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Irreducible Bases in Icosahedral Group Space

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The irreducible bases in the icosahedral group space are calculated explicitly by reducing the regular representation. The symmetry-adapted bases of the system with $\mathbf{I}$ or $\mathbf{I}_h$ 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 recalculated by the irreducible bases.

1. INTRODUCTION

Fullerenes (Kroto, 1998; Huffman, 1991; Pennis, 1991), such as $B_{12}H_{12}$, $C_{20}H_{20}$, and C_{60}, are intriguing cagelike molecules of carbon atoms with icosahedral symmetry. This discovery (Rohlfing, *et al.*, 1984; Kroto *et al.*, 1985; Weeks and Harter; 1989) has drawn the attention of chemists and physicists (Deng and Yang, 1993; Friedberg and Lee, 1992; Chen and Yang, 1993). With the development of experimental techniques in high-resolution spectroscopy, much new data on vibrational spectra of polyatomic molecules with the symmetry $\mathbf{I}_h$ have been 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 have been studied in some detail (Clougherty and Gorman, 1996; Martınez-Torres, 1996; Varga *et al.*, 1996; Fowler and Ceulemans, 1985, 1993).

As is well known, symmetry analysis provides a powerful tool for classifying energy levels and organizing experimental data. In explaining the

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vibrational spectra of polyatomic molecules, the symmetry-adapted bases (SAB) play an important role in simplifying the calculations (Lemus and Frank, 1994; Mo *et al.*, 1996; Chen *et al.* 1996). The SABs are defined as the orthogonal bases that belong to given rows of given irreducible representations of the symmetry group. In such studies, SABs of the system with $\mathbf{I}_h$ symmetry have been widely used. Therefore, the properties of the $\mathbf{I}_h$ group are worth studying in some detail, although the dimension of the $\mathbf{I}_h$ group space is 120.

Early work on the **I** group was mainly concerned with the construction of the representations of **I** subduced by D^l of the $SO(3)$ group and the 3j and 6j symbols (McLellan, 1961; Golding, 1973; Pooler, 1980; Brown, 1987a,b). Liu *et al.* (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 have been 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 SABs 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 $\mathbf{I}_h$ by reducing the regular representation of **I**:

$$R\psi^{\Gamma}_{\mu\nu} = \sum_{\rho} \psi^{\Gamma}_{\rho\nu} D^{\Gamma}_{\rho\mu}(R), \qquad \psi^{\Gamma}_{\mu\nu}R = \sum_{\rho} D^{\Gamma}_{\nu\rho}(R)\psi^{\Gamma}_{\mu\rho}, \qquad R \in I \tag{1}$$

where D^{Γ} 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 $\psi^{\Gamma}_{\mu\nu}F(x)$:

$$R\{\psi^{\Gamma}_{\mu\nu}F(x)\} = \sum_{\rho} \{\psi^{\Gamma}_{\rho\nu}F(x)\}\ D^{\Gamma}_{\rho\mu}(R) \tag{2}$$

This is a unified and straightforward way to calculate the SAB of the system with the $\mathbf{I}_h$ 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). This 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 Section 2 we will give our notations. In Section 3 the irreducible bases in the **I** group space are calculated explicitly, and the irreducible bases of $\mathbf{I}_h$ are easily calculated from those of **I**. Three examples are given to explain how to calculate the SAB in terms of these irreducible bases. A short conclusion is given in Section 4.

2. 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, $0 \le j \le 5$, and their opposite vertices by B_j. The z and y axes point from the center O to A_0 and the midpoint of $A_2 B_5$, respectively.

The group **I** has 6 fivefold axes, 10 threefold axes, and 15 twofold axes. One of the fivefold axes is directed along the z axis, and the rest point from B_j to A_j ($1 \le j \le 5$) with the polar angle θ_1 and azimuthal angles $\varphi_j^{(1)}$. The rotations through $2\pi/5$ around those fivefold axes are denoted by T_j, $0 \le j \le 5$. The threefold axes join the centers of two opposite faces. The polar angles of the first and last 5 axes are denoted by θ_2 and θ_3, respectively, and the azimuthal angles by $\varphi_j^{(2)}$. The rotations through $2\pi/3$ around those threefold axes are denoted by R_j, $1 \le j \le 10$. The twofold axes join the midpoints of two opposite edges. The polar and azimuthal angles of the first, next, and last 5 axes are θ_4, $\varphi_j^{(1)}$, θ_5, $\varphi_j^{(2)}$, π, and $\varphi_j^{(3)}$, respectively. The rotations through π around those twofold axes are denoted by S_j, $1 \le j \le 15$. Those angles θ_i and $\varphi_j^{(i)}$ are given as follows:

$$\begin{gathered}
\tan\theta_1 = 2, \qquad \tan\theta_2 = 3 - \sqrt{5} = 2p^{2}, \qquad \tan\theta_3 = 3 + \sqrt{5} = 2p^{-2} \\
\tan\theta_4 = (\sqrt{5} - 1)/2 = p, \qquad \tan\theta_5 = (\sqrt{5} + 1)/2 = p^{-1} \\
\varphi_j^{(1)} = 2(j-1)\,\pi/5, \qquad \varphi_j^{(2)} = (2j-1)\,\pi/5, \qquad \varphi_j^{(3)} = (4j-3)\,\pi/10 \\
p = \eta + \eta^{-1}, \qquad p^{-1} = 1 + \eta + \eta^{-1}, \qquad \eta = \exp(-i2\,\pi/5)
\end{gathered} \tag{3}$$

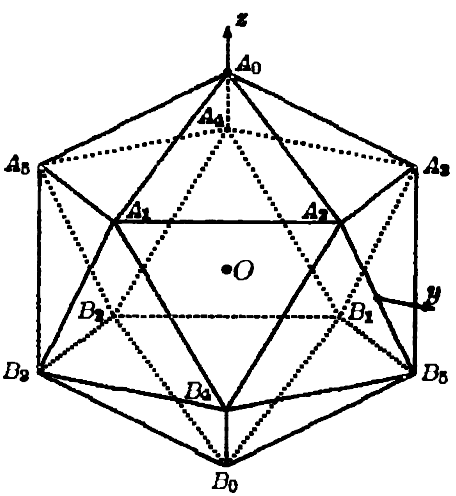

Fig. 1. Icosahedron with $\mathbf{I}_h$ symmetry.

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

$$R = T_0^a R_6^b S_1^c S_{12}^d \tag{4}$$

Due to the relations

$$R_6 = S_1 T_0^2 S_1 T_0^4, \qquad S_{12} = R_6^2 S_1 R_6 \tag{5}$$

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

3. 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:

$$T_0 \Phi_{\mu\nu} = \eta^\mu \Phi_{\mu\nu}, \qquad \Phi_{\mu\nu} T_0 = \eta^\nu \Phi_{\mu\nu}$$
$$\eta = \exp(-i2\pi/5), \qquad \mu, \nu \bmod 5 \tag{6}$$

The eigenstates can be easily calculated by the projection operator P_μ (Hamermesh, 1962, p. 113):

$$\Phi_{\mu\nu} = c\, P_\mu R P_\nu, \qquad P_\mu = \frac{1}{5} \sum_{\lambda=-2}^{2} \eta^{-\mu\lambda} T_0^\lambda \tag{7}$$

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 $\Phi_{\mu\nu}^{(i)}$:

$$\Phi_{\mu\mu}^{(1)} = (E + \eta^{-\mu} T_0 + \eta^{-2\mu} T_0^2 + \eta^{2\mu} T_0^3 + \eta^\mu T_0^4)/\sqrt{5}$$
$$\Phi_{\mu\mu}^{(2)} = (S_{11} + \eta^{-\mu} S_{14} + \eta^{-2\mu} S_{12} + \eta^{2\mu} S_{15} + \eta^\mu S_{13})/\sqrt{5}$$
$$\begin{aligned}\Phi_{\mu\nu}^{(3)} = \{&(S_5 + \eta^{-\mu} R_5^2 + \eta^{-2\mu} T_1^4 + \eta^{2\mu} T_4 + \eta^\mu R_4) \\ &+ \eta^{(\mu-\nu)}(S_4 + \eta^{-\mu} R_4^2 + \eta^{-2\mu} T_5^4 + \eta^{2\mu} T_3 + \eta^\mu R_3) \\ &+ \eta^{2(\mu-\nu)}(S_3 + \eta^{-\mu} R_3^2 + \eta^{-2\mu} T_4^4 + \eta^{2\mu} T_2 + \eta^\mu R_2) \\ &+ \eta^{-2(\mu-\nu)}(S_2 + \eta^{-\mu} R_2^2 + \eta^{-2\mu} T_3^4 + \eta^{2\mu} T_1 + \eta^\mu R_1) \\ &+ \eta^{-(\mu-\nu)}(S_1 + \eta^{-\mu} R_1^2 + \eta^{-2\mu} T_2^4 + \eta^{2\mu} T_5 + \eta^\mu R_5)\}/5\end{aligned} \tag{8}$$
$$\Phi_{\mu\nu}^{(4)} = \{(S_{10} + \eta^{-\mu} T_1^3 + \eta^{-2\mu} R_6^2 + \eta^{2\mu} R_9 + \eta^\mu T_5^2)$$

$$+ \eta^{(\mu-\nu)}(S_9 + \eta^{-\mu}T_5^3 + \eta^{-2\mu}R_{10}^2 + \eta^{2\mu}R_8 + \eta^{\mu}T_4^2)$$
$$+ \eta^{2(\mu-\nu)}(S_8 + \eta^{-\mu}T_4^3 + \eta^{-2\mu}R_9^2 + \eta^{2\mu}R_7 + \eta^{\mu}T_3^2)$$
$$+ \eta^{-2(\mu-\nu)}(S_7 + \eta^{-\mu}T_3^3 + \eta^{-2\mu}R_8^2 + \eta^{2\mu}R_6 + \eta^{\mu}T_2^2)$$
$$+ \eta^{-(\mu-\nu)}(S_6 + \eta^{-\mu}T_2^3 + \eta^{-2\mu}R_7^2 + \eta^{2\mu}R_{10} + \eta^{\mu}T_1^2)\}/5$$

where and hereafter the subscript $\bar{\mu}$ denotes $-\mu$. These bases $\Phi_{\mu\nu}^{(i)}$ should be combined into the irreducible bases $\psi_{\mu\nu}^{\Gamma}$ that belong to the given irreducible representation Γ. The combinations can be determined from the condition that $\psi_{\mu\nu}^{\Gamma}$ should be the eigenstate of a class operator W, which was called CSCO-I in Chen and Ping (1997). The eigenvalues α_Γ can be calculated from the characters in the irreducible representation Γ [see (3-170) in Hamermesh (1962)]

$$W = \sum_{j=0}^{5}(T_j + T_j^4), \qquad W\psi_{\mu\nu}^{\Gamma} = \psi_{\mu\nu}^{\Gamma}W = \alpha_\Gamma\psi_{\mu\nu}^{\Gamma} \tag{9}$$

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

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

$$\psi_{\mu\nu}^{\Gamma} = N^{-1/2}\sum_{i=1}^{4} C_i\Phi_{\mu\nu}^{(i)} \tag{10}$$

where N is the normalization factor. In those bases $\psi_{\mu\nu}^{\Gamma}$, the representation matrices are diagonal with the diagonal elements η^{μ} [see (6)]. In principle, each $\psi_{\mu\nu}^{\Gamma}$ 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:

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

$$D^{T_2}(S_1) = \frac{1}{\sqrt{5}}\begin{pmatrix} -p & \sqrt{2} & p^{-1} \\ \sqrt{2} & -1 & \sqrt{2} \\ p^{-1} & \sqrt{2} & -p \end{pmatrix}$$

$$D^G(S_1) = \frac{1}{\sqrt{5}}\begin{pmatrix} -1 & -p & -p^{-1} & 1 \\ -p & 1 & -1 & -p^{-1} \\ -p^{-1} & -1 & 1 & -p \\ 1 & -p^{-1} & -p & -1 \end{pmatrix} \tag{11}$$

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

where the row (column) indices μ of the irreducible representations Γ are put in the following order: 0 for A; 1, 0, and 1 for T_1; 2, 0, and 2 for T_2; 2, 1, 1, and 2 for G; and 2, 1, 0, 1, and 2 for H. The representation matrices of some irreducible representations of **I** coincide with those in the subduced representations of D^l of $SO(3)$:

$$D^0(R) = D^A(R), \qquad D^1(R) = D^{T_1}(R), \qquad D^2(R) = D^H(R)$$
$$X^{-1}D^3(R)X = D^{T_2}(R) \oplus D^G(R), \qquad R \in \mathbf{I} \tag{12}$$

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

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

The group $\mathbf{I}_h$ 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 $\mathbf{I}_h$ are denoted as Γ_g (even) and Γ_u (odd) with the following irreducible bases:

$$\psi^{\Gamma_g}_{\mu\nu} = 2^{-1/2}(E + P)\,\psi^{\Gamma_u}_{\mu\nu}, \qquad \psi^{\Gamma}_{\mu\nu} = 2^{-1/2}(E - P)\,\psi^{\Gamma}_{\mu\nu} \tag{13}$$

Now we are in the position to construct the symmetry-adapted bases (SABs). For a given polyatomic molecule with **I** or $\mathbf{I}_h$ symmetry, its vibrational states are described by the vibration quanta occupying its bonds. Applying the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ to the vibrational states, we obtain the SABs generally. The only problem is to determine the actions of group elements R on the vibrational states according to the geometric meaning of R. In fact, the action of R only permutes, but does not change the vibration quanta. When some quanta are equal to each other, some SAB may be vanishing, or linearly

Table I. Irreducible Bases in the Group Space of **I**

$$\psi^{\Gamma}_{\mu\nu} = N^{-1/2} \sum_{i=1}^{4} C_i \Phi^{(i)}_{\mu\nu}, \qquad \eta = \exp(-i2\pi/5), \qquad p = \eta + \eta^{-1}$$

$$\phi^{A}_{00} = (\Phi^{(1)}_{00} + \Phi^{(2)}_{00} + \sqrt{5}\Phi^{(3)}_{00} + \sqrt{5}\Phi^{(4)}_{00})/\sqrt{12}$$

$\Gamma = T_1$

μ	ν	C_1	C_2	C_3	C_4	N
1	1	1		$-p^{-1}$	$-p$	4
0	1			$-\eta^{-1}$	η^2	2
1	1		η^{-2}	$-\eta^{-2}p$	$-\eta^{-1}p^{-1}$	4
1	0			$-\eta$	η^{-2}	2
0	0	1	-1	1	-1	4
1	0			η^{-1}	$-\eta^2$	2
1	1		η^2	$-\eta^2 p$	ηp^{-1}	4
0	1			η	$-\eta^{-2}$	2
1	1	1		$-p^{-1}$	$-p$	4

$\Gamma = T_2$

μ	ν	C_1	C_2	C_3	C_4	N
2	2	1		$-p$	$-p^{-1}$	4
0	2			η^{-2}	$-\eta^{-1}$	2
2	2		$-\eta$	ηp^{-1}	$\eta^{-2}p$	4
2	2	0		η^2	$-\eta$	2
0	0	1	-1	-1	1	4
2	0			η^{-2}	$-\eta^{-1}$	2
2	2		$-\eta^{-1}$	$\eta^{-1}p^{-1}$	$\eta^2 p$	4
0	2			η^2	$-\eta$	2
2	2	1		$-p$	$-p^{-1}$	4

$\Gamma = G$

μ	ν	C_1	C_2	C_3	C_4	N
2	2	1		-1	1	3
1	2			$-\eta^{-1}p$	$-\eta^2 p^{-1}$	3
1	2			$-\eta^2 p^{-1}$	$-\eta p$	3
2	2		η	η	$-\eta^{-2}$	3
2	1			ηp	$-\eta^{-2}p^{-1}$	3
1	1	1		1	-1	3
1	1		η^{-2}	$-\eta^{-2}$	η^{-1}	3
2	1			$-\eta^2 p^{-1}$	$-\eta p$	3

$\Gamma = G$

μ	ν	C_1	C_2	C_3	C_4	N
2	1			$-\eta^{-2}p^{-1}$	$-\eta^{-1}p$	3
1	1		η^2	$-\eta^2$	η	3
1	1	1		1	-1	3
2	1			$-\eta^{-1}p$	$-\eta^2 p^{-1}$	3
2	2		η^{-1}	η^{-1}	$-\eta^2$	3
1	1			$-\eta^{-2}p^{-1}$	$-\eta^{-1}p$	3
1	1			$-\eta p$	$-\eta^{-2}p^{-1}$	3
2	1			-1	1	3

$\Gamma = H$

μ	ν	C_1	C_2	C_3	C_4	N
2	2	$\sqrt{5}$		P^{-2}	p^2	12
1	2			$\eta^{-1}p^{-1}$	$-\eta^2 p$	3
0	2			η^{-2}	η^{-1}	2
1	2			$\eta^2 p$	$-\eta p^{-1}$	3
2	2		$\sqrt{5}\eta$	ηp^2	$\eta^{-2}p^{-2}$	12
2	1			ηp^{-1}	$-\eta^{-2}p$	3
1	1	$\sqrt{5}$		p^2	p^{-2}	12
0	1			$-\eta^{-1}$	$-\eta^2$	2
1	1		$-\sqrt{5}\eta^{-2}$	$-\eta^{-2}p^{-2}$	$-\eta^{-1}p^2$	12
2	1			$-\eta^2 p$	ηp^{-1}	3
2	0			η^2	η	2
1	0			$-\eta$	$-\eta^{-2}$	2
0	0	$\sqrt{5}$	$\sqrt{5}$	-1	-1	12

$\Gamma = H$

μ	ν	C_1	C_2	C_3	C_4	N
1	0			η^{-1}	η^2	2
0	2			η^{-2}	η^{-1}	2
2	1			$\eta^{-2}p$	$-\eta^{-1}p^{-1}$	3
1	2		$-\sqrt{5}\eta^2$	$-\eta^2 p^{-2}$	$-\eta p^2$	12
0	1			η	η^{-2}	2
1	1	$\sqrt{5}$		p^2	p^{-2}	12
2	1			$-\eta^{-1}p^{-1}$	$\eta^2 p$	3
2	2		$\sqrt{5}\eta^{-1}$	$\eta^{-1}p^2$	$\eta^2 p^{-2}$	12
1	2			$-\eta^{-2}p$	$\eta^{-1}p^{-1}$	3
0	2			η^2	η	2
1	2			$-\eta p^{-1}$	$\eta^{-2}p$	3
2	2	$\sqrt{5}$		p^{-2}	p^2	12

dependent on other states. Let us give three examples to explain the general method of calculating SABs.

Example 1. The eigenvalues and eigenfunctions of the Hückel Hamiltonian for carbon-60. Deng and Yang (1992) calculated this problem by computer. Now we calculate the same problem in terms of the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ 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 $\mathbf{I}_h$ in the following meaning:

$$R\,|1,\,0,\,1\rangle = PR'\,|1,\,0,\,1\rangle = |a,\,b,\,c\rangle, \qquad R \text{ and } PR' \to |a,\,b,\,c\rangle. \tag{14}$$

where $R \in \mathbf{I}$ and $R' \in \mathbf{I}$. Introduce the new notation for the states

$$|R\rangle = P|R'\rangle = |PR'\rangle \equiv |a,\,b,\,c\rangle, \qquad P|a,\,b,\,c\rangle = |\bar{a},\,b,\,c\rangle, \tag{15}$$

where the correspondence between $|a = 1,\,b,\,c\rangle$ and the elements R and PR' of $\mathbf{I}_h$ is as follows:

$$|R\rangle = |1,\,b,\,c\rangle, \qquad |R'\rangle = |\bar{1},\,b,\,c\rangle. \tag{16}$$

$R(R')$	$c=1$	$c=2$	$c=3$	$c=4$	$c=5$	$c=6$
$b=0$	$E(S_{12})$	$S_1(S_8)$	$R^2_5(T^2_4)$	$R_1(T^3_3)$	$T^4_5(R_9)$	$T_2(R^2_7)$
$b=1$	$T_0(S_{15})$	$R^3_1(T^3_4)$	$T^4_1(S_9)$	$S_2(R^8_8)$	$T_3(T^2_5)$	$R_2(R_{10})$
$b=2$	$T^2_0(S_{13})$	$T^4_2(R^2_9)$	$T_4(T^3_5)$	$R^2_2(R_6)$	$R_3(S_{10})$	$S_3(T^2_1)$
$b=3$	$T^3_0(S_{11})$	$T_5(R_7)$	$R_4(R^2_{10})$	$T^4_3(T^2_2)$	$S_4(T^3_1)$	$R^2_3(S_6)$
$b=4$	$T^4_0(S_{14})$	$R_5(T^2_3)$	$S_5(R_8)$	$T_1(S_7)$	$R^2_4(R^2_6)$	$T^4_4(T^3_2)$

Substituting (16) into (8), we obtain

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

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

$$\begin{aligned}
&2^{-1/2}|\psi^{Ag}_{00}\rangle = |\psi^{A}_{00}\rangle, \quad |\psi^{T_1g}_{\mu 1}\rangle = |\psi^{T_1g}_{\mu\bar{1}}\rangle, \quad |\psi^{T_1u}_{\mu 1}\rangle = -|\psi^{T_1u}_{u\bar{1}}\rangle, \quad 2^{-1/2}|\psi^{T_1u}_{\mu 0}\rangle = |\psi^{T_1}_{\mu 0}\rangle \\
&|\psi^{T_1g}_{\mu 2}\rangle = -|\psi^{T_1g}_{\mu\bar{2}}\rangle, \quad |\psi^{T_2u}_{\mu 2}\rangle = |\psi^{T_2u}_{\mu\bar{2}}\rangle, \quad 2^{-1/2}|\psi^{T_2u}_{\mu 0}\rangle = |\psi^{T_2}_{\mu 0}\rangle, \quad |\psi^{Gg}_{\mu 2}\rangle = |\psi^{G_g}_{\mu\bar{2}}\rangle \\
&|\psi^{Gg}_{\mu 1}\rangle = |\psi^{G_g}_{\mu 1}\rangle, \quad |\psi^{Gu}_{\mu 2}\rangle = -|\psi^{G_u}_{\mu\bar{2}}\rangle, \quad |\psi^{Gu}_{\mu 1}\rangle = -|\psi^{G_u}_{\mu\bar{1}}\rangle, \quad |\psi^{Hg}_{\mu 2}\rangle = |\psi^{H_g}_{\mu\bar{2}}\rangle \\
&|\psi^{Hg}_{\mu 1}\rangle = -|\psi^{H_g}_{\mu\bar{1}}\rangle, \quad 2^{-1/2}|\psi^{Hg}_{\mu 0}\rangle = |\psi^{H}_{\mu 0}\rangle, \quad |\psi^{Hu}_{\mu 2}\rangle = -|\psi^{H_u}_{\mu\bar{2}}\rangle, \quad |\psi^{Hu}_{\mu 1}\rangle = |\psi^{H_u}_{\mu\bar{1}}\rangle
\end{aligned} \tag{18}$$

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

$$|\psi^{\Gamma}_{\mu 0}\rangle = P|\psi^{\Gamma}_{\mu 0}\rangle \qquad \text{or} \qquad |\psi^{\Gamma}_{\mu 0}\rangle = -P|\psi^{\Gamma}_{\mu 0}\rangle$$

There are 90 bonds, 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 equal to $-\alpha$, and that of the 30 *hh* bonds is equal to $(\alpha - 2)$. Now, since the states of C_{60} are denoted by the elements R of $\mathbf{I}$, the action of Hamiltonian on the states can be written from (16) and the figure in Deng and Yang (1992); for example,

$$\begin{aligned} H|E\rangle &= -\alpha|T_0\rangle - \alpha|T_0^4\rangle + (\alpha - 2)|S_1\rangle \\ H|T_0\rangle &= -\alpha|E\rangle - \alpha|T_0^2\rangle + (\alpha - 2)|R_1^2\rangle \\ H|T_0^4\rangle &= -\alpha|E\rangle - \alpha|T_0^3\rangle + (\alpha - 2)|R_5\rangle \\ H|S_1\rangle &= -\alpha|R_1\rangle - \alpha|R_5^2\rangle + (\alpha - 2)|E\rangle \end{aligned} \tag{19}$$

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 $|\psi_{\mu 1}^{T_{1u}}\rangle$ and $|\psi_{\mu 0}^{T_1}\rangle$ for the representation T_{1u}:

$$\begin{aligned} |\psi_{11}^{T_{1u}}\rangle &= 8^{-1/2}\{|\Phi_{11}^{(1)}\rangle - \eta^2|\Phi_{11}^{(2)}\rangle - p^{-1}|\Phi_{11}^{(3)}\rangle + p\eta^2|\Phi_{11}^{(3)}\rangle \\ &\quad - p|\Phi_{11}^{(4)}\rangle + p^{-1}\eta|\Phi_{11}^{(4)}\rangle\} \\ &= (200)^{-1/2}\{\sqrt{5}(|E\rangle + \eta^{-1}|T_0\rangle + \eta|T_0^4\rangle) + (-p^{-1} + p)|S_1\rangle + \cdots\} \\ |\psi_{10}^{T_1}\rangle &= 2^{-1/2}\{-\eta|\Phi_{10}^{(3)}\rangle + \eta^{-2}|\Phi_{10}^{(4)}\rangle\} = (50)^{-1/2}\{-|S_1\rangle + \cdots\} \\ |\psi_{01}^{T_{1u}}\rangle &= 2^{-1}\{-\eta^{-1}|\Phi_{01}^{(3)}\rangle - \eta|\Phi_{01}^{(3)}\rangle + \eta^2|\Phi_{01}^{(4)}\rangle + \eta^{-2}|\Phi_{01}^{(4)}\rangle\} \\ &= (10)^{-1}\{-2|S_1\rangle + \cdots\} \\ |\psi_{00}^{T_1}\rangle &= 2^{-1}\{|\Phi_{00}^{(1)}\rangle - |\Phi_{00}^{(2)}\rangle + |\Phi_{00}^{(3)}\rangle - |\Phi_{00}^{(4)}\rangle\} \\ &= (10)^{-1}\{\sqrt{5}(|E\rangle + |T_0\rangle + |T_0^4\rangle) + |S_1\rangle + \cdots\} \end{aligned} \tag{20}$$

where we only list the terms of $|E\rangle$, $|T_0\rangle$, $|T_0^4\rangle$, and $|S_1\rangle$ which are relevant to the calculation. Comparing the coefficients of the term $|E\rangle$ on both sides of the equations

$$\begin{aligned} H|\psi_{11}^{T_{1u}}\rangle &= H_{11}|\psi_{11}^{T_{1u}}\rangle + H_{01}|\psi_{10}^{T_1}\rangle \\ H|\psi_{10}^{T_1}\rangle &= H_{10}|\psi_{11}^{T_{1u}}\rangle + H_{00}|\psi_{10}^{T_1}\rangle \\ H|\psi_{01}^{T_{1u}}\rangle &= H_{11}|\psi_{01}^{T_{1u}}\rangle + H_{01}|\psi_{00}^{T_1}\rangle \\ H|\psi_{00}^{T_1}\rangle &= H_{10}|\psi_{01}^{T_{1u}}\rangle + H_{00}|\psi_{00}^{T_1}\rangle \end{aligned} \tag{21}$$

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

$$H^{T_{1u}} = \frac{1}{2\sqrt{5}} \begin{pmatrix} -\alpha(7-\sqrt{5})+4 & -4(\alpha-2) \\ -4(\alpha-2) & -2\alpha(2\sqrt{5}-1)-4 \end{pmatrix} \tag{22}$$

$$E^{T_{1u}} = -\alpha\,(3+\sqrt{5})/4 \pm \frac{1}{4}\{18\alpha^2\,(3-\sqrt{5}) - 16\alpha\,(5-\sqrt{5}) + 64\}^{1/2}$$

The advantage of this method is that the eigenfunctions of the Hamiltonian can be obtained simultaneously.

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

$$H^{A_g} = -\alpha - 2, \qquad H^{T_{1g}} = -\alpha(\sqrt{5}+1)/2 + 2,$$

$$H^{T_{2g}} = \alpha(\sqrt{5}-1)/2 + 2$$

$$H^{T_{2u}} = \frac{1}{2\sqrt{5}} \begin{pmatrix} \alpha(7+\sqrt{5})-4 & 4(\alpha-2) \\ 4(\alpha-2) & -2\alpha(2\sqrt{5}+1)+4 \end{pmatrix},$$

$$H^{G_g} = \begin{pmatrix} \alpha(\sqrt{5}+1)/2 & -(\alpha-2) \\ -(\alpha-2) & -\alpha(\sqrt{5}-1)/2 \end{pmatrix} \tag{23}$$

$$H^{G_u} = \frac{1}{2\sqrt{5}} \begin{pmatrix} \alpha(\sqrt{5}+1)+8 & 2(\alpha-2) \\ 2(\alpha-2) & \alpha(\sqrt{5}-1)-8 \end{pmatrix},$$

$$H^{H_u} = \frac{1}{2\sqrt{5}} \begin{pmatrix} \alpha(7+\sqrt{5})-4 & 4(\alpha-2) \\ 4(\alpha-2) & -\alpha(7-\sqrt{5})+4 \end{pmatrix}$$

$$H^{H_g} = \frac{1}{10} \begin{pmatrix} \alpha(5\sqrt{5}+11)-12 & 4(\alpha-2) & 4\sqrt{3}(\alpha-2) \\ 4(\alpha-2) & -\alpha(5\sqrt{5}-11)-12 & -4\sqrt{3}(\alpha-2) \\ 4\sqrt{3}(\alpha-2) & -4\sqrt{3}(\alpha-2) & -22\alpha+4 \end{pmatrix}$$

The dimensions of the submatrices H^{Γ} are one or two except for H^{H_g}, so that the energy levels of the Hückel Hamiltonian can be calculated by hand:

$$E^{A_g} = -\alpha - 2, \qquad E^{T_{1g}} = -\alpha(\sqrt{5}+1)/2 + 2,$$

$$E^{T_{2g}} = \alpha(\sqrt{5}-1)/2 + 2$$

$$E^{T_{2u}} = -\alpha(3-\sqrt{5})/4 \pm \frac{1}{4}\{18\alpha^2(3+\sqrt{5}) - 16\alpha(5+\sqrt{5}) + 64\}^{1/2} \tag{24}$$

$$E^{G_g} = \alpha/2 \pm 2^{-1}(9\alpha^2 - 16\alpha + 16)^{1/2},$$

$$E^{G_u} = \alpha/2 \pm 2^{-1}(\alpha^2 + 16)^{1/2}$$

$$E^{Hu} = \alpha/2 \pm 2^{-1}(13\alpha^2 - 24\alpha + 16)^{1/2}$$

and E^{Hg} is the root of the following equation:

$$x^3 + 2x^2 + x(-6\alpha^2 + 8\alpha - 4) + (\alpha^3 - 12\alpha^2 + 16\alpha - 8) = 0 \qquad (25)$$

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

Example 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 each carbon atom of carbon-60. In addition to (a, b, c), we introduce a new index λ to identify those four carbon atoms. The carbon atom in the center is labeled by $\lambda = 1$, the carbon on the hexagon is labeled by 2, and the carbons on the two neighbor pentagons are 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 λ in terms of the generalized notation in (15):

$$|R, \lambda\rangle = |PR', \sigma(\lambda)\rangle = |a, b, c, \lambda\rangle, \qquad P|a, b, c, \lambda\rangle = |\bar{a}, b, c, \sigma(\lambda)\rangle$$
$$\sigma(1) = 1, \qquad \sigma(2) = 2, \qquad \sigma(3) = 4, \qquad \sigma(4) = 3 \qquad (26)$$

From (8) we have

$$P|\Phi^{(1)}_{\mu\mu}, \lambda\rangle = \eta^{2\mu}|\Phi^{(2)}_{\mu\mu}, \sigma(\lambda)\rangle, \qquad P|\Phi^{(3)}_{\mu\nu}, \lambda\rangle = \eta^{2\mu-\nu}|\Phi^{(4)}_{\mu\nu}, \sigma(\lambda)\rangle \qquad (27)$$

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

$$\begin{aligned}
|A_{1g}, 0, 1\rangle &= |\psi^A_{00}, 1\rangle = 60^{-1/2}\{|E,1\rangle + \cdots\} \\
|A_{1g}, 0, 2\rangle &= |\psi^A_{00}, 2\rangle = 60^{-1/2}\{|E, 2\rangle + |T_0, 2\rangle + |T^4_0, 2\rangle + \cdots\} \\
|A_{1g}, 0, 3\rangle &= 2^{-1/2}\{|\psi^A_{00}, 3\rangle + |\psi^A_{00}, 4\rangle\} \\
&= 120^{-1/2}\{|E, 3\rangle + |E, 4\rangle + |T^4_0, 3\rangle + |T_0, 4\rangle \\
&\quad + |S_1, 3\rangle + |S_1, 4\rangle + \cdots\} \\
|A_{1u}, 0, 1\rangle &= 2^{-1/2}\{|\psi^A_{00}, 3\rangle - |\psi^A_{00}, 4\rangle\} \\
&= 120^{-1/2}\{|E, 3\rangle - |E, 4\rangle + |T^4_0, 3\rangle - |T_0, 4\rangle \\
&\quad + |S_1, 3\rangle - |S_1, 4\rangle + \cdots\}
\end{aligned} \qquad (28)$$

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

$$\begin{aligned} H|E, 1\rangle &= -\alpha|E, 3\rangle - \alpha|E, 4\rangle + (\alpha - 2)|E, 2\rangle \\ H|E, 2\rangle &= -\alpha|T_0, 2\rangle - \alpha|T_0^4, 2\rangle + (\alpha - 2)|E, 1\rangle \\ H|E, 3\rangle &= -\alpha|E, 1\rangle - \alpha|S_1, 4\rangle + (\alpha - 2)|T_0, 4\rangle \\ H|E, 4\rangle &= -\alpha|E, 1\rangle - \alpha|S_1, 3\rangle + (\alpha - 2)|T_0^4, 3\rangle \end{aligned} \tag{29}$$

and for bond arrangement (b)

$$\begin{aligned} H|E, 1\rangle &= -\alpha|E, 3\rangle - \alpha|E, 4\rangle + (\alpha - 2)|E, 2\rangle \\ H|E, 2\rangle &= -\alpha|T_0, 2\rangle - \alpha|T_0^4, 2\rangle + (\alpha - 2)|E, 1\rangle \\ H|E, 3\rangle &= -\alpha|E, 1\rangle + (\alpha - 2)|S_1, 4\rangle - \alpha|T_0, 4\rangle \\ H|E, 4\rangle &= -\alpha|E, 1\rangle + (\alpha - 2)|S_1, 3\rangle - \alpha|T_0^4, 3\rangle \end{aligned} \tag{30}$$

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

$$\begin{aligned} &|E, 1\rangle, \quad |E, 2\rangle, \quad |E, 3\rangle, \quad |E, 4\rangle, \quad |T_0, 2\rangle \\ &|T_0, 4\rangle, \quad |T_0^4, 2\rangle, \quad |T_0^4, 3\rangle, \quad |S_1, 3\rangle, \quad |S_1, 4\rangle \end{aligned} \tag{31}$$

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

$$\begin{aligned} H^{A_{1g}}(a) = H^{A_{1g}}(b) &= \begin{pmatrix} 0 & \alpha - 2 & -\sqrt{2}\alpha \\ \alpha - 2 & -2\alpha & 0 \\ -\sqrt{2}\alpha & 0 & -2 \end{pmatrix}, \\ H^{A_{1u}}(a) = H^{A_{1u}}(b) &= 2 \end{aligned} \tag{32}$$

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.

$$\begin{aligned} |T_{1g}, \mu, \lambda\rangle &= 2^{-1/2}\{|\psi_{\mu 1}^{T_1}, \lambda\rangle + |\psi_{\mu 1}^{T_1}, \sigma(\lambda)\rangle\} \\ |T_{2g}, \mu, \lambda\rangle &= 2^{-1/2}\{|\psi_{\mu 2}^{T_2}, \lambda\rangle - |\psi_{\mu 2}^{T_2}, \sigma(\lambda)\rangle\} \\ |T_{1g}, \mu, 5\rangle &= 2^{-1/2}\{|\psi_{\mu 0}^{T_1}, 3\rangle - |\psi_{\mu 0}^{T_1}, 4\rangle\} \\ |T_{2g}, \mu, 5\rangle &= 2^{-1/2}\{|\psi_{\mu 0}^{T_2}, 3\rangle - |\psi_{\mu 0}^{T_2}, 4\rangle\} \end{aligned} \tag{33}$$

$$
\begin{aligned}
|T_{1u}, \mu, \lambda\rangle &= 2^{-1/2}\{|\psi^{T_1}_{\mu 1}, \lambda\rangle - |\psi^{T_1}_{\mu 1}, \sigma(\lambda)\rangle\} \\
|T_{2u}, \mu, \lambda\rangle &= 2^{-1/2}\{|\psi^{T_2}_{\mu 2}, \lambda\rangle + |\psi^{T_2}_{\mu 2}, \sigma(\lambda)\rangle\} \\
|T_{1u}, \mu, 5\rangle &= 2^{-1/2}\{|\psi^{T_1}_{\mu 0}, 3\rangle + |\psi^{T_1}_{\mu 0}, 4\rangle\} \\
|T_{2u}, \mu, 5\rangle &= 2^{-1/2}\{|\psi^{T_2}_{\mu 0}, 3\rangle + |\psi^{T_2}_{\mu 0}, 4\rangle\} \\
|T_{1u}, \mu, 6\rangle &= |\psi^{T_1}_{\mu 0}, 1\rangle, \qquad |T_{2u}, \mu, 6\rangle = |\psi^{T_2}_{\mu 0}, 1\rangle, \\
|T_{1u}, \mu, 7\rangle &= |\psi^{T_1}_{\mu 0}, 2\rangle, \qquad |T_{2u}, \mu, 7\rangle = |\psi^{T_2}_{\mu 0}, 2\rangle,
\end{aligned} \tag{34}
$$

where λ runs from 1 to 4, and $\sigma(\lambda)$ is 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):

$$
\begin{aligned}
H^{T_{1g}}(a)_{22} &= H^{T_{1g}}(b)_{22} = H^{T_{1u}}(a)_{22} = H^{T_{1u}}(b)_{22} = -\alpha p \\
H^{T_{1g}}(a)_{33} &= H^{T_{1g}}(a)_{44} = -H^{T_{1u}}(a)_{33} = -H^{T_{1u}}(a)_{44} = \alpha p/\sqrt{5} \\
H^{T_{1g}}(b)_{33} &= H^{T_{1g}}(b)_{44} = -H^{T_{1u}}(b)_{33} = -H^{T_{1u}}(b)_{44} = -(\alpha - 2)p/\sqrt{5} \\
H^{T_{1g}}(a)_{55} &= -H^{T_{1u}}(a)_{55} = -(\alpha - 2) + \alpha/\sqrt{5} \\
H^{T_{1g}}(b)_{55} &= -H^{T_{1u}}(b)_{55} = \alpha - (\alpha - 2)/\sqrt{5} \\
H^{T_{1u}}(a)_{77} &= H^{T_{1u}}(b)_{77} = -2\alpha \\
H^{T_{1g}}(a)_{12} &= H^{T_{1g}}(b)_{12} = H^{T_{1u}}(a)_{12} = H^{T_{1u}}(b)_{12} = H^{T_{1u}}(a)_{67} \\
&= H^{T_{1u}}(b)_{67} = \alpha - 2 \\
H^{T_{1g}}(a)_{13} &= H^{T_{1g}}(a)_{14} = H^{T_{1g}}(b)_{13} = H^{T_{1g}}(b)_{14} = H^{T_{1u}}(a)_{13} = H^{T_{1u}}(a)_{14} \\
&= H^{T_{1u}}(b)_{13} = H^{T_{1u}}(b)_{14} = -\alpha \\
H^{T_{1g}}(a)_{34} &= H^{T_{1u}}(a)_{34} = (\alpha - 2)\eta^{-1} + \alpha p^{-1}/\sqrt{5} \\
H^{T_{1g}}(b)_{34} &= H^{T_{1u}}(b)_{34} = -\alpha\eta^{-1} - (\alpha - 2)p^{-1}/\sqrt{5} \\
-H^{T_{1g}}(a)_{35} &= H^{T_{1g}}(a)_{45} = H^{T_{1u}}(a)_{35} = H^{T_{1u}}(a)_{45} = \alpha\sqrt{2/5} \\
-H^{T_{1g}}(b)_{35} &= H^{T_{1g}}(b)_{45} = H^{T_{1u}}(b)_{35} = H^{T_{1u}}(b)_{45} = -(\alpha - 2)\sqrt{2/5} \\
H^{T_{1u}}(a)_{56} &= H^{T_{1u}}(b)_{56} = -\alpha\sqrt{2}
\end{aligned} \tag{35}
$$

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

For the representations G and H we have

$$\begin{aligned}
|G_g, \mu, \lambda\rangle &= 2^{-1/2}\{|\psi^G_{\mu 2}, \lambda\rangle + |\psi^G_{\mu 2}, \sigma(\lambda)\rangle\} \\
|G_u, \mu, \lambda\rangle &= 2^{-1/2}\{|\psi^G_{\mu 2}, \lambda\rangle - |\psi^G_{\mu 2}, \sigma(\lambda)\rangle\} \\
|G_g, \mu, 4+\lambda\rangle &= 2^{-1/2}\{|\psi^G_{\mu 1}, \lambda\rangle + |\psi^G_{\mu 1}, \sigma(\lambda)\rangle\} \\
|G_u, \mu, 4+\lambda\rangle &= 2^{-1/2}\{|\psi^G_{\mu 1}, \lambda\rangle - |\psi^G_{\mu 1}, \sigma(\lambda)\rangle\}
\end{aligned} \tag{36}$$

$$\begin{aligned}
H^{G_g}(a)_{22} &= H^{G_g}(b)_{22} = H^{G_u}(a)_{22} = H^{G_u}(b)_{22} = \alpha p^{-1} \\
H^{G_g}(a)_{66} &= H^{G_g}(b)_{66} = H^{G_u}(a)_{66} = H^{G_u}(b)_{66} = -\alpha p \\
H^{G_g}(a)_{33} &= H^{G_g}(a)_{44} = -H^{G_g}(a)_{77} = -H^{G_g}(a)_{88} \\
&= -H^{G_u}(a)_{33} = -H^{G_u}(a)_{44} = H^{G_u}(a)_{77} = H^{G_u}(a)_{88} \\
&= -\alpha/\sqrt{5} \\
H^{G_g}(b)_{33} &= H^{G_g}(b)_{44} = -H^{G_g}(b)_{77} = -H^{G_g}(b)_{88} \\
&= -H^{G_u}(b)_{33} = -H^{G_u}(b)_{44} = H^{G_u}(b)_{77} = H^{G_u}(b)_{88} \\
&= (\alpha - 2)/\sqrt{5} \\
H^{G_g}(a)_{12} &= H^{G_g}(a)_{56} = H^{G_u}(a)_{12} = H^{G_u}(a)_{56} \\
&= H^{G_g}(b)_{12} = H^{G_g}(b)_{56} = H^{G_u}(b)_{12} = H^{G_u}(b)_{56} = \alpha - 2 \\
H^{G_g}(a)_{13} &= H^{G_g}(a)_{14} = H^{G_g}(a)_{57} = H^{G_g}(a)_{58} = H^{G_u}(a)_{13} = H^{G_u}(a)_{14} \\
&= H^{G_u}(a)_{57} = H^{G_u}(a)_{58} = H^{G_g}(b)_{13} = H^{G_g}(b)_{14} \\
&= H^{G_g}(b)_{57} = H^{G_g}(b)_{58} = H^{G_u}(b)_{13} = H^{G_u}(b)_{14} \\
&= H^{G_u}(b)_{57} = H^{G_u}(b)_{58} = -\alpha \\
H^{G_g}(a)_{34} &= H^{G_u}(a)_{34} = (\alpha - 2)\eta^{-2} + \alpha/\sqrt{5} \\
H^{G_g}(b)_{34} &= H^{G_u}(b)_{34} = -\alpha\eta^{-2} - (\alpha - 2)/\sqrt{5} \\
H^{G_g}(a)_{78} &= H^{G_u}(a)_{78} = (\alpha - 2)\eta^{-1} - \alpha/\sqrt{5} \\
H^{G_g}(b)_{78} &= H^{G_u}(b)_{78} = -\alpha\eta^{-1} + (\alpha - 2)/\sqrt{5} \\
H^{G_g}(a)_{37} &= H^{G_g}(a)_{48} = -H^{G_u}(a)_{37} = -H^{G_u}(a)_{48} = \alpha p^{-1}/\sqrt{5} \\
H^{G_g}(b)_{37} &= H^{G_g}(b)_{48} = -H^{G_u}(b)_{37} = -H^{G_u}(b)_{48} = -(\alpha - 2)p^{-1}/\sqrt{5} \\
H^{G_g}(a)_{38} &= H^{G_g}(a)_{47} = H^{G_u}(a)_{38} = H^{G_u}(a)_{47} = \alpha p/\sqrt{5}
\end{aligned} \tag{37}$$

$$
\begin{aligned}
H^{G_g}(b)_{38} &= H^{G_g}(b)_{47} = H^{G_u}(b)_{38} = H^{G_u}(b)_{47} = -(\alpha - 2)p/\sqrt{5} \\
|H_g, \mu, \lambda\rangle &= 2^{-1/2}\{|\psi^H_{\mu 2}, \lambda\rangle + |\psi^H_{\mu 2}, \sigma(\lambda)\rangle\} \\
|H_u, \mu, \lambda\rangle &= 2^{-1/2}\{|\psi^H_{\mu 2}, \lambda\rangle - |\psi^H_{\mu 2}, \sigma(\lambda)\rangle\} \\
|H_g, \mu, 4 + \lambda\rangle &= 2^{-1/2}\{|\psi^H_{\mu 1}, \lambda\rangle - |\psi^H_{\mu 1}, \sigma(\lambda)\rangle\} \\
|H_u, \mu, 4 + \lambda\rangle &= 2^{-1/2}\{|\psi^H_{\mu 1}, \lambda\rangle + |\psi^H_{\mu 1}, \sigma(\lambda)\rangle\} \qquad (38) \\
|H_g, \mu, 9\rangle &= 2^{-1/2}\{|\psi^H_{\mu 0}, 3\rangle + |\psi^H_{\mu 0}, 4\rangle\} \\
|H_u, \mu, 9\rangle &= 2^{-1/2}\{|\psi^H_{\mu 0}, 3\rangle - |\psi^H_{\mu 0}, 4\rangle\} \\
|H_g, \mu, 10\rangle &= |\psi^H_{\mu 0}, 1\rangle \\
|H_g, \mu, 11\rangle &= |\psi^H_{\mu 0}, 2\rangle \\
H^{H_g}(a)_{22} &= H^{H_g}(b)_{22} = H^{H_u}(a)_{22} = H^{H_u}(b)_{22} = \alpha p^{-1} \\
H^{H_g}(a)_{66} &= H^{H_g}(b)_{66} = H^{H_u}(a)_{66} = H^{H_u}(b)_{66} = -\alpha p \\
H^{H_g}(a)_{33} &= H^{H_g}(a)_{44} = -H^{H_u}(a)_{33} = -H^{H_u}(a)_{44} = -\alpha p^2/5 \\
H^{H_g}(b)_{33} &= H^{H_g}(b)_{44} = -H^{H_u}(b)_{33} = -H^{H_u}(b)_{44} = (\alpha - 2)\, p^2/5 \\
H^{H_g}(a)_{77} &= H^{H_g}(a)_{88} = -H^{H_u}(a)_{77} = -H^{H_u}(a)_{88} = -\alpha p^{-2}/5 \\
H^{H_g}(b)_{77} &= H^{H_g}(b)_{88} = -H^{H_u}(b)_{77} = -H^{H_u}(b)_{88} = (\alpha - 2)\, p^{-2}/5 \\
H^{H_g}(a)_{99} &= -H^{H_u}(a)_{99} = (\alpha - 2) + \alpha/5 \\
H^{H_g}(b)_{99} &= -H^{H_u}(b)_{99} = -\alpha - (\alpha - 2)/5 \\
H^{H_g}(a)_{11,11} &= H^{H_g}(b)_{11,11} = -2\alpha \\
H^{H_g}(a)_{12} &= H^{H_g}(a)_{56} = H^{H_g}(a)_{10,11} = H^{H_u}(a)_{12} = H^{H_u}(a)_{56} \\
&= H^{H_g}(b)_{12} = H^{H_g}(b)_{56} = H^{H_g}(b)_{10,11} = H^{H_u}(b)_{12} \qquad (39) \\
&= H^{H_u}(b)_{56} = \alpha - 2 \\
H^{H_g}(a)_{13} &= H^{H_g}(a)_{14} = H^{H_g}(a)_{57} = H^{H_g}(a)_{58} = H^{H_u}(a)_{13} = H^{H_u}(a)_{14} \\
&= H^{H_u}(a)_{57} = H^{H_u}(a)_{58} = H^{H_g}(b)_{13} = H^{H_g}(b)_{14} \\
&= H^{H_g}(b)_{57} = H^{H_g}(b)_{58} \\
&= H^{H_u}(b)_{13} = H^{H_u}(b)_{14} = H^{H_u}(b)_{57} = H^{H_u}(b)_{58} = -\alpha \\
H^{H_g}(a)_{34} &= H^{H_u}(a)_{34} = (\alpha - 2)\,\eta^{-2} - \alpha p^{-2}/5 \\
H^{H_g}(b)_{34} &= H^{H_u}(b)_{34} = -\alpha\eta^{-2} + (\alpha - 2)p^{-2}/5
\end{aligned}
$$

$$
\begin{aligned}
H^{H_g}(a)_{78} &= H^{H_u}(a)_{78} = (\alpha - 2)\,\eta^{-1} - \alpha p^2/5 \\
H^{H_g}(b)_{78} &= H^{H_u}(b)_{78} = -\alpha\eta^{-1} + (\alpha - 2)p^2/5 \\
H^{H_g}(a)_{37} &= H^{H_g}(a)_{48} = -H^{H_u}(a)_{37} = -H^{H_u}(a)_{48} = 2\alpha p/5 \\
H^{H_g}(b)_{37} &= H^{H_g}(b)_{48} = -H^{H_u}(b)_{37} = -H^{H_u}(b)_{48} = -2(\alpha - 2)p/5 \\
H^{H_g}(a)_{38} &= H^{H_g}(a)_{47} = H^{H_u}(a)_{38} = H^{H_u}(a)_{47} = -2\alpha p^{-1}/5 \\
H^{H_g}(b)_{38} &= H^{H_g}(b)_{47} = H^{H_u}(b)_{38} = H^{H_u}(b)_{47} = 2(\alpha - 2)\,p^{-1}/5 \\
H^{H_g}(a)_{39} &= H^{H_g}(a)_{49} = -H^{H_g}(a)_{79} = -H^{H_g}(a)_{89} \\
&= -H^{H_u}(a)_{39} = H^{H_u}(a)_{49} = H^{H_u}(a)_{79} = -H^{H_u}(a)_{89} \\
&= -\alpha\sqrt{6}/5 \\
H^{H_g}(b)_{39} &= H^{H_g}(b)_{49} = -H^{H_g}(b)_{79} = -H^{H_g}(b)_{89} \\
&= -H^{H_u}(b)_{39} = H^{H_u}(b)_{49} = H^{H_u}(b)_{79} = -H^{H_u}(b)_{89} \\
&= (\alpha - 2)\sqrt{6}/5 \\
H^{H_g}(a)_{9,10} &= H^{H_g}(b)_{9,10} = -\alpha\sqrt{2}
\end{aligned}
$$

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.

Example 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 $\psi^{\Gamma}_{\mu\nu}$ on the states, we obtain the SAB as follows:

$$\psi^{\Gamma}_{\mu\nu}|n_0n_1n_2n_3n_4n_5m_0m_1m_2m_3m_4m_5\rangle \tag{40}$$

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

$$
\begin{aligned}
&\overset{T_0}{\longrightarrow} \\
A_0, A_1, A_2, A_3, A_4, A_5 &\rightarrow A_0, A_2, A_3, A_4, A_5, A_1 \\
&\overset{S_{11}}{\longrightarrow} \\
A_0, A_1, A_2, A_3, A_4, A_5 &\rightarrow B_0, B_4, B_3, B_2, B_1, B_5 \\
&\overset{S_5}{\longrightarrow} \\
A_0, A_1, A_2, A_3, A_4, A_5 &\rightarrow A_5, A_4, B_2, B_3, A_1, A_0 \\
&\overset{S_{10}}{\longrightarrow} \\
A_0, A_1, A_2, A_3, A_4, A_5 &\rightarrow B_3, A_5, B_2, B_0, B_4, A_1
\end{aligned}
$$

Under the applications of T_0, S_{11}, S_5, and S_{10}, the state $|n_0n_1n_2n_3n_4n_5m_0m_1m_2m_3m_4m_5\rangle$ becomes

$$\begin{aligned} T_0&: \quad |n_0n_5n_1n_2n_3n_4m_0m_5m_1m_2m_3m_4\rangle \\ S_{11}&: \quad |m_0m_4m_3m_2m_1m_5n_0n_4n_3n_2n_1n_5\rangle \\ S_5&: \quad |n_5n_4m_2m_3n_1n_0m_5m_4n_2n_3m_1m_0\rangle \\ S_{10}&: \quad |m_3n_5m_2m_0m_4n_1n_3m_5n_2n_0n_4m_1\rangle \end{aligned} \tag{41}$$

When 12 quanta are all different from each other, we obtain 60 SABs that are divided into 16 sets with given irreducible representations. If some quanta are equal to each other, the number of 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 nonregular (Chen and Ping, 1997).

4. 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 SABs can be calculated generally and simply. This is a standard method in group theory (Hamermesh, 1962), and is widely used in 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 the **I** group space will be useful in future calculations for molecules with **I** and $\mathbf{I}_h$ symmetry.

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