Irreducible bases in icosahedral group space

Shi-Hai Dong

Institute of High Energy Physics, P.O. Box 918(4), Beijing 100039, The People’s Republic of China

Xi-Wen Hou

Institute of High Energy Physics, P.O. Box 918(4), Beijing 100039,
and Department of Physics, University of Three Gorges, Yichang 443000, The People’s Republic of China

Mi Xie

Department of Physics, Tianjin Normal University, Tianjin 300074

Zhong-Qi Ma *

Institute of High Energy Physics, P.O.Box 918(4), Beijing 100039, The People’s Republic of China

The irreducible bases in the icosahedral group space are calculated explicitly by reducing the regular representation. The symmetry adapted bases of the system with I or I_h symmetry can be calculated easily and generally by applying those irreducible bases to wavefunctions of the system, if they are not vanishing. As examples, the submatrices of the Hückel Hamiltonians for Carbon-60 and Carbon-240 are re-calculated by the irreducible bases.

Keywords: Irreducible bases  icosahedral group  Carbon-60

Running head: Irreducible bases in icosahedral group space

*Electronic address: MAZQ@BEPC3.IHEP.AC.CN
I. INTRODUCTION

Fullerenes (Kroto 1988, Huffman 1991, Pennis 1991), such as $B_{12}H_{12}, C_{20}H_{20}$ and $C_{60}$, are intriguing cage-like molecules of carbon atoms with the icosahedral symmetry. This discovery (Rohlfing et al. 1984, Kroto et al. 1985, Weeks and Harter 1989) has greatly drawn attentions of chemists and physicists (Deng and Yang 1992, Chou and Yang 1993, Friedberg and Lee 1992). With the development of experimental techniques in high resolution spectroscopy, many new data on vibrational spectra of polyatomic molecules with the symmetry $I_h$ were observed and analyzed (Negri and Orlandi 1996, Olthof et al. 1996, Giannozzi and Baroni 1994, Schettino et al. 1994, Gunnarsson et al. 1995, Doye and Wales 1996, Wang et al. 1996, Tang et al. 1996, Tang and Huang 1997). The vibrational modes, the force fields, and the spin-orbit coupling coefficients for icosahedral molecules were studied in some detail (Clougherty and Gorman 1996, Martínez-Torres et al. 1996, Varga et al. 1996, Fowler and Ceulemans 1985).

As is well known, symmetry analysis provides a powerful tool for classifying energy levels and organizing experimental data. In explaining the vibrational spectra of polyatomic molecules, the symmetry adapted bases (SAB) play an important role in simplifying the calculations (Lemus and Frank 1994, Ma et al. 1996, Chen et al. 1996). The SAB are defined as the orthogonal bases that belong to given rows of given irreducible representations of the symmetry group. In those studies, SAB of the system with the $I_h$ symmetry were widely used. Therefore, the properties of the $I_h$ group are worthy to be studied in some detail, although the dimension of the $I_h$ group space is 120.

Early works on $I$ group are mainly concerned with the construction of the representations of $I$ subduced by $D^I$ of SO(3) group and the 3j- and 6j-symbols (McLellan 1961, Golding 1973, Pooler 1980, Brown 1987). Liu-Ping-Chen (1990) enumerated the 60 elements of icosahedral group $I$, listed its group table, and calculated the irreducible representation matrices of all the 60 elements explicitly. The character tables of the point groups and the double point groups were listed (Altmann and Herzig 1994, Balasubramanian 1996). Recently, Chen and Ping (1997) constructed the point-group symmetrized boson representation, and gave the explicit expressions of the SAB for seven important cases of the molecule $B_{12}H_{12}$.

As another approach, in this paper we will explicitly calculate the irreducible bases $\psi^\Gamma_{\mu\nu}$ in the group spaces of $I$ and $I_h$ by reducing the regular representation of $I$:

$$R \psi^\Gamma_{\mu\nu} = \sum_\rho \psi^\Gamma_{\rho\nu} D^\Gamma_{\rho\mu}(R), \quad R \psi^\Gamma_{\mu\nu} R = \sum_\rho D^\Gamma_{\rho\mu}(R) \psi^\Gamma_{\rho\nu}, \quad R \in I.$$  \hspace{1cm} (1)

where $D^\Gamma$ is an irreducible representation of $I$, and $\psi^\Gamma_{\mu\nu}$ is a combination of the group elements. Applying those irreducible bases to any function $F(x)$, if it is not vanishing, one will obtain the SAB $\psi^\Gamma_{\mu\nu} F(x)$:

$$R \{ \psi^\Gamma_{\mu\nu} F(x) \} = \sum_\rho \{ \psi^\Gamma_{\rho\nu} F(x) \} D^\Gamma_{\rho\mu}(R).$$  \hspace{1cm} (2)

It is an unified and straightforward way to calculate the SAB of the system with the $I_h$ symmetry.
By the way, we would like to point out that the rank of group $I$ is two, not three (McLellan 1961, Liu et al. 1990, Lomont 1959). It means that all 60 elements of $I$ can be expressed as the products of only two generators.

The plan of this paper is as follows. In Sec. II we will give our notations. In Sec. III the irreducible bases in the $I$ group space are calculated explicitly, and the irreducible bases of $I_h$ are easy to be calculated from those of $I$. Three examples are given to explain how to calculate the SAB in terms of those irreducible bases. A short conclusion is given in Sec. IV.

**II. NOTATIONS AND GENERATORS OF GROUP I**

A regular icosahedron is shown in Fig. 1. The vertices on the upper part are labeled by $A_j, 0 \leq j \leq 5$, and their opposite vertices by $B_j$. The $z$ and $y$ axes point from the center $O$ to $A_0$ and the midpoint of $A_2B_5$, respectively.

![Fig. 1](image-url)

The group $I$ has 6 five-fold axes, 10 three-fold axes, and 15 two-fold axes. One of the five-fold axes directs along $z$ axis, and the rest point from $B_j$ to $A_j$ $(1 \leq j \leq 5)$ with the polar angle $\theta_1$ and azimuthal angles $\varphi_j^{(1)}$. The rotations through $2\pi/5$ around those five-fold axes are denoted by $T_j$, $0 \leq j \leq 5$. The three-fold axes join the centers of two opposite faces. The polar angles of the first and last 5 axes are denoted by $\theta_2$ and $\theta_3$, respectively, and the azimuthal angles by $\varphi_j^{(2)}$. The rotations through $2\pi/3$ around those three-fold axes are denoted by $R_j, 1 \leq j \leq 10$. The two-fold axes join the midpoints of two opposite edges. The polar and azimuthal angles of the first, next and last 5 axes are $\theta_4, \theta_5, \varphi_j^{(1)}, \varphi_j^{(2)}, \pi$, and $\varphi_j^{(3)}$, respectively. The rotations through $\pi$ around those two-fold axes are denoted by $S_j, 1 \leq j \leq 15$. Those angles $\theta_i$ and $\varphi_j^{(i)}$ are given as follows:

\[
\begin{align*}
\tan \theta_1 &= 2, & \tan \theta_2 &= 3 - \sqrt{5}, & \tan \theta_3 &= 3 + \sqrt{5} = 2\eta^2, \\
\tan \theta_4 &= (\sqrt{5} - 1)/2 = p, & \tan \theta_5 &= (\sqrt{5} + 1)/2 = p^{-1}, \\
\varphi_j^{(1)} &= 2(j - 1)\pi/5, & \varphi_j^{(2)} &= (2j - 1)\pi/5, & \varphi_j^{(3)} &= (4j - 3)\pi/10, \\
p &= \eta + \eta^{-1}, & p^{-1} &= 1 + \eta + \eta^{-1}, & \eta &= \exp(-i2\pi/5).
\end{align*}
\]

(3)

It is easy to see from Fig. 1 that 12 elements $E, S_8, S_{12}, S_1, R_6^{\pm 1}, R_2^{\pm 1}, R_4^{\pm 1}$ and $R_{10}^{\pm 1}$ construct a subgroup $T$. Now, any element $R$ of $I$ can be expressed as a product of $T_0^a$ and an element $R_0^b S_{12}^c$ of the subgroup $T$:

\[
R = T_0^a R_0^b S_{12}^c.
\]

(4)

Owing to the relations:

\[
R_6 = S_1 T_0^2 S_1 T_0^4, \quad S_{12} = R_0^2 S_1 R_0,
\]

(5)

$T_0$ and $S_1$ are the generators of group $I$. The rank of $I$ is two.

**III. IRREDUCIBLE BASES IN $I$ AND $I_h$ GROUP SPACES**
It is convenient to choose the irreducible representations of $I$ such that the representation matrices of one generator $T_0$ are diagonal. Assume that the bases $\Phi_{\mu\nu}$ in the $I$ group space are the eigenstates of left-action and right-action of $T_0$:

$$T_0 \Phi_{\mu\nu} = \eta^\mu \Phi_{\mu\nu}, \quad \Phi_{\mu\nu} T_0 = \eta^\nu \Phi_{\mu\nu}, \quad \eta = \exp(-i2\pi/5), \quad \mu, \nu \ \mod \ 5.$$  (6)

The eigenstates can be easily calculated by the projection operator $P_\mu$ (see p.113 in Hamermesh 1962):

$$\Phi_{\mu\nu} = c \ P_\mu \ R \ P_\nu, \quad P_\mu = \frac{1}{5} \sum_{\lambda=-2}^{0} \eta^{-\mu \lambda} T_0^\lambda,$$  (7)

where $c$ is a normalization factor. The choice of the group element $R$ in (7) will not affect the results except for the factor $c$. In the following we choose $E$, $S_{11}$, $S_5$ and $S_{10}$ as the group element $R$, respectively, and obtain four independent sets of bases $\Phi^{(i)}_{\mu\nu}$:

$$\Phi^{(1)}_{\mu\nu} = \left( E + \eta^{-\mu} T_0 + \eta^{-2\mu} T_0^3 + \eta^{2\mu} T_0^3 + \eta^\mu T_0^5 \right) / \sqrt{5},$$

$$\Phi^{(2)}_{\mu\nu} = \left\{ S_{11} + \eta^{-\mu} S_{14} + \eta^{-2\mu} S_{12} + \eta^{2\mu} S_{15} + \eta^\mu S_{13} \right\} / \sqrt{5},$$

$$\Phi^{(3)}_{\mu\nu} = \left\{ (S_5 + \eta^{-\mu} R_6^2 + \eta^{-2\mu} T_4^2 + \eta^{2\mu} R_4^2 + \eta^\mu T_2^2) + \eta^{-2(\mu-\nu)} (S_2 + \eta^{-\mu} R_2^2 + \eta^{-2\mu} T_2^2 + \eta^{2\mu} R_2 + \eta^\mu R_1) ight.$$\n
$$+ \eta^{-2(\mu-\nu)} (S_2 + \eta^{-\mu} R_2^2 + \eta^{-2\mu} T_2^2 + \eta^{2\mu} R_2 + \eta^\mu R_1) + \eta^{-(\mu-\nu)} (S_1 + \eta^{-\mu} R_2^2 + \eta^{-2\mu} T_2^2 + \eta^{2\mu} T_3 + \eta^\mu R_5) \right\} / 5,$$  (8)

$$\Phi^{(4)}_{\mu\nu} = \left\{ (S_0 + \eta^{-\mu} T_2^2 + \eta^{-2\mu} R_6^2 + \eta^{2\mu} R_6 + \eta^\mu T_2^2) + \eta^{2(\mu-\nu)} (S_7 + \eta^{-\mu} R_2^2 + \eta^{-2\mu} R_2 + \eta^{2\mu} R_6 + \eta^\mu T_2^2) ight.$$\n
$$+ \eta^{2(\mu-\nu)} (S_7 + \eta^{-\mu} R_2^2 + \eta^{-2\mu} R_2 + \eta^{2\mu} R_6 + \eta^\mu T_2^2) + \eta^{-(\mu-\nu)} (S_0 + \eta^{-\mu} T_2^2 + \eta^{-2\mu} R_6^2 + \eta^{2\mu} R_6 + \eta^\mu T_2^2) \right\} / 5,$$

where and hereafter the subscript $\overline{\nu}$ denotes $-\nu$. Those bases $\Phi^{(i)}_{\mu\nu}$ should be combined into the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ that belong to the given irreducible representation $\Gamma$. The combinations can be determined from the condition that $\psi^{\Gamma}_{\mu\nu}$ should be the eigenstate of a class operator $W$, which was called CSCO-I by Chen and Ping (1997). The eigenvalues $\alpha_\Gamma$ can be calculated from the characters in the irreducible representations $\Gamma$ (see (3-170) in Hamermesh 1962):

$$W = \sum_{j=0}^{5} (T_j + T_j^3), \quad W \psi^{\Gamma}_{\mu\nu} = \psi^{\Gamma}_{\mu\nu} W = \alpha_\Gamma \psi^{\Gamma}_{\mu\nu},$$  (9)

$$\alpha_A = 12, \quad \alpha_{T_1} = 4p^{-1}, \quad \alpha_{T_2} = -4p, \quad \alpha_G = -3, \quad \alpha_H = 0.$$  

Now we calculate the matrix form of $W$ in the bases $\Phi^{(i)}_{\mu\nu}$, and diagonalize it. $\psi^{\Gamma}_{\mu\nu}$ are just the eigenvectors of the matrix form of $W$:

$$\psi^{\Gamma}_{\mu\nu} = N^{-1/2} \sum_{i=1}^{4} C_i \Phi^{(i)}_{\mu\nu},$$  (10)
where \( N \) is the normalization factor. In those bases \( \psi^\Gamma_{\mu\nu} \), the representation matrices are diagonal with the diagonal elements \( \eta^\mu \) (see (6)). In principle, each \( \psi^\Gamma_{\mu\nu} \) contains a free phase, and the representation matrices of another generator \( S_1 \) depend upon the choice of phases. We choose the phases such that the representation matrices of \( S_1 \) are as follows:

\[
D^A(S_1) = 1, \quad D^{T_1}(S_1) = \frac{1}{\sqrt{5}} \begin{pmatrix} -p^{-1} & -\sqrt{2} & -p \\ -\sqrt{2} & 1 & \sqrt{2} \\ -p & \sqrt{2} & -p^{-1} \end{pmatrix},
\]

\[
D^{T_2}(S_1) = \frac{1}{\sqrt{5}} \begin{pmatrix} -p & \sqrt{2} & p^{-1} \\ \sqrt{2} & -1 & \sqrt{2} \\ p^{-1} & \sqrt{2} & -p \end{pmatrix}, \quad D^G(S_1) = \frac{1}{\sqrt{5}} \begin{pmatrix} -1 & -p & -p^{-1} & 1 \\ -p & 1 & -1 & -p^{-1} \\ -p^{-1} & -1 & 1 & -p \\ 1 & -p^{-1} & -p & -1 \end{pmatrix},
\]

\[
D^H(S_1) = \frac{1}{5} \begin{pmatrix} p^{-2} & 2p^{-1} & \sqrt{6} & 2p & p^2 \\ 2p^{-1} & p^2 & -\sqrt{6} & -p^2 & -2p \\ \sqrt{6} & -\sqrt{6} & -1 & \sqrt{6} & \sqrt{6} \\ 2p & -p^{-2} & \sqrt{6} & p^2 & -2p^{-1} \\ p^2 & -2p & \sqrt{6} & -2p^{-1} & p^{-2} \end{pmatrix}.
\]

where the row (column) indices \( \mu \) of the irreducible representations \( \Gamma \) are put in the following order: 0 for \( A \), 1, 0, and \( \overline{1} \) for \( T_1 \), 2, 0, and \( \overline{2} \) for \( T_2 \), 2, 1, \( \overline{1} \), and \( \overline{2} \) for \( G \), and 2, 1, 0, \( \overline{1} \), and \( \overline{2} \) for \( H \). The representation matrices of some irreducible representations of \( I \) coincide with those in the subduced representations of \( D^\ell \) of SO(3):

\[
D^0(R) = D^A(R), \quad D^1(R) = D^{T_1}(R), \quad D^2(R) = D^H(R), \quad X^{-1}D^3(R)X = D^{T_2}(R) \oplus D^G(R), \quad R \in I,
\]

\[
X = \begin{pmatrix} 0 & 0 & -\sqrt{2/5} & 0 & 0 & 0 & \sqrt{3/5} \\ \sqrt{3/5} & 0 & 0 & -\sqrt{2/5} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \sqrt{3/5} & 0 & 0 & 0 & \sqrt{2/5} \\ \sqrt{2/5} & 0 & 0 & \sqrt{3/5} & 0 & 0 & 0 \end{pmatrix}.
\]

The normalization factors \( N \) and combination coefficients \( C_i \) in the expression (10) of \( \psi^\Gamma_{\mu\nu} \) are listed in Table I.

| Table 1 |

The group \( I_h \) is the direct product of \( I \) and the inversion group \{ \( E \), \( P \) \}, where \( P \) is the inversion operator. According to the parity, the irreducible representations of \( I_h \) are denoted as \( \Gamma_g \) (even) and \( \Gamma_u \) (odd) with the following irreducible bases:

\[
\psi^\Gamma_{\mu\nu} = 2^{-1/2} (E + P) \psi^\Gamma_{\mu\nu}, \quad \psi^{\Gamma_g}_{\mu\nu} = 2^{-1/2} (E - P) \psi^\Gamma_{\mu\nu}.
\]
The only problem is to determine the actions of group elements to the geometric meaning of linearly dependent on other states. Let us give three examples to explain the general method of calculating SAB.

**Ex. 1.** The eigenvalues and eigenfunctions of the Hückel Hamiltonian for Carbon-60.

Deng and Yang (1992) have calculated this problem by computer. Now we calculate the same problem in terms of the irreducible bases $\psi^\Gamma_{\nu\mu}$ even by hand. It is easy to see from Fig. 1 in Deng and Yang (1992) that there is one-to-two correspondence between their states $|a, b, c\rangle$ and the group elements $R$ and $PR'$ of $I_h$ in the following meaning:

$$R \ |1, 0, 1\rangle = PR' \ |1, 0, 1\rangle = |a, b, c\rangle, \quad R \text{ and } PR' \rightarrow |a, b, c\rangle. \quad (14)$$

where $R \in I$ and $R' \in I$. Introduce the new notation for the states:

$$|R\rangle = P \ |R'\rangle \equiv |a, b, c\rangle, \quad P |a, b, c\rangle = |\pi, b, c\rangle, \quad (15)$$

where the correspondence between $|a = 1, b\rangle$ and the elements $R$ and $PR'$ of $I_h$ is listed as follows:

$$R(R') |c = 1 \rangle = |c = 2 \rangle = |c = 3 \rangle = |c = 4 \rangle = |c = 5 \rangle = |c = 6 \rangle$$

$\begin{array}{ccccccc}
|b = 0 & E(S_{12}) & S_1(S_b) & R_2^a(T_4^a) & R_1(T_3^a) & T_3(T_2^a) & T_2(R_2^a) \\
|b = 1 & T_5(S_{15}) & R_2^a(T_4^a) & T_4(S_b) & S_2(R_2^a) & T_5(T_2^a) & R_2(R_1^a) \\
|b = 2 & T_5(S_{13}) & T_5(T_3^a) & R_1(R_2^a) & S_3(T_4^a) & R_3(S_{10}) & S_3(T_2^a) \\
|b = 3 & T_5(S_{11}) & T_5(R_7) & R_4(R_{10}^a) & T_7(T_2^a) & S_4(T_3^a) & R_3(S_b) \\
|b = 4 & T_5(S_{14}) & R_5(T_2^a) & S_5(S_b) & T_1(S_7) & R_3(R_2^a) & T_4(T_2^a) \\
\end{array}$

Substituting (16) into (8), we obtain:

$$P \ |\Phi^{(1)}_{\mu\nu}\rangle = \eta^{2\mu} \ |\Phi^{(2)}_{\mu\nu}\rangle, \quad P \ |\Phi^{(3)}_{\mu\nu}\rangle = \eta^{2\mu-\nu} \ |\Phi^{(4)}_{\mu\nu}\rangle. \quad (17)$$

Thus, some bases in (13) become vanishing or linearly dependent on other bases. The independent bases are listed as follows:

$$2^{-1/2} \ |\psi^{A_0}_{\mu\nu}\rangle = |\psi^{A}_{\mu\nu}\rangle, \quad |\psi^{T_1}_{\mu\nu}\rangle = |\psi^{T_2}_{\mu\nu}\rangle, \quad |\psi^{T_4}_{\mu\nu}\rangle = -|\psi^{T_4}_{\mu\nu}\rangle, \quad 2^{-1/2} \ |\psi^{T_4}_{\nu\mu}\rangle = |\psi^{T_1}_{\mu\nu}\rangle,$$

$$|\psi^{T_2}_{\mu\nu}\rangle = -|\psi^{T_2}_{\mu\nu}\rangle, \quad |\psi^{T_3}_{\mu\nu}\rangle = |\psi^{T_3}_{\mu\nu}\rangle, \quad 2^{-1/2} \ |\psi^{T_3}_{\nu\mu}\rangle = |\psi^{T_3}_{\mu\nu}\rangle, \quad |\psi^{G_3}_{\mu\nu}\rangle = |\psi^{G_3}_{\mu\nu}\rangle,$$

$$2^{-1/2} \ |\psi^{G_3}_{\mu\nu}\rangle = -|\psi^{G_3}_{\mu\nu}\rangle, \quad |\psi^{G_2}_{\mu\nu}\rangle = -|\psi^{G_2}_{\mu\nu}\rangle, \quad |\psi^{G_3}_{\mu\nu}\rangle = -|\psi^{G_2}_{\mu\nu}\rangle, \quad |\psi^{H_3}_{\mu\nu}\rangle = -|\psi^{H_3}_{\mu\nu}\rangle,$$

$$2^{-1/2} \ |\psi^{H_3}_{\mu\nu}\rangle = |\psi^{H_3}_{\mu\nu}\rangle, \quad |\psi^{H_2}_{\mu\nu}\rangle = -|\psi^{H_2}_{\mu\nu}\rangle, \quad |\psi^{H_3}_{\mu\nu}\rangle = -|\psi^{H_2}_{\mu\nu}\rangle, \quad |\psi^{H_3}_{\mu\nu}\rangle = |\psi^{H_2}_{\mu\nu}\rangle. \quad (18)$$

where an additional normalization factor $2^{-1/2}$ has to be introduced when

$$|\psi^{G_3}_{\mu\nu}\rangle = P |\psi^{G_3}_{\mu\nu}\rangle \quad \text{or} \quad |\psi^{G_3}_{\mu\nu}\rangle = -P |\psi^{G_3}_{\mu\nu}\rangle.$$
There are 90 bonds that are divided into two types (Deng and Yang 1992). The \( hp \) bonds separate a hexagon from a pentagon, and the others are called the \( hh \) bonds. Following the notation in Deng and Yang (1992), the Hückel interaction of the 60 \( hp \) bonds are equal to \(-\alpha\), and that of the 30 \( hh \) bonds equal to \((\alpha - 2)\). Now, since the states of \( C_6 \) are denoted by the elements \( R \) of \( I \), the action of Hamiltonian on the states can be written from (16) and the Figure in Deng and Yang (1992), for example:

\[
H |E\rangle = -\alpha |T_0\rangle - \alpha |T_0^4\rangle + (\alpha - 2) |S_1\rangle,
\]
\[
H |T_0\rangle = -\alpha |E\rangle - \alpha |T_0^5\rangle + (\alpha - 2) |R_5\rangle,
\]
\[
H |T_0^4\rangle = -\alpha |E\rangle - \alpha |T_0^3\rangle + (\alpha - 2) |R_5\rangle,
\]
\[
H |S_1\rangle = -\alpha |R_1\rangle - \alpha |R_5^2\rangle + (\alpha - 2) |E\rangle.
\]

We are only interested in the properties of \( H \) acting on \( |E\rangle \) and vice versa. The matrix of the Hamiltonian in the irreducible bases (18) is a hermitian and block one, which can be calculated by the standard method of group theory (Hamermesh 1962). For example, there are two sets of bases \( |\psi_{\mu_1}\rangle \) and \( |\psi_{\mu_0}\rangle \) for the representation \( T_{1u} \): 

\[
|\psi_{T_{1u}}^{11}\rangle = 8^{-1/2} \left\{ (\Phi_{11}^{(1)}) - \eta^2 (\Phi_{11}^{(2)}) - p^{-1} (\Phi_{11}^{(3)}) - p (\Phi_{11}^{(4)}) - p^{-1} \eta (\Phi_{11}^{(4)}) \right\}
\]
\[
|\psi_{T_{1u}}^{10}\rangle = (200)^{-1/2} \left\{ \sqrt{5} (|E\rangle + \eta^{-1} |T_0\rangle + \eta |T_0^3\rangle) + (-p^{-1} + p) |S_1\rangle + \cdots \right\},
\]
\[
|\psi_{T_{1u}}^{01}\rangle = 2^{-1/2} \left\{ -\eta (\Phi_{10}^{(3)}) + \eta p (\Phi_{10}^{(4)}) \right\} = (50)^{-1/2} \left\{ -|S_1\rangle + \cdots \right\},
\]
\[
|\psi_{T_{1u}}^{00}\rangle = 2^{-1} \left\{ |\Phi_{00}^{(1)}\rangle - |\Phi_{00}^{(2)}\rangle + |\Phi_{00}^{(3)}\rangle - |\Phi_{00}^{(4)}\rangle \right\}
\]
\[
= (10)^{-1} \left\{ \sqrt{5} (|E\rangle + |T_0\rangle + |T_0^4\rangle) + |S_1\rangle + \cdots \right\},
\]

where we only list the terms \(|E\rangle\), \(|T_0\rangle\), \(|T_0^4\rangle\), and \(|S_1\rangle\), which are relevant to the calculation.

Comparing the coefficients of the term \(|E\rangle\) on both sides of the following equations:

\[
H |\psi_{T_{1u}}^{11}\rangle = H_{11} |\psi_{T_{1u}}^{11}\rangle + H_{01} |\psi_{T_{1u}}^{10}\rangle,
\]
\[
H |\psi_{T_{1u}}^{10}\rangle = H_{10} |\psi_{T_{1u}}^{11}\rangle + H_{00} |\psi_{T_{1u}}^{10}\rangle,
\]
\[
H |\psi_{T_{1u}}^{01}\rangle = H_{11} |\psi_{T_{1u}}^{01}\rangle + H_{01} |\psi_{T_{1u}}^{00}\rangle,
\]
\[
H |\psi_{T_{1u}}^{00}\rangle = H_{10} |\psi_{T_{1u}}^{01}\rangle + H_{00} |\psi_{T_{1u}}^{00}\rangle,
\]

we obtain the submatrix of \( H \) for the representation \( T_{1u} \), which is of two dimensions:

\[
H_{T_{1u}} = \frac{1}{2\sqrt{5}} \begin{pmatrix}
-\alpha (7 - \sqrt{5}) + 4 & -4(\alpha - 2) \\
-4(\alpha - 2) & -2\alpha (2\sqrt{5} - 1) - 4
\end{pmatrix},
\]

\[
E_{T_{1u}} = \alpha (3 + \sqrt{5}) / 4 \pm \frac{1}{4} \left\{ 18\alpha^2 \left( 3 - \sqrt{5} \right) - 16\alpha \left( 5 - \sqrt{5} \right) + 64 \right\}^{1/2}.
\]

The advantage of this method is that the eigenfunctions of the Hamiltonian are able to be obtained simultaneously.

In the same way we can easily calculate the submatrices of the Hückel Hamiltonian for other
representations:

\[
\begin{align*}
H_{A_2} &= -\alpha - 2, & H_{T_{3s}} &= -\alpha \left(\sqrt{5} + 1\right)/2 + 2, & H_{T_{2s}} &= \alpha \left(\sqrt{5} - 1\right)/2 + 2, \\
H_{T_{2s}} &= \frac{1}{2\sqrt{5}} \begin{pmatrix}
\alpha(7 + \sqrt{5}) - 4 & 4(\alpha - 2) \\
4(\alpha - 2) & -2\alpha(2\sqrt{5} + 1) + 4
\end{pmatrix}, & H_{G_2} &= \frac{1}{2\sqrt{5}} \begin{pmatrix}
\alpha(\sqrt{5} + 1)/2 & -\alpha - 2 \\
-\alpha - 2 & -\alpha(\sqrt{5} - 1)/2
\end{pmatrix}, \\
H_{G_2} &= \frac{1}{2\sqrt{5}} \begin{pmatrix}
\alpha(\sqrt{5} + 1) + 8 & 2(\alpha - 2) \\
2(\alpha - 2) & \alpha(\sqrt{5} - 1) - 8
\end{pmatrix}, & H_{H_{s}} &= \frac{1}{2\sqrt{5}} \begin{pmatrix}
\alpha(7 + \sqrt{5}) - 4 & 4(\alpha - 2) \\
4(\alpha - 2) & -\alpha(\sqrt{5} - 1) - 4
\end{pmatrix}, \\
H_{H_{s}} &= \frac{1}{10} \begin{pmatrix}
\alpha(5\sqrt{5} + 11) - 12 & 4(\alpha - 2) & 4\sqrt{3}(\alpha - 2) \\
4(\alpha - 2) & -\alpha(5\sqrt{5} - 11) - 12 & -4\sqrt{3}(\alpha - 2) \\
4\sqrt{3}(\alpha - 2) & -4\sqrt{3}(\alpha - 2) & -22\alpha + 4
\end{pmatrix}.
\end{align*}
\]

The dimensions of the submatrices \( H^\Gamma \) are one or two except for \( H^{H_{s}} \), so that the energy levels of the Hückel Hamiltonian are able to be calculated by hand:

\[
\begin{align*}
E_{A_2} &= -\alpha - 2, & E_{T_{3s}} &= -\alpha \left(\sqrt{5} + 1\right)/2 + 2, & E_{T_{2s}} &= \alpha \left(\sqrt{5} - 1\right)/2 + 2, \\
E_{T_{2s}} &= -\alpha \left(3 - \sqrt{5}\right)/4 \pm \frac{1}{4} \left\{ 18\alpha^2 \left(3 + \sqrt{5}\right) - 16\alpha \left(5 + \sqrt{5}\right) + 64 \right\}^{1/2}, \\
E_{G_2} &= \alpha/2 \pm 2^{-1} \left(9\alpha^2 - 16\alpha + 16\right)^{1/2}, & E_{G_2} &= \alpha/2 \pm 2^{-1} \left(5\alpha^2 + 16\right)^{1/2}, \\
E_{H_{s}} &= \alpha/2 \pm 2^{-1} \left(13\alpha^2 - 24\alpha + 16\right)^{1/2},
\end{align*}
\]

and \( E^{H_{s}} \) is the root of the following equation:

\[
x^3 + 2x^2 + x \left(-6\alpha^2 + 8\alpha - 4\right) + \left(\alpha^3 - 12\alpha^2 + 16\alpha - 8\right) = 0.
\]

The results coincide with that given in Deng and Yang (1992) except for a misprint in (32) of Deng and Yang (1992) \((Q_{3\gamma_-} \text{ and } Q_{3\gamma_-} \text{ should be switched, but Fig. 2 in Deng and Yang (1992) is correct.})\)

**Ex. 2.** The submatrices of the Hückel Hamiltonian for carbon-240.

It can be seen from Fig. 1 of Chou and Yang (1993) that, in comparison with each atom of Carbon-60, Carbon-240 contains three more carbon atoms distributed symmetrically around that carbon atom of Carbon-60. In addition to \((a, b, c)\), we introduce a new index \(\lambda\) to identify those four carbon atoms. The carbon atom in the center is labeled by \(\lambda = 1\), the carbon on the hexagon labeled by 2, and the carbons on the two neighbor pentagons labeled by 3 and 4, respectively. Each carbon atom corresponds to a state, denoted by \(|a, b, c, \lambda\rangle\), or by a group element \(R\) and \(\lambda\) in terms of the generalized notation in (15):

\[
|R, \lambda\rangle = |PR', \sigma(\lambda)\rangle = |a, b, c, \lambda\rangle, \quad P |a, b, c, \lambda\rangle = |\overline{a}, b, c, \sigma(\lambda)\rangle,
\]

\[
\sigma(1) = 1, \quad \sigma(2) = 2, \quad \sigma(3) = 4, \quad \sigma(4) = 3.
\]

From (8) we have:

\[
P|\Phi^{(1)}_{\mu\nu}, \lambda\rangle = \eta^{2\mu} |\Phi^{(2)}_{\mu\nu}, \sigma(\lambda)\rangle, \quad P|\Phi^{(3)}_{\mu\nu}, \lambda\rangle = \eta^{2\mu-\nu} |\Phi^{(4)}_{\mu\nu}, \sigma(\lambda)\rangle.
\]

Following (10), (13) and (18), we are able to combine \(|\Phi^{(j)}_{\mu\nu}, \lambda\rangle\) into the SAB \(|\Gamma, \mu, \tau\rangle\). For example,
we have three independent SAB for \( \Gamma = A_{1g} \) and one for \( \Gamma = A_{1u} \):

\[
\begin{align*}
|A_{1g}, 0, 1 \rangle &= |\psi_{0,0}^{A_{1g}} 1, \rangle = 60^{-1/2} \{ |E, 1 \rangle + \cdots \}, \\
|A_{1g}, 0, 2 \rangle &= |\psi_{0,0}^{A_{1g}} 2, \rangle = 60^{-1/2} \{ |E, 2 \rangle + |T_0, 2 \rangle + |T_0^4, 2 \rangle + \cdots \}, \\
|A_{1g}, 0, 3 \rangle &= 2^{-1/2} \{ |\psi_{0,0}^{A_{1g}} 3, \rangle + |\psi_{0,0}^{A_{1g}} 4, \rangle \} \\
&= 120^{-1/2} \{ |E, 3 \rangle + |E, 4 \rangle + |T_0^4, 3 \rangle + |T_0, 4 \rangle + |S_1, 3 \rangle + |S_1, 4 \rangle + \cdots \}, \\
|A_{1u}, 0, 1 \rangle &= 2^{-1/2} \{ |\psi_{0,0}^{A_{1u}} 3, \rangle - |\psi_{0,0}^{A_{1u}} 4, \rangle \} \\
&= 120^{-1/2} \{ |E, 3 \rangle - |E, 4 \rangle + |T_0^4, 3 \rangle - |T_0, 4 \rangle + |S_1, 3 \rangle - |S_1, 4 \rangle + \cdots \},
\end{align*}
\] (28)

In the bases \( |R, \lambda \rangle \), the matrix of the Hückel Hamiltonian \( H \) is hermitian. We are only interested in the property of \( H \) acting on the states \( |E, \lambda \rangle \) and vice versa. For bond arrangement (a) we have:

\[
\begin{align*}
H \ |E, 1 \rangle &= -\alpha \ |E, 3 \rangle - \alpha \ |E, 4 \rangle + (\alpha - 2) \ |E, 2 \rangle \\
H \ |E, 2 \rangle &= -\alpha \ |T_0, 2 \rangle - \alpha \ |T_0^4, 2 \rangle + (\alpha - 2) \ |E, 1 \rangle \\
H \ |E, 3 \rangle &= -\alpha \ |E, 1 \rangle - \alpha \ |S_1, 4 \rangle + (\alpha - 2) \ |T_0, 4 \rangle \\
H \ |E, 4 \rangle &= -\alpha \ |E, 1 \rangle - \alpha \ |S_1, 3 \rangle + (\alpha - 2) \ |T_0^4, 3 \rangle
\end{align*}
\] (29)

and for bond arrangement (b):

\[
\begin{align*}
H \ |E, 1 \rangle &= -\alpha \ |E, 3 \rangle - \alpha \ |E, 4 \rangle + (\alpha - 2) \ |E, 2 \rangle \\
H \ |E, 2 \rangle &= -\alpha \ |T_0, 2 \rangle - \alpha \ |T_0^4, 2 \rangle + (\alpha - 2) \ |E, 1 \rangle \\
H \ |E, 3 \rangle &= -\alpha \ |E, 1 \rangle + (\alpha - 2) \ |S_1, 4 \rangle - \alpha \ |T_0, 4 \rangle \\
H \ |E, 4 \rangle &= -\alpha \ |E, 1 \rangle + (\alpha - 2) \ |S_1, 3 \rangle - \alpha \ |T_0^4, 3 \rangle
\end{align*}
\] (30)

Therefore, in the expansions of (28) we only need list 10 relevant states:

\[
|E, 1 \rangle, \ |E, 2 \rangle, \ |E, 3 \rangle, \ |E, 4 \rangle, \ |T_0, 2 \rangle, \\
|T_0, 4 \rangle, \ |T_0^4, 2 \rangle, \ |T_0^4, 3 \rangle, \ |S_1, 3 \rangle, \ |S_1, 4 \rangle
\] (31)

From (28), (29) and (30) we obtain the submatrices of the Hückel Hamiltonian for the representations \( A_{1g} \) and \( A_{1u} \):

\[
H^{A_{1g}}(a) = H^{A_{1g}}(b) = \begin{pmatrix}
0 & \alpha - 2 & -\sqrt{2}\alpha \\
\alpha - 2 & -2\alpha & 0 \\
-\sqrt{2}\alpha & 0 & -2
\end{pmatrix}, \quad H^{A_{1u}}(a) = H^{A_{1u}}(b) = 2.
\] (32)

In the cases \( A_{1g} \) and \( A_{1u} \), the submatrices of \( H \) are same for both bond arrangements (a) and (b). There are more SAB belonging to other irreducible representations. However, the calculations are still simple enough to complete by hand. In the following we list the independent SAB for each irreducible representation and the nonvanishing matrix elements of the Hamiltonian.

\[
\begin{align*}
|T_{1g}, \mu, \lambda \rangle &= 2^{-1/2} \{ |\psi_{\mu, \lambda}^{T_{1g}}, \lambda \rangle + |\psi_{\mu, \lambda}^{T_{1g}}, \mu \rangle, \sigma(\lambda) \} \\
|T_{1g}, \mu, 5 \rangle &= 2^{-1/2} \{ |\psi_{\mu, \lambda}^{T_{1g}}, 3 \rangle - |\psi_{\mu, \lambda}^{T_{1g}}, 4 \rangle \}, \\
|T_{2g}, \mu, \lambda \rangle &= 2^{-1/2} \{ |\psi_{\mu, \lambda}^{T_{2g}}, \lambda \rangle - |\psi_{\mu, \lambda}^{T_{2g}}, \mu \rangle, \sigma(\lambda) \} \\
|T_{2g}, \mu, 5 \rangle &= 2^{-1/2} \{ |\psi_{\mu, \lambda}^{T_{2g}}, 3 \rangle - |\psi_{\mu, \lambda}^{T_{2g}}, 4 \rangle \}, \\
|T_{1u}, \mu, \lambda \rangle &= 2^{-1/2} \{ |\psi_{\mu, \lambda}^{T_{1u}}, \lambda \rangle - |\psi_{\mu, \lambda}^{T_{1u}}, \mu \rangle, \sigma(\lambda) \} \\
|T_{1u}, \mu, 5 \rangle &= 2^{-1/2} \{ |\psi_{\mu, \lambda}^{T_{1u}}, 3 \rangle + |\psi_{\mu, \lambda}^{T_{1u}}, 4 \rangle \}, \\
|T_{2u}, \mu, \lambda \rangle &= 2^{-1/2} \{ |\psi_{\mu, \lambda}^{T_{2u}}, \lambda \rangle + |\psi_{\mu, \lambda}^{T_{2u}}, \mu \rangle, \sigma(\lambda) \} \\
|T_{2u}, \mu, 5 \rangle &= 2^{-1/2} \{ |\psi_{\mu, \lambda}^{T_{2u}}, 3 \rangle + |\psi_{\mu, \lambda}^{T_{2u}}, 4 \rangle \}, \\
|T_{1u}, \mu, 6 \rangle &= |\psi_{\mu, \lambda}^{T_{1u}}, 1 \rangle, \\
|T_{1u}, \mu, 7 \rangle &= |\psi_{\mu, \lambda}^{T_{1u}}, 2 \rangle, \\
|T_{2u}, \mu, 6 \rangle &= |\psi_{\mu, \lambda}^{T_{2u}}, 1 \rangle, \\
|T_{2u}, \mu, 7 \rangle &= |\psi_{\mu, \lambda}^{T_{2u}}, 2 \rangle.
\] (33)

where $\lambda$ runs from 1 to 4, and $\sigma(\lambda)$ was given in (26). Since the submatrices of the Hamiltonian are all hermitian, we only list the nonvanishing matrix elements in the up-triangle part (the row index is not larger than the column index).

\[
\begin{align*}
H_{T_1^u}(a)_{22} &= H_{T_1^u}(b)_{22} = H_{T_1^u}(a)_{22} = H_{T_1^u}(b)_{22} = -\alpha p, \\
H_{T_1^u}(a)_{33} &= -H_{T_1^u}(a)_{44} = -H_{T_1^u}(a)_{33} = -H_{T_1^u}(a)_{44} = \alpha p/\sqrt{5}, \\
H_{T_1^u}(b)_{33} &= H_{T_1^u}(b)_{44} = -H_{T_1^u}(b)_{33} = -H_{T_1^u}(b)_{44} = - (\alpha - 2)p/\sqrt{5},
\end{align*}
\]

\[
\begin{align*}
H_{T_1^u}(a)_{55} &= -H_{T_1^u}(a)_{55} = - (\alpha - 2) + \alpha/\sqrt{5}, \\
H_{T_1^u}(b)_{55} &= -H_{T_1^u}(b)_{55} = \alpha - (\alpha - 2)/\sqrt{5}, \\
H_{T_1^u}(a)_{77} &= H_{T_1^u}(b)_{77} = -2\alpha, \\
H_{T_1^u}(a)_{12} &= H_{T_1^u}(b)_{12} = H_{T_1^u}(a)_{12} = H_{T_1^u}(b)_{12} = H_{T_1^u}(a)_{67} = H_{T_1^u}(b)_{67} = \alpha - 2, \\
H_{T_1^u}(a)_{13} &= H_{T_1^u}(a)_{14} = H_{T_1^u}(b)_{13} = H_{T_1^u}(b)_{14} = H_{T_1^u}(a)_{13} = H_{T_1^u}(a)_{14} \\
&= H_{T_1^u}(b)_{13} = H_{T_1^u}(b)_{14} = -\alpha, \\
H_{T_1^u}(a)_{34} &= H_{T_1^u}(a)_{34} = (\alpha - 2)\eta^{-1} + \alpha p^{-1}/\sqrt{5}, \\
H_{T_1^u}(b)_{34} &= H_{T_1^u}(b)_{34} = -\alpha\eta^{-1} - (\alpha - 2)p^{-1}/\sqrt{5}, \\
-H_{T_1^u}(a)_{35} &= H_{T_1^u}(a)_{45} = H_{T_1^u}(a)_{35} = H_{T_1^u}(a)_{45} = \alpha \sqrt{2/5}, \\
-H_{T_1^u}(b)_{35} &= H_{T_1^u}(b)_{45} = H_{T_1^u}(b)_{35} = H_{T_1^u}(b)_{45} = - (\alpha - 2)\sqrt{2/5}, \\
H_{T_1^u}(a)_{56} &= H_{T_1^u}(b)_{56} = -\alpha \sqrt{2}.
\end{align*}
\]

After the replacement of $\sqrt{5}$ by $-\sqrt{5}$ from the submatrices for $T_1$ representation, we obtain those for $T_2$.

For the representations $G$ and $H$ we have

\[
\begin{align*}
|G_\mu, \lambda \rangle &= 2^{-1/2} \left\{ |G_{\mu^2}, \lambda \rangle + |G_{\mu^2}, \sigma(\lambda) \rangle \right\}, & |G_\mu, \mu, \lambda \rangle &= 2^{-1/2} \left\{ |G_{\mu^2}, \lambda \rangle - |G_{\mu^2}, \sigma(\lambda) \rangle \right\}, \\
|G_\mu, \mu + 4, \lambda \rangle &= 2^{-1/2} \left\{ |G_{\mu^2}, \lambda \rangle + |G_{\mu^2}, \sigma(\lambda) \rangle \right\}, & |G_\mu, \mu, 4 + \lambda \rangle &= 2^{-1/2} \left\{ |G_{\mu^2}, \lambda \rangle - |G_{\mu^2}, \sigma(\lambda) \rangle \right\}.
\end{align*}
\]
\begin{align*}
H^G_s(a)_{22} &= H^G_s(b)_{22} = H^G_u(a)_{22} = H^G_u(b)_{22} = \alpha p^{-1}, \\
H^G_s(a)_{66} &= H^G_s(b)_{66} = H^G_u(a)_{66} = H^G_u(b)_{66} = -\alpha p, \\
H^G_s(a)_{33} &= H^G_s(a)_{44} = -H^G_s(a)_{77} = -H^G_s(a)_{88} \\
&= -H^G_u(a)_{33} = -H^G_u(a)_{44} = H^G_u(a)_{77} = H^G_u(a)_{88} = -\alpha/\sqrt{5}, \\
H^G_s(b)_{33} &= H^G_s(b)_{44} = -H^G_s(b)_{77} = -H^G_s(b)_{88} \\
&= -H^G_u(b)_{33} = -H^G_u(b)_{44} = H^G_u(b)_{77} = H^G_u(b)_{88} = (\alpha - 2)/\sqrt{5}, \\
H^G_s(a)_{12} &= H^G_s(a)_{56} = H^G_u(a)_{12} = H^G_u(a)_{56} \\
&= H^G_s(b)_{12} = H^G_u(b)_{12} = H^G_u(b)_{56} = \alpha - 2, \\
H^G_s(a)_{13} &= H^G_s(a)_{14} = H^G_s(a)_{57} = H^G_u(a)_{13} = H^G_u(a)_{14} \\
&= H^G_u(a)_{57} = H^G_u(a)_{58} = H^G_s(b)_{13} = H^G_s(b)_{14} = H^G_u(b)_{57} = H^G_u(b)_{58} = -\alpha, \\
H^G_s(a)_{34} &= H^G_u(a)_{34} = (\alpha - 2)\eta^{-2} + \alpha/\sqrt{5}, \\
H^G_s(b)_{34} &= H^G_u(b)_{34} = -\alpha\eta^{-2} - (\alpha - 2)/\sqrt{5}, \\
H^G_s(a)_{78} &= H^G_u(a)_{78} = (\alpha - 2)\eta^{-1} - \alpha/\sqrt{5}, \\
H^G_s(b)_{78} &= H^G_u(b)_{78} = -\alpha\eta^{-1} + (\alpha - 2)/\sqrt{5}, \\
H^G_s(a)_{37} &= H^G_u(a)_{48} = -H^G_u(a)_{37} = -H^G_u(a)_{48} = \alpha p^{-1}/\sqrt{5}, \\
H^G_s(b)_{37} &= H^G_u(b)_{48} = -H^G_u(b)_{37} = -H^G_u(b)_{48} = -(\alpha - 2)p^{-1}/\sqrt{5}, \\
H^G_s(a)_{38} &= H^G_s(a)_{47} = H^G_u(a)_{38} = H^G_u(a)_{47} = \alpha p/\sqrt{5}, \\
H^G_s(b)_{38} &= H^G_u(b)_{47} = H^G_u(b)_{38} = H^G_u(b)_{47} = -(\alpha - 2)p/\sqrt{5}.
\end{align*}

\begin{align*}
|H_g, \mu, \lambda\rangle &= 2^{-1/2} \left\{ |\psi^H_{\mu1}\rangle_1 + |\psi^H_{\mu3}\rangle_3, |\psi^H_{\mu1}\rangle_1 - |\psi^H_{\mu3}\rangle_3 \right\}, \\
|H_u, \mu, \lambda\rangle &= 2^{-1/2} \left\{ |\psi^H_{\mu2}\rangle_2 - |\psi^H_{\mu3}\rangle_3, |\psi^H_{\mu2}\rangle_2 + |\psi^H_{\mu3}\rangle_3 \right\}, \\
|H_g, \mu, 4 + \lambda\rangle &= 2^{-1/2} \left\{ |\psi^H_{\mu1}\rangle_1 + |\psi^H_{\mu1}\rangle_1 \right\}, \\
|H_u, \mu, 4 + \lambda\rangle &= 2^{-1/2} \left\{ |\psi^H_{\mu2}\rangle_2 + |\psi^H_{\mu2}\rangle_2 \right\}, \\
|H_g, \mu, 9\rangle &= 2^{-1/2} \left\{ |\psi^H_{\mu0}\rangle_0 + |\psi^H_{\mu0}\rangle_0 \right\}, \\
|H_u, \mu, 9\rangle &= 2^{-1/2} \left\{ |\psi^H_{\mu1}\rangle_1 - |\psi^H_{\mu1}\rangle_1 \right\}, \\
|H_g, \mu, 10\rangle &= |\psi^H_{\mu0}\rangle_0, \\
|H_g, \mu, 11\rangle &= |\psi^H_{\mu0}\rangle_0.
\end{align*}

(38)
vibration quanta are denoted by $\psi_{\mu}$. Applying the irreducible bases $R_{ij}$, the symmetry adapted bases of $H_{ij}$ are denoted by $H_{ij}(a)_{ij} = \frac{1}{5} \left( g_{ij}(a)_{ij} - \psi_{ij}(a)_{ij} \right)$.

Applying $R_{ij}$, we obtain the SAB as follows:

$$H_{ij}(a)_{ij} = H_{ij}(b)_{ij} = H_{ij}(a)_{ij} = \frac{1}{5} \left( g_{ij}(a)_{ij} - \psi_{ij}(a)_{ij} \right)$$

The secular equations can be calculated by a standard program in Mathematica, and coincide with those given in Chou and Yang (1993) except for one dropped zero there. The coefficient of the term $\lambda^6 \alpha_5$ in $Q_{5+}$ is 100, not 10.

**Ex. 3.** The symmetry adapted bases of $B_{12}H_{12}$. A state in $B_{12}H_{12}$ is described by the vibration quanta in the 12 bonds. Those numbers of the vibration quanta are denoted by $n_j$ and $m_j$ for the bonds $OA_j$ and $OB_j$, $0 \leq j \leq 5$, respectively. Applying the irreducible bases $\psi_{\mu}$ on the states, we obtain the SAB as follows:

$$\psi_{\mu} \ |n_0n_1n_2n_3n_4n_5m_0m_1m_2m_3m_4m_5 \rangle$$

where the action of a group element $R$ of $I$ on the state can be calculated from the definition of $R$.
and from Fig. 1. For example,

\[ A_0, A_1, A_2, A_3, A_4, A_5 \xrightarrow{T_0} A_0, A_2, A_3, A_4, A_5, A_1, \]
\[ A_0, A_1, A_2, A_3, A_4, A_5 \xrightarrow{S_{11}} B_0, B_4, B_3, B_2, B_1, B_5, \]
\[ A_0, A_1, A_2, A_3, A_4, A_5 \xrightarrow{S_5} A_5, A_4, B_2, B_3, A_1, A_0, \]
\[ A_0, A_1, A_2, A_3, A_4, A_5 \xrightarrow{S_{10}} B_3, A_5, B_2, B_0, B_4, A_1. \]

Under the applications of \( T_0, S_{11}, S_5 \) and \( S_{10} \), the state \( |n_0 n_1 n_3 n_4 n_5 m_0 m_1 m_2 m_3 m_4 m_5\rangle \) becomes:

\[ T_0 : |n_0 n_5 n_1 n_2 n_3 n_4 m_0 m_5 m_2 m_3 m_4\rangle, \]
\[ S_{11} : |m_0 m_4 m_3 m_2 m_1 m_5 n_0 n_4 n_3 n_2 n_1 n_5\rangle, \]
\[ S_5 : |n_5 m_2 m_3 n_1 n_0 m_4 m_5 n_2 n_3 m_1 m_0\rangle, \]
\[ S_{10} : |m_3 m_5 m_2 m_0 m_4 n_1 n_3 m_5 n_2 n_0 n_4 m_1\rangle. \]  

When 12 quanta are all different from each other, we obtain 60 SAB that are divided into 16 sets with given irreducible representations. If some quanta are equal to each other, the number of the independent sets may decrease. Since the dimensions of the representations are less than 60 for the seven important cases discussed in Chen and Ping (1997), those representations were called non-regular (Chen and Ping 1997).

**IV. CONCLUSION**

The symmetry adapted bases are very useful in calculating the eigenvalues and eigenstates of a Hamiltonian with given symmetry. From the irreducible bases in the group space of the symmetry group of the system, the SAB can be calculated generally and simply. This is a standard method in group theory (Hamermesh 1962), and widely used in the problems of vibrations of a polyatomic molecule (Lemus and Frank 1994, Ma et al. 1996, Chen et al. 1996). The explicit form of the irreducible bases of \( I \) group space are useful in the future calculations for the molecules with \( I \) and \( I_h \) symmetry.

**ACKNOWLEDGMENTS**

The authors would like to thank Professor Jin-Quan Chen for useful discussion. This work was supported by the National Natural Science Foundation of China and Grant No. LWTZ-1298 of Chinese Academy of Sciences.

**REFERENCES**

Altmann, S. L., and Herzig, P. (1994). *Point-Group Theory Tables*, Oxford University Press, Oxford.

Balasubramanian, K. (1996). *Chemical Physics Letters*, 260, 476.

Brown, W. B. (1987). *Chemical Physics Letters*, 136, 128 and 139, 612.

Chen, J. Q., Klein, A., and Ping, J. L. (1996). *Journal of Mathematical Physics*, 37, 2400.

Chen, J. Q., and Ping, J. L. (1997). *Journal of Mathematical Physics*, 38, 387.

Chou, T. T., and Yang, C. N. (1993). *Physics Letters A*, 183, 221.

Clougherty, D. P., and Gorman, J. P. (1996). *Chemical Physics Letters*, 251, 353.
Deng, Y., and Yang, C. N. (1992). *Physics Letters A*, 170, 116.
Doye J. P. K., and Wales, D. J. (1996). *Chemical Physics Letters*, 262, 167.
Fowler P. W., and Ceulemans, A. (1985). *Molecular Physics*, 54, 767.
Friedberg, H. R., and Lee, T. D. (1992). *Physical Review B*, 46, 14150.
Giannozzi, P., and Baroni, S. (1994). *Journal of Chemical Physics*, 100, 8537.
Golding, R. M. (1973). *Molecular Physics*, 26, 661.
Gunnarsson, O., Handschuh, H., Bechthold, P. S., Kessler, B., Gantefoer, G., and Eberhardt, W. (1995). *Physical Review Letters*, 74, 1875.
Hamermesh, M. (1962). *Group Theory and its Application to Physical Problems*, Addison-Wesley Pub. Co. Reading.
Huffman, D. R. (1991). *Physics Today*, Nov. 22.
Kroto, H. W. (1988). *Science*, 242, 1139.
Kroto, H. W., Heath, J. R., O’Brien, S. C., Curl, R. F., and Smalley, R. E. (1985). *Nature*, 318, 162.
Lemus R., and Frank, A. (1994). *Journal of Chemical Physics*, 101, 8321.
Liu, F., Ping, J. L., and Chen, J. Q. (1990). *Journal of Mathematical Physics*, 31, 1065.
Lomont, J. S. (1959). *Applications of Finite Groups*, Academic Press, New York, p.32 and p.312.
Ma, Z. Q., Hou, X. W., and Xie, M. (1996). *Physical Review A*, 53, 2173.
Martínez-Torres, E., López-González, J. J., Fernández-Gómez, M., Brendsdal, E., and Cyvin, S. J. (1996). *Chemical Physics Letters*, 253, 32.
McLellan, A. G. (1961). *Journal of Chemical Physics*, 34, 1350.
Negri, F., and Orlandi, G. (1996). *Journal of Physics B*, 29, 5049.
Olthof, E. H. T., van der Avoird, A., and Wormer, P. E. S. (1996). *Journal of Chemical Physics*, 104, 832.
Pennis, E. (1991). *Science News*, 140, 120.
Pooler, D. R. (1980). *Journal of Physics A*, 13, 1197.
Rohlfing, E. A., Cox, D. M., and Kaldor, A. (1984) *Journal of Chemical Physics*, 81, 3322.
Schettino, V., Salvi, P. R., Bini, R., and Cardini, G. (1994). *Journal of Chemical Physics*, 101, 11079.
Tang, A. C., and Huang, F. Q. (1997). *International Journal of Quantum Chemistry*, 63, 367.
Tang, A. C., Huang, F. Q., and Liu, R. Z. (1996). *Physical Review B*, 53, 7442.
Varga, F., Nemes, L., and Watson, J. K. G. (1996). *Journal of Physics B*, 29, 5043.
Wang, Z., Day, P., and Pachter, R. (1996). *Chemical Physics Letters*, 248, 121.
Weeks, D. E., and Harter, W. G. (1989). *Journal of Chemical Physics*, 90, 4744.