_1 has the maximum trace. Furthermore, using matrix S_1^{-1} , the combination coefficients of AOs to form HAOs of the central atom can be determined.

Since the bond strength F_j of bond $M-L_j$ is, according to Mulliken⁸, equal to the overlap integral between the orbital of ligand L_j and the corresponding best HAO of central atom M , we have an universal formula of the bond strength which may be expressed in the following form:

$$F_j = (S_1)_{jj} = \langle \omega_j | \psi_j \rangle = (SS^T)_{jj}^{1/2} = [U^T D(\sqrt{\lambda}) U]_{jj} = \sum_{n=1}^k \sqrt{\lambda_n} u_{nj}^2 \quad (4)$$

$j = 1, 2, \dots, k$

2. COMMENT ON MATRIX SS^T

We have seen in the procedure outlined above that the most important step is to find an unitary matrix for the diagonalization of the symmetric matrix SS^T . After this step is completed, the successive steps will be easy. We now discuss the elements of matrix SS^T under some approximations for the case of $k > 2$. The spherical function $Y_{lm}(\vartheta, \varphi)$ is utilized in its complex form. We shall consider a Hermitian matrix of order k constructed by overlap matrix S (Eq. (2)):

$$SS^* = \begin{pmatrix} \sum_{i=1}^n |\langle \omega_1 \chi_i \rangle|^2 & \sum_{i=1}^n \langle \omega_1 \chi_i \rangle \langle \omega_2 \chi_i \rangle^* & \cdots & \sum_{i=1}^n \langle \omega_1 \chi_i \rangle \langle \omega_k \chi_i \rangle^* \\ \sum_{i=1}^n \langle \omega_2 \chi_i \rangle \langle \omega_1 \chi_i \rangle^* & \sum_{i=1}^n |\langle \omega_2 \chi_i \rangle|^2 & \cdots & \sum_{i=1}^n \langle \omega_2 \chi_i \rangle \langle \omega_k \chi_i \rangle^* \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^n \langle \omega_k \chi_i \rangle \langle \omega_1 \chi_i \rangle^* & \sum_{i=1}^n \langle \omega_k \chi_i \rangle \langle \omega_2 \chi_i \rangle^* & \cdots & \sum_{i=1}^n |\langle \omega_k \chi_i \rangle|^2 \end{pmatrix} \quad (5)$$

where symbol $+$ means a complex-conjugate transpose.

Assume that the radial parts of χ_i are all equal and could be neglected, that is, only their angular parts of atom M are to be considered. We set

$$\chi_i = \sqrt{4\pi} Y_i(\vartheta, \varphi) = \sqrt{4\pi} Y_{lm}(\vartheta, \varphi), \quad i = 1, 2, \dots, n \quad (6)$$

The second approximation is that the projection method is employed, i. e. the function of ligand L_p is only to determine the direction of bond $M-L_p$, to define the projected value of χ_i in that direction and the actual value of the overlap integral $\langle \omega_p \chi_i \rangle$ is not necessary, then

$$\begin{aligned} \langle \omega_p \chi_i \rangle &= \sqrt{4\pi} \langle \omega_p Y_i \rangle \sqrt{4\pi} Y_{lm}(\vartheta_p, \varphi_p) \\ &= \sqrt{(2l+1) \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \varphi_p) e^{im\varphi_p} \end{aligned} \quad (7)$$

Now the off-diagonal element of matrix SS^T is

$$\begin{aligned} (SS^+)_{pq} &= \sum_{i=1}^n \langle \omega_p \chi_i \rangle \langle \omega_q \chi_i \rangle^* \\ &= \sum_{i=1}^n 4\pi Y_i(\vartheta_p, \varphi_p) Y_i^*(\vartheta_q, \varphi_q) \\ &= \sum_{i=1}^n (2l+1) \frac{(l-m)!}{(l+m)!} P_l^m(\cos \vartheta_p) P_l^m(\cos \vartheta_q) e^{im(\varphi_p - \varphi_q)} \end{aligned}$$

The symbol of summation means that it is necessary to sum up all AOs which participate in the HAO. If a group of orbitals with definite orbital angular momentum quantum number l is chosen to participate in HAO, there are $(2l+1)$ AOs contained in the sum, but all AOs of $l=0$ through to $l=l_{\max}$ need not be taken into account, namely

$$\sum_{i=1}^n = \sum_{l=0}^{l_{\max}} \sum_{m=-l}^l \quad (8)$$

Hence, we write

$$\begin{aligned} (SS^+)_{pq} &= \sum_l (2l+1) \sum_{m=-l}^l \frac{(l-m)!}{(l+m)!} P_l^m(\cos \vartheta_p) P_l^m(\cos \vartheta_q) e^{im(\varphi_p - \varphi_q)} \\ &= \sum_l (2l+1) P_l(\cos \alpha), \end{aligned} \quad (9)$$

where $\alpha = \angle L_p M L_q$ is the angle between the bonds of $M-L_p$ and $M-L_q$, *i. e.* the angle between the orientations of (ϑ_p, φ_p) and (ϑ_q, φ_q) and it satisfies the trigonometric identity

$$\cos \alpha = \cos \vartheta_p \cos \vartheta_q + \sin \vartheta_p \sin \vartheta_q \cos(\varphi_p - \varphi_q). \quad (10)$$

We have used the addition formula of spherical harmonics⁹ to deduce Eq. (9), which is a general relationship and applicable to all off-diagonal elements of matrix SS^+ .

The off-diagonal elements of SS^+ are real since they are composed of Legendre polynomials. The value of $(SS^+)_{pq}$ is only determined by bond angle $\alpha = \angle L_p M L_q$ under the approximations mentioned above. Therefore, if the angles between any two $M-L_p$ and $M-L_q$ bonds in molecule ML_k are equal, the off-diagonal elements of matrix SS^+ have the same value.

Considering the diagonal elements of SS^+ , in this situation, $\vartheta_p = \vartheta_q$, $\varphi_p = \varphi_q$, $\alpha = 0$, $\cos \alpha = 1$ and $P_l(1) = 1$. Eq. (9) becomes

$$(SS^+)_{pp} = \sum_l (2l+1). \quad (11)$$

Thus, the diagonal elements are independent of the bond angle. In fact, they are equal to the number of AOs taking part in the hybridization. We

also see that diagonal elements of SS^+ are real, implying that the matrix is real and symmetrical. In fact, we usually use the real form of AOs, so that matrix SS^+ may be generally written as SS^T .

3. DIAGONALIZATION OF SS^T

Let's assume that the angles between any two bonds $M-L_p$ and $M-L_q$ are equal. Setting

$$\begin{aligned}
 (SS^T)_{pp} &= \sum_{i=1}^n \langle \omega_p \chi_i \rangle^2 = \sum_l (2l + 1) = a, \\
 (SS^T)_{pq} &= \sum_{i=1}^n \langle \omega_p \chi_i \rangle \langle \omega_q \chi_i \rangle = \sum_l (2l + 1) P_l(\cos a) = c
 \end{aligned}
 \tag{12}$$

matrix SS^T has the same form as that of the determinant considered in Eq. (A-1) (See Appendix):

$$SS^T = \begin{pmatrix} a & c & c & \cdots & c \\ c & a & c & \cdots & c \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ c & c & c & \cdots & a \end{pmatrix} (k).
 \tag{13}$$

In order to find the eigenvalues λ of SS^T , we take

$$\begin{vmatrix} x & -1 & -1 & \cdots & -1 \\ -1 & x & -1 & \cdots & -1 \\ -1 & -1 & x & \cdots & -1 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ -1 & -1 & -1 & \cdots & x \end{vmatrix} = 0,
 \tag{14}$$

(k)

where $x = (a - \lambda)/(-c)$ or the eigenvalue $\lambda = a + cx$. Using Eq. (A-2) (See Appendix) we have

$$x_1 = k - 1 \quad \text{and} \quad x_i = -1, \quad (i = 2, 3, \dots, k)$$

thus, from the relationship of λ and x , we find:

$$\begin{cases} \lambda_1 = a + (k - 1)c \\ \lambda_2 = \lambda_3 = \dots = \lambda_k = a - c \end{cases}
 \tag{15}$$

Hence, the corresponding diagonal matrix takes the following form:

$$D(\lambda) = \begin{pmatrix} a + (k - 1)c & & & & \\ & & & & 0 \\ & & & & \\ & & & & \\ & & & & \end{pmatrix}
 \tag{16}$$

and

$$D(\sqrt{\lambda}) = \begin{pmatrix} \sqrt{a + (k-1)c} & & & 0 \\ & \sqrt{a-c} & & \\ & & \ddots & \\ & & & \sqrt{a-c} \end{pmatrix} (k), \quad (17)$$

where the sign of square roots $\sqrt{\lambda}$ is taken as positive to satisfy the requirement of the maximum overlap principle, and we obtain

$$\text{Tr } S_1 = \text{Tr } D(\sqrt{\lambda}) = \sqrt{a + (k-1)c} + (k-1)\sqrt{a-c} = \text{maximum} \quad (18)$$

Since equivalent hybridization is considered, HAOs have the same bond strength but differ only in the direction in space, and one gets:

$$F_1 = F_2 = \dots = F_k = F$$

and therefore

$$F = \frac{1}{k} \text{Tr } S_1 = \frac{1}{k} [\sqrt{a + (k-1)c} + (k-1)\sqrt{a-c}]. \quad (19)$$

Parameter k is the number of ligands, and a is the total number of AOs taking part in the HAOs. Both of them are constants, but the value of c , from Eq. (12), is a variable depending on the bond angle α if the approximation of the projection method is adopted. We may take the condition of $\partial F/\partial c = 0$ to find the characteristic angles at which the bond strength has a maximum. The results shows that the value of F reaches a maximum if

$$c = \sum_l (2l+1) P_l(\cos \alpha) = 0 \quad (20)$$

is satisfied, so that

$$F_{\max} = \sqrt{a} = \sqrt{\sum (2l+1)}. \quad (21)$$

The value of F_{\max} is determined only by the number of AOs used in constructing the HAOs. All the results obtained in the previous work for $k = 2$ are effective for the systems of $k > 2$.

4. MATRIX OF EIGENVECTORS

Inserting the first eigenvalue λ_1 into matrix equation of SS^T

$$(SS^T) U_1^T = \lambda_1 U_1^T, \quad \lambda_1 = a + (k-1)c$$

and using the condition of normalization

$$u_{11}^2 + u_{21}^2 + \dots + u_{k1}^2 = \sum_{i=1}^k u_{i1}^2 = 1,$$

this result is readily obtained:

$$k u_{i1}^2 = 1$$

and therefore

$$u_{i1} = \frac{1}{\sqrt{k}} \quad (22)$$

in which the positive sign has been taken, and the first eigenvector is

$$U_1 = (1/\sqrt{k} \quad 1/\sqrt{k} \dots 1/\sqrt{k}).$$

Since from the second to the k -th all eigenvalues are of the same value, $\lambda_2 = a - c$, after inserting λ_2 into the matrix equation of SS^T , it becomes a matrix composed of c for every element. This means that the basis vectors may be chosen as $(1 - 1 0 \dots 0)$, $(1 0 - 1 \dots 0)$, $(1 0 0 - 1 \dots 0)$, $\dots (1 0 0 \dots -1)$, and an arbitrary vector in the vector space can be expressed by the linear combination of the basis. We use the Schmidt orthogonalization process to form the eigenvectors of $U_2^T, U_3^T, \dots U_k^T$, the j -th row vector being

$$U_j = (1/\sqrt{j(j-1)} \quad 1/\sqrt{j(j-1)} \dots 1/\sqrt{j(j-1)} - \sqrt{(j-1)/j} \quad 0 \dots 0) \tag{23}$$

and the whole matrix of the eigenvectors is

$$U^T = \begin{pmatrix} \frac{1}{\sqrt{k}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{20}} & \dots & \frac{1}{\sqrt{k(k-1)}} \\ \frac{1}{\sqrt{k}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{20}} & \dots & \frac{1}{\sqrt{k(k-1)}} \\ \frac{1}{\sqrt{k}} & 0 & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{20}} & \dots & \frac{1}{\sqrt{k(k-1)}} \\ \frac{1}{\sqrt{k}} & 0 & 0 & -\frac{3}{\sqrt{12}} & \frac{1}{\sqrt{20}} & \dots & \frac{1}{\sqrt{k(k-1)}} \\ \frac{1}{\sqrt{k}} & 0 & 0 & 0 & -\frac{4}{\sqrt{20}} & \dots & \frac{1}{\sqrt{k(k-1)}} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{k}} & 0 & 0 & 0 & \dots & \dots & -\frac{k-1}{\sqrt{k(k-1)}} \end{pmatrix} \tag{24}$$

From Eq. (3), we obtain

$$S_1 = U^T \begin{pmatrix} \sqrt{\lambda_1} & & & & & & \\ & \sqrt{\lambda_2} & & & & & \\ & & \sqrt{\lambda_2} & & & & \\ & & & \ddots & & & \\ & & & & \ddots & & \\ & & & & & \ddots & \\ & & & & & & \sqrt{\lambda_2} \end{pmatrix} U, \quad \begin{cases} \sqrt{\lambda_1} = \sqrt{a + (k-1)c} \\ \sqrt{\lambda_2} = \sqrt{a - c} \end{cases}$$

the diagonal elements in the resultant matrix S_1 are in the same form as

$$\frac{\sqrt{\lambda_1}}{k} + \sqrt{\lambda_2} \left[\frac{1}{2 \cdot 1} + \frac{1}{3 \cdot 2} + \frac{1}{4 \cdot 3} + \frac{1}{5 \cdot 4} + \dots + \frac{1}{k(k-1)} \right]$$

Comparing this with Eq. (A-3) (See Appendix) yields

$$(S_1)_{jj} = \frac{\sqrt{\lambda_1}}{k} + \left(\frac{k-1}{k} \right) \sqrt{\lambda_2} = \frac{1}{k} [\sqrt{\lambda_1} + (k-1) \sqrt{\lambda_2}] \tag{25}$$

The off-diagonal elements of S_1 have similar forms to

$$\frac{\sqrt{\lambda_1}}{k} + \sqrt{\lambda_2} \left[-\frac{1}{2 \cdot 1} + \frac{1}{3 \cdot 2} + \frac{1}{4 \cdot 3} + \frac{1}{5 \cdot 4} + \dots + \frac{1}{k(k-1)} \right], \quad (\sim p = 2)$$

$$\frac{\sqrt{\lambda_1}}{k} + \sqrt{\lambda_2} \left[-\frac{2}{3 \cdot 2} + \frac{1}{4 \cdot 3} + \frac{1}{5 \cdot 4} + \frac{1}{6 \cdot 5} + \dots + \frac{1}{k(k-1)} \right], \quad (\sim p = 3)$$

$$\frac{\sqrt{\lambda_1}}{k} + \sqrt{\lambda_2} \left[-\frac{3}{4 \cdot 3} + \frac{1}{5 \cdot 4} + \frac{1}{6 \cdot 5} + \frac{1}{7 \cdot 6} + \dots + \frac{1}{k(k-1)} \right], \quad (\sim p = 4)$$

Comparing the above results with Eq. (A-4) (See appendix), we have

$$(S_1)_{ij(i \neq j)} = \frac{1}{k} (\sqrt{\lambda_1} - \sqrt{\lambda_2}).$$

Thus, the whole matrix of S_1 is

$$S_1 = \frac{1}{k} \begin{pmatrix} \sqrt{\lambda_1} + (k-1)\sqrt{\lambda_2} & \sqrt{\lambda_1} - \sqrt{\lambda_2} & \dots & \sqrt{\lambda_1} - \sqrt{\lambda_2} \\ \sqrt{\lambda_1} - \sqrt{\lambda_2} & \sqrt{\lambda_1} + (k-1)\sqrt{\lambda_2} & \dots & \sqrt{\lambda_1} - \sqrt{\lambda_2} \\ \vdots & \vdots & \ddots & \vdots \\ \sqrt{\lambda_1} - \sqrt{\lambda_2} & \sqrt{\lambda_1} - \sqrt{\lambda_2} & \dots & \sqrt{\lambda_1} + (k-1)\sqrt{\lambda_2} \end{pmatrix} \quad (27)$$

and therefore the bond strength for every single bond is

$$F = \frac{1}{k} [\sqrt{\lambda_1} + (k-1)\sqrt{\lambda_2}] = \frac{1}{k} [\sqrt{a + (k-1)c} + (k-1)\sqrt{a-c}], \quad (28)$$

this is in accordance with Eq. (19) for the case of equivalent hybridization. It should be noted that identical bond angles imply equivalent hybridization, but we cannot inversely say that the bond angles should be identical given equivalent hybridization. For example, in octahedral coordination the hybrid orbitals of the central atom may be equivalent, but the bond angles are different (the angles between the bonds at neighbouring sites are 90° while the angle between the bonds at the opposite sites is 180°).

The equations derived above are quite general and may be useful in some other theoretical work, but in practice, there are few kinds of molecules that satisfy the condition that the bond angles should be identical. Among these are the trigonal pyramid, including trigonal planar geometry, for $k = 3$, and tetrahedral geometry for $k = 4$.

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APPENDIX

First let us consider a determinant

$$D = \begin{vmatrix} a & c & c & \dots & c \\ c & a & c & \dots & c \\ c & c & a & \dots & c \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ c & c & c & \dots & a \end{vmatrix} \quad (n) \quad (\text{A-1})$$

the characteristic of which is that $n-1$ off-diagonal elements in every row are equal to the same value of c , except for the diagonal ones. Adding the second, third, ... and n -th columns to the first column yields

$$D = [a + (n-1)c] \begin{vmatrix} 1 & c & c & \dots & c \\ 1 & a & c & \dots & c \\ 1 & c & a & \dots & c \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ 1 & c & c & \dots & a \end{vmatrix} \quad (n)$$

Multiplying the first row by (-1) and adding it to every other rows gives

$$D = [a + (n-1)c] \begin{vmatrix} 1 & c & c & \dots & c \\ 0 & a-c & 0 & \dots & 0 \\ 0 & 0 & a-c & \dots & 0 \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ 0 & 0 & 0 & \dots & a-c \end{vmatrix} \quad (n) \quad (\text{A-2})$$

$$D = [a + (n-1)c] (a-c)^{n-1}.$$

Second, we consider the sum of a series:

$$\begin{aligned} \sum_{j=2}^k \frac{1}{j(j-1)} &= \frac{1}{2 \cdot 1} + \frac{1}{3 \cdot 2} + \frac{1}{4 \cdot 3} + \dots + \frac{1}{k(k-1)} \\ &= \left(1 - \frac{1}{2}\right) + \left(\frac{1}{2} - \frac{1}{3}\right) + \left(\frac{1}{3} - \frac{1}{4}\right) + \dots + \left(\frac{1}{k-1} - \frac{1}{k}\right) \\ &= 1 - \frac{1}{k} = \frac{k-1}{k}. \end{aligned} \quad (\text{A-3})$$

In the same way, we obtain

$$\begin{aligned} -\frac{1}{p} + \sum_{j=p+1}^k \frac{1}{j(j-1)} &= -\frac{1}{p} + \frac{1}{p(p+1)} + \frac{1}{(p+2)(p+1)} + \dots + \frac{1}{k(k-1)} \\ &= \left(1 - \frac{1}{p}\right) + \left(\frac{1}{p} - \frac{1}{p+1}\right) + \left(\frac{1}{p+1} - \frac{1}{p+2}\right) + \dots + \left(\frac{1}{k-1} - \frac{1}{k}\right) - 1 \\ &= 1 - \frac{1}{k} - 1 = -\frac{1}{k}. \end{aligned} \quad (\text{A-4})$$

SAŽETAK**Hibridizacija u ML_k ($k > 2$) sustavima***Frank Liu i Chang-Guo Zhan*

Razmatrana je matrična metoda maksimalnog prekrivanja (Murrell) i razjašnjena mnoga posebna svojstva matrica koje se koriste u računima.