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Reduced projection operators and algebraic expressions for the symmetry-adapted functions of the icosahedral group

Peng-Dong Fan,[a] Jin-Quan Chen[a]* and J. P. Draayer[b]

[a]*Department of Physics, Nanjing University, Nanjing 210093, People's Republic of China, and* [b]*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA.*
E-mail: jqchen@chenwang.nju.edu.cn

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Abstract

The algebraic expressions for the reduced projection operators $\wp_{\mu}^{(\lambda)\bar{\mu}} = \sum_{i=1}^{4} u_i \hat{\beta}_i$ for the irreducible representation (irrep) λ of the icosahedral group I are found by using the double-induced technique and eigenfunction method, where $\hat{\beta}_i$ are the double-coset generators of I with respect to the cyclic subgroup C_5. Simple algebraic expressions are derived for the symmetry-adapted functions (SAF's) by applying the reduced projection operators $\wp_{\mu}^{(\lambda)\bar{\mu}}$ to $Y_{l\bar{m}}$. The SAF's are functions of the angular momentum l, the quantum numbers λ, μ of the group chain $I \supset C_5$ and the multiplicity label $\bar{m}$. In this way, the SAF problem of the group I is solved once for all instead of for one angular momentum l each time.

1. Introduction

The icosahedral group is the most complicated molecular point group and has been the subject of many studies (Speiser, 1937; Laporte, 1948; Cohan, 1958; McLellian, 1961). The discovery of the quasicrystal and the fullerence C_{60} has revived the interest in the group (Hu *et al.*, 1987; Liu *et al.*, 1990; Chen & Ping, 1997; Prandl *et al.*, 1996). The symmetry-adapted functions (SAF's) of the icosahedral groups are important in physical applications (see for example Prandl *et al.*, 1996, and references therein). In some cases, high-order SAF's are also required. Low-order SAF's for the icosahedral group are available in McLellian (1961) and Butler (1981) ($j = 0, \frac{1}{2}, 1, \ldots, 8$), and in the papers by Laporte (1948) and Michel (1992), Cohan (1958) and Elcoro *et al.* (1994), with $l_{\max} = 10$, 12 and 16, respectively. In Altmann & Herzig (1994), the SAF's of the group chain $I \supset T \supset C_2$ are tabulated for l up to 15 with 12 digits.

Except in Butler (1981), where a building-up procedure is used, the conventional method for constructing SAF's is the projection-operator method. The construction of the SAF's for a high-symmetry group, such as the octahedral group and icosahedral group, by the projection-operator method is extremely difficult (Halonen & Child, 1983; Herman, 1997). Recently, Prandl *et al.* (1996) proposed a recursive method for constructing the SAF's of the group I and totally symmetric SAF's are obtained for angular momentum l up to 30. The extension of the recursive method to the irreps other than the identity representation is possible but it does not alleviate the difficulty of the original projection-operator method to a substantial extent. It is highly desirable to have algebraic expressions for the SAF's so that they can be obtained easily for any angular momentum l.

Recently, by using the double-induced technique and the eigenfunction method, algebraic solutions of the tetrahedral group T have been found (Chen & Fan, 1998*a*,*b*). Simple algebraic expressions of the projection operators (or irreducible symmetry operators), irreducible matrices, SAF's and Clebsch–Gordan (CG) coefficients are derived for the group T. The *elegance and simplicity* of the results lie in the fact that the projection operators, SAF's and CG coefficients are *functions of only the quantum numbers of the group chain* [the analogy of (j, m) for the group chain $SO_3 \supset SO_2$], without involving any irreducible matrix elements. Another advantage is that the solutions for both the single-valued and double-valued representations (reps) are obtained in a unified way.

In Chen & Fan (1998*b*), it is shown that, for constructing the SAF's and CG coefficients, the projection operator can be replaced by the so-called reduced projection operator (or effective irreducible symmetry operator, as it was originally called), which is extremely simple in structure, and enables us to obtain algebraic instead of numerical expressions for the SAF's and CG coefficients of any molecular point group.

In this paper, we will apply the same method to the icosahedral group. Although both single- and double-valued reps can be obtained simultaneously, owing to space limitations we will treat the single-valued case only, while leaving the double-valued case to another paper.

The outline of the paper is as follows: The Euler angles for the icosahedral group are given in §2. The double-induced technique is reviewed in §3, and the reduced projection operator of the group I is introduced

Table 1. *The rotation axes of the group I*

$C_{5,1}$ $1' \to 1$	$C_{5,2}$ $2' \to 2$	$C_{5,3}$ $3' \to 3$	$C_{5,4}$ $4' \to 4$	$C_{5,5}$ $5' \to 5$	$C_{5,6}$ $6' \to 6$		
$C_{3,1}$ △126†	$C_{3,2}$ △236	$C_{3,3}$ △346	$C_{3,4}$ △456	$C_{3,5}$ △516			
$C_{3,6}$ ▽124′‡	$C_{3,7}$ ▽235′	$C_{3,8}$ ▽341′	$C_{3,9}$ ▽452′	$C_{3,10}$ ▽513′			
$C_{2,1}$ 16§	$C_{2,2}$ 14′	$C_{2,3}$ 45	$C_{2,4}$ 35′	$C_{2,5}$ 36	$C_{2,6}$ 26	$C_{2,7}$ 12	$C_{2,8}$ 24′
$C_{2,9}$ 25′	$C_{2,10}$ 23	$C_{2,11}$ 46	$C_{2,12}$ 56	$C_{2,13}$ 15	$C_{2,14}$ 13′	$C_{2,15}$ 34	

† △126 means an axis from the origin to the center of the triangle 126. ‡ ▽124′ means an axis from the origin to the center of the triangle 124′. § 16 is the axis from the origin to the midpoint of the line connecting 1 and 6.

in §4. The algebraic expressions for the reduced projection operator are derived in §5. The irreducible matrices of double-coset generators, the SAF's and the relation between the double-induced representation and the symmetrized boson representation (Chen & Ping, 1997) are shown in §§6–8, respectively. The final section is a *Discussion and summary*.

2. The Euler angles of the icosahedral group

The vertices of an icosahedron are labeled as in Fig. 1. The vertices of the upper (lower) part are labeled 1–6(1′–6′). We use the same notation and ordering for the symmetry axes and elements of the group I as in Chen & Ping (1997). The group I has:

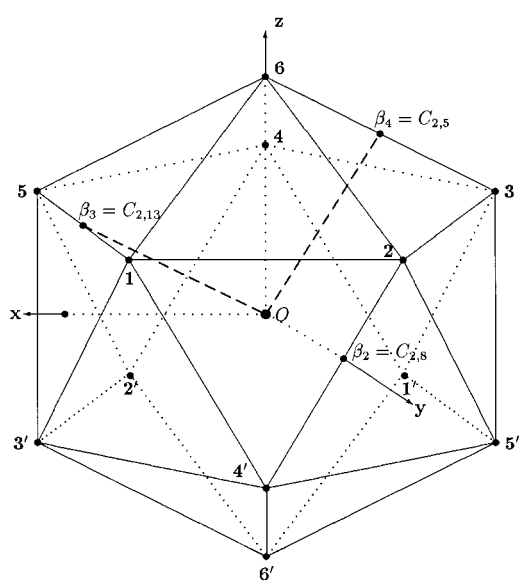

Fig. 1. The coordinate system and labels of the vertices for the I group, with β_i standing for the double-coset generators $\hat{\beta}_i$, $i = 2, \ldots, 4$.

6 fivefold axes (joining the two opposite vertices), $C_{5,j}$, $j = 1, \ldots, 6$;

10 threefold axes (joining the center of two opposite faces), $C_{3,j}$, $j = 1, \ldots, 10$;

15 twofold axes (joining the midpoints of the opposite edges), $C_{2,j}$, $j = 1, \ldots, 15$, as listed in Table 1. The indices for the 60 elements are listed in Table 2.

The Euler angles of the 60 elements have been given by Cohan (1958) and are valid only for single-valued representations. To avoid the ambiguity in assigning the Euler angles to each element of a double point group, a new way of determining the Euler angles has been proposed in Chen & Fan (1998*a*). The Euler angles of the 60 elements found in this way are given in Table 2. With the Euler angles and the rotation matrices $D^{1/2}(\alpha, \beta, \gamma)$ (Rose, 1957), the group table of the double point group $I^{\dagger}$ has been constructed in Fan *et al.* (1999), and is available upon request.

The main steps in Chen & Fan (1998*a*) for deriving the algebraic expressions of a point group are summarized in the next section, but now specified to the $I \supset C_5$ case.

3. The double-induced technique

The SAF is a linear combination of spherical harmonics $|lm\rangle = Y_{lm}$, which transforms as an irreducible basis of a point group. A key for constructing the SAF's is to find the projection operator. The normalized projection operator for the group chain $I \supset C_5$ is defined as

$$\mathcal{P}_{\mu}^{(\lambda)\bar{\mu}} = (h_{\lambda}/60)^{1/2} \sum_{a=1}^{60} D_{\mu\bar{\mu}}^{(\lambda)}(R_a)^* R_a, \qquad (1)$$

where h_{λ} is the dimension of the irrep λ, $D^{(\lambda)}(R_a)$ is the irreducible matrix of the element R_a and μ is the quantum number of the cyclic group C_5 generated from $C_{5z} = C_{5,6}$. Applying the projection operator $\mathcal{P}_{\mu}^{(\lambda)\bar{\mu}}$ to $|l\bar{m}\rangle$, we can get the SAF's $\psi_{\mu}^{\lambda} = \mathcal{P}_{\mu}^{(\lambda)\bar{\mu}}|l\bar{m}\rangle$.

Table 2. *Euler angles of $I^{\dagger}$*

Elements		α	β	γ	Elements		α	β	γ	Elements		α	β	γ
1	E	0	0	0	21	$C_{5,5}^{2-}$	0	$\pi-\omega$	$17\pi/5$	41	$C_{3,4}$	$7\pi/5$	ω	$16\pi/5$
2	$C_{5,6}$	0	0	$2\pi/5$	22	$C_{5,3}^{2}$	$4\pi/5$	$\pi-\omega$	$19\pi/5$	42	$C_{3,10}^{-}$	$2\pi/5$	$\pi-\omega$	$17\pi/5$
3	$C_{5,6}^{-}$	0	0	$18\pi/5$	23	$C_{5,3}^{2-}$	$6\pi/5$	$\pi-\omega$	$11\pi/5$	43	$C_{3,10}$	$8\pi/5$	$\pi-\omega$	$13\pi/5$
4	$C_{5,1}$	$9\pi/5$	ω‡	$12\pi/5$	24	$C_{5,2}^{2}$	$2\pi/5$	$\pi-\omega$	$\pi/5$	44	$C_{3,3}$	π	ω	$18\pi/5$
5	$C_{5,1}^{-}$	$3\pi/5$	ω	$16\pi/5$	25	$C_{5,2}^{2-}$	$4\pi/5$	$\pi-\omega$	$13\pi/5$	45	$C_{3,3}^{-}$	$7\pi/5$	ω	2π
6	$C_{5,4}$	π	ω	$16\pi/5$	26	$C_{3,1}$	$\pi/5$	ω	$2\pi/5$	46	$C_{2,1}$	$\pi/5$	ω	$4\pi/5$
7	$C_{5,4}^{-}$	$9\pi/5$	ω	2π	27	$C_{3,1}^{-}$	$3\pi/5$	ω	$14\pi/5$	47	$C_{2,2}$	0	π	$2\pi/5$
8	$C_{5,5}$	$7\pi/5$	ω	$14\pi/5$	28	$C_{3,6}$	0	$\pi-\omega$	$\pi/5$	48	$C_{2,3}$	$8\pi/5$	$\pi-\omega$	$17\pi/5$
9	$C_{5,5}^{-}$	$\pi/5$	ω	$18\pi/5$	29	$C_{3,6}^{-}$	$4\pi/5$	$\pi-\omega$	3π	49	$C_{2,4}$	0	π	$16\pi/5$
10	$C_{5,3}$	$3\pi/5$	ω	$18\pi/5$	30	$C_{3,9}$	0	$\pi-\omega$	$19\pi/5$	**50**§	$C_{2,5}$	π	ω	0
11	$C_{5,3}^{-}$	$7\pi/5$	ω	$12\pi/5$	31	$C_{3,9}$	$6\pi/5$	$\pi-\omega$	3π	51	$C_{2,6}$	$3\pi/5$	ω	$2\pi/5$
12	$C_{5,2}$	$\pi/5$	ω	0	32	$C_{3,7}$	$2\pi/5$	$\pi-\omega$	$19\pi/5$	52	$C_{2,7}$	$2\pi/5$	$\pi-\omega$	$3\pi/5$
13	$C_{5,2}^{-}$	π	ω	$14\pi/5$	33	$C_{3,7}^{-}$	$6\pi/5$	$\pi-\omega$	$13\pi/5$	**53**§	$C_{2,8}$	0	π	0
14	$C_{5,6}^{2}$	0	0	$4\pi/5$	34	$C_{3,2}$	$3\pi/5$	ω	0	54	$C_{2,9}$	0	π	$18\pi/5$
15	$C_{5,6}^{2-}$	0	0	$16\pi/5$	35	$C_{3,2}^{-}$	π	ω	$12\pi/5$	55	$C_{2,10}$	$4\pi/5$	$\pi-\omega$	$\pi/5$
16	$C_{5,1}^{2}$	0	$\pi-\omega$	$3\pi/5$	36	$C_{3,5}$	$9\pi/5$	ω	$14\pi/5$	56	$C_{2,11}$	$7\pi/5$	ω	$18\pi/5$
17	$C_{5,1}^{2-}$	$2\pi/5$	$\pi-\omega$	3π	37	$C_{3,5}^{-}$	$\pi/5$	ω	$16\pi/5$	57	$C_{2,12}$	$9\pi/5$	ω	$16\pi/5$
18	$C_{5,4}^{2}$	$6\pi/5$	$\pi-\omega$	$17\pi/5$	38	$C_{3,8}^{-}$	$8\pi/5$	$\pi-\omega$	$11\pi/5$	**58**§	$C_{2,13}$	0	$\pi-\omega$	π
19	$C_{5,4}^{2-}$	$8\pi/5$	$\pi-\omega$	$9\pi/5$	39	$C_{3,8}$	$4\pi/5$	$\pi-\omega$	$17\pi/5$	59	$C_{2,14}$	0	π	$4\pi/5$
20	$C_{5,5}^{2}$	$8\pi/5$	$\pi-\omega$	3π	40	$C_{3,4}^{-}$	$9\pi/5$	ω	$8\pi/5$	60	$C_{2,15}$	$6\pi/5$	$\pi-\omega$	$19\pi/5$

‡ $\omega=\cos^{-1}(1/5^{1/2})$. § The elements **50**, **53**, **58** are the coset generators β_4, β_2, β_3, respectively.

The double-induced technique is based on the double-coset decomposition and the eigenfunction method used for obtaining the analytic solutions of the rotation group in the group chain $SO(3)\supset SO(2)$. Recall that the $SO_3\supset SO_2$ projection operator

$$\mathcal{P}^{(j)}_{m\bar{m}}=[(2j+1)/8\pi^2]\times\int\sin\beta\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}\gamma\,D^{(j)}_{m\bar{m}}(\alpha\beta\gamma)^{*}R(\alpha\beta\gamma)\qquad(2a)$$

can be found by solving the following set of eigenequations (Eisenberg & Greiner, 1970; Chen, 1989)

$$(\mathbf{J}^2,J_z,\bar{J}_z)\mathcal{P}^{(j)}_{m\bar{m}}=[j(j+1),m,\bar{m}]\mathcal{P}^{(j)}_{m\bar{m}},\qquad(2b)$$

where $\bar{J}_z$ is the projection of the angular momentum along the intrinsic z axis (Bohr & Mottelson, 1969; Eisenberg & Greiner, 1970) and the quantum numbers m and $\bar{m}$ are referred to as the external and intrinsic quantum numbers.

Now let us give the counterpart of equation (2*b*) for the icosahedral group I. The 60 elements R_a of I span the group space with scalar product defined as

$$\langle R_a|R_b\rangle=\delta_{ab}.\qquad(2c)$$

In analogy with (2*b*), the projection operator $\mathcal{P}^{(\lambda)\bar{\mu}}_{\mu}$ can be found from the following set of eigenvalue equations (Chen, 1989):

$$\big(C,C_{5z},\bar{C}_{5z}\big)\mathcal{P}^{(\lambda)\bar{\mu}}_{\mu}=\big(\lambda,\rho_{\mu},\rho_{\bar{\mu}}\big)\mathcal{P}^{(\lambda)\bar{\mu}}_{\mu},\qquad(2d)$$

where C and C_{5z} are the CSCO (complete set of commuting operators) of I and C_5. The CSCO of a finite group G (Chen, 1989) is the analogy of the set of Casimir operators of a Lie group, and whose eigenvalue, called the quantum number of the group G, can uniquely label the inequivalent irreps. The CSCO's of most pure rotation point groups consist of only a single class operator. The CSCO of I is

$$C=\sum_{j=1}^{6}[C_{5,j}+C_{5,j}^{-}],\quad C_{5,j}^{-}\equiv C_{5,j}^{-1},\qquad(3)$$

which has five distinct eigenvalues

$$12,\quad -8c_2,\quad -8c_4,\quad -3,\quad 0,$$

with

$$c_{\mu}=\cos 2\mu\pi/5,\quad c_2=-(5^{1/2}+1)/4,\quad c_4=(5^{1/2}-1)/4,$$

corresponding to the five irreps, A, F_1, F_2, G, H, in Mulliken notation, as shown in Table 3. The CSCO of C_5 is C_{5z} with the eigenvalues

$$\rho\equiv\rho_{\mu}=\exp(-2\pi\mu i/5),\quad \mu=0,\pm1,\pm2.\qquad(4)$$

The operator $\bar{C}_{5z}$ is the so-called intrinsic operator. A general intrinsic operator $\bar{R}$ is defined in Chen (1989) by

$$\bar{R}S=SR\quad\text{for any } S\in G.\qquad(5a)$$

Notice that (5*a*) is the defining equation for the intrinsic operator $\bar{R}$ rather than an operator identity. Therefore,

$$\bar{R}_aR_bR_c\ldots R_d=\bar{R}_a(R_bR_c\ldots R_d)=R_bR_c\ldots R_dR_a.\qquad(5b)$$

The set of operators $(C,C_{5z},\bar{C}_{5z})$ is the analogy of $(\mathbf{J}^2,J_z,\bar{J}_z)$.

The eigenvector of C_{5z} is the projection operator of C_5,

$$P^{\mu}=\sum_{k=0}^{4}(\rho_{\mu}^{*})^k(C_{5z})^k,\quad C_{5z}=\exp[-(2\pi J_z/5)i].\qquad(6)$$

Table 3. *The eigenvalues* (λ, ρ) *of* (C, C_5)

$\rho = \exp(-2\mu\pi i/5)$.

	A	F_1	F_2	G	H
λ	12	$2+5^{1/2}$	$2-5^{1/2}$	-3	0
μ	0	(1, 0, −1)	(2, 0, −2)	(2, 1, −1, −2)	(2, 1, 0, −1, −2)

The steps for finding the eigenvectors of (2d) by the double-induced technique are as follows:

Step 1. Make the double coset decomposition of I with respect to the subgroup C_5:

$$I = \sum_{i=1}^{4} C_5\hat{\beta}_i C_5 = C_5(\hat{\beta}_1 + \hat{\beta}_2) + C_5(\hat{\beta}_3 + \hat{\beta}_4)C_5, \quad (7a)$$

with the coset generators chosen as

$$\hat{\beta}_1 = e, \ \hat{\beta}_2 = C_{2,8}, \ \hat{\beta}_3 = C_{2,13}, \ \hat{\beta}_4 = C_{2,5}. \quad (7b)$$

Let M_i be the number of times an element appears in the double coset $C_5\hat{\beta}_i C_5$. It can be easily shown that

$$M_i = \begin{cases} 5, & i = 1, 2 \\ 1, & i = 3, 4. \end{cases} \quad (8)$$

Step 2. Sandwiching the coset generators between P^{μ} and $P^{\bar{\mu}}$ gives us the simultaneous eigenvectors $\phi^i_{\mu\bar{\mu}}$ of C_{5z} and $\bar{C}_{5z}$ [due to (5a) and the fact that $P^{\bar{\mu}}C_{5z} = C_{5z}P^{\bar{\mu}} = \rho_{\bar{\mu}}P^{\bar{\mu}}$], which are orthonormal with the scalar product defined in (2c).

$$\phi^i_{\mu\bar{\mu}} = 5^{-1}M_i^{-1/2}P^{\mu}\hat{\beta}_i P^{\bar{\mu}}, \quad i = 1, 2, 3, 4, \quad (9)$$

with

$$\phi^1_{\mu\bar{\mu}} = \delta_{\mu\bar{\mu}}\phi^1_{\mu}, \quad \phi^2_{\mu\bar{\mu}} = \delta_{\mu-\bar{\mu}}\phi^2_{\mu}. \quad (10)$$

The $\phi^i_{\mu\bar{\mu}}$, $i = 1, 2, 3, 4$, form is called the double induced representation, which is a representation of I induced from the irrep $(\mu, \bar{\mu})$ of the group $C_5 \times \bar{C}_5$, where the intrinsic group $\bar{C}_5$ is the group generated from $\bar{C}_{5z}$.

To find the eigenvectors of the CSCO of I, we need steps 3 and 4.

Step 3. Construct the representation matrix M of the CSCO of the group I in the double-induced representation,

$$M_{ij}(\mu, \bar{\mu}) = \langle\phi^i_{\mu\bar{\mu}}|C|\phi^j_{\mu\bar{\mu}}\rangle. \quad (11)$$

Step 4. The projection operators can be expressed as

$$\mathcal{P}^{(\lambda)\bar{\mu}}_{\mu} = \sum_{i=1}^{4} u^{(\lambda)}_{i,\mu\bar{\mu}}\phi^i_{\mu\bar{\mu}}. \quad (12a)$$

The coefficients $u_i \equiv u^{(\lambda)}_{i,\mu\bar{\mu}}$ are determined from the following matrix equation:

$$M(\mu, \bar{\mu})\mathbf{u}^{(\lambda)}_{\mu\bar{\mu}} = \lambda\mathbf{u}^{(\lambda)}_{\mu\bar{\mu}}, \quad (12b)$$

where $\mathbf{u} = \{u_1, \ldots, u_q\}_{\text{column}}$ are orthonormalized column vectors.

Step 5. The determination of the phases of the projection operators. For each multidimensional irrep λ, we first choose the phases for the SAF's associated with the lowest possible l, as shown in the first two rows of Table 5. These SAF's are necessarily multiplicity free and they are associated with $l = 1, 2, 3$ for the irreps F_1, H, F_2 and G. Then the phases of the projection operators are determined by the request that the projected states $\mathcal{P}^{(\lambda)\bar{\mu}}_{\mu}|l\bar{m}\rangle$ for the above lowest possible l have the same phases as the SAF's with the chosen phases.

4. The reduced projection operator

In the double-coset decomposition, elements R_a of the group I can be expressed as

$$R_a = C^s_{5z}\hat{\beta}_i C^t_{5z}, \quad s, t = 0, 1, \ldots, 4, \quad (13a)$$

and the irreducible matrix elements can be factorized,

$$D^{(\lambda)}_{\mu\bar{\mu}}(R_a) = \rho^s_{\mu}d^{(\lambda)}_{\mu\bar{\mu}}(\hat{\beta}_i)\rho^t_{\bar{\mu}}, \quad (13b)$$

where $d^{(\lambda)}(\hat{\beta}_i) = D^{(\lambda)}(\hat{\beta}_i)$ [in analogy with the rotation matrix $d^j(\beta) = D^j(0, \beta, 0)$]. Substituting (13$a$) into (1) and using

$$\sum_{a=1}^{60} = \sum_{i=1}^{4} M_i^{-1} \sum_{s,t=0}^{4},$$

the projection operator (1) can be written as

$$\mathcal{P}^{(\lambda)\bar{\mu}}_{\mu} = (h_{\lambda}/60)^{1/2}P^{\mu}\wp^{(\lambda)\bar{\mu}}_{\mu}P^{\bar{\mu}}, \quad (14a)$$

$$\wp^{(\lambda)\bar{\mu}}_{\mu} = \sum_{i=1}^{4} M_i^{-1}d^{(\lambda)}_{\mu\bar{\mu}}(\hat{\beta}_i)^*\hat{\beta}_i. \quad (14b)$$

From (9), (12a) and (14), we obtain the relation between the eigenvectors $\mathbf{u}$ and irreducible matrices of the coset generators,

$$u^{(\lambda)}_{i,\mu\bar{\mu}} = (5h_{\lambda}/12)^{1/2}M_i^{-1/2}d^{(\lambda)}_{\mu\bar{\mu}}(\hat{\beta}_i)^*. \quad (15)$$

The operator $\wp^{(\lambda)\bar{\mu}}_{\mu}$ is called the reduced projection operator. The SAF's can be obtained by applying the projection operator (14a) to $|l\bar{m}\rangle = Y_{l\bar{m}}$ [the spherical harmonics defined according to Rose (1957)]:

$$\psi^{\lambda}_{\mu} = \mathcal{P}^{(\lambda)\bar{\mu}}_{\mu}|l\bar{m}\rangle. \quad (16a)$$

Using

$$P^{\mu}|lm\rangle = \sum_{k=0}^{4}(\rho_{\mu}^{*}\rho_{m})^{k}|lm\rangle = 5\dot{\delta}_{\mu,m}|lm\rangle,$$
$$\dot{\delta}_{\mu,m} = \begin{cases} 1, & \mu \doteq m \\ 0, & \text{otherwise}, \end{cases} \qquad (16b)$$

where $\mu \doteq m$ means $\mu = m \,(\mathrm{mod}\, 5)$, and ignoring the irrelevant constant factor, we get

$$\psi_{\mu}^{(\lambda)} = \mathcal{P}_{\mu}^{(\lambda)\bar{\mu}}|l\bar{m}\rangle = \sum_{m}{}' \sum_{i=1}^{4} M_{i}^{-1} d_{\mu\bar{\mu}}^{(\lambda)}(\hat{\beta}_{i})^{*} d_{m\bar{m}}^{(l)}(\hat{\beta}_{i})|lm\rangle, \quad \bar{m} \doteq \bar{\mu}, \qquad (17)$$

where $\sum'$ means that the summation is subjected to the condition $m \doteq \mu$.

Equation (17) shows that, acting on $|lm\rangle$, the projection operator $\mathcal{P}_{\mu}^{(\lambda)\bar{\mu}}$ can be replaced by the reduced projection operator $\wp_{\mu}^{(\lambda)\bar{\mu}}$ so long as we impose the magnetic quantum number conservation rules $\bar{m} \doteq \bar{\mu}$ for the trial state $|l\bar{m}\rangle$ and $m \doteq \mu$ for the final state, which are stipulated by the projection operators $P^{\bar{\mu}}$ and P^{μ}, respectively.

It is to be noted that the reduced projection operator (14*b*) contains only 4 instead of 60 terms for the group I, and thus is a drastic simplification of the usual form (1). It is this fact that makes the projection-operator method extremely simple and powerful once the reduced projection operator is used.

5. The algebraic expression of the $I \supset C_5$ projection operators

We now proceed to derive the algebraic expresion for the projection operator following the steps in §3.

5.1. *The $I \supset C_5$ projection operator*

According to (7*b*), (8) and (9), the four basis vectors of the double-induced representation are

$$\phi_{\mu,\bar{\mu}}^{1} = [1/5(5)^{1/2}]P^{\mu}eP^{\bar{\mu}}, \quad \phi_{\mu,\bar{\mu}}^{2} = [1/5(5)^{1/2}]P^{\mu}C_{2,8}P^{\bar{\mu}},$$
$$\phi_{\mu,\bar{\mu}}^{3} = \tfrac{1}{5}P^{\mu}C_{2,13}P^{\bar{\mu}}, \quad \phi_{\mu,\bar{\mu}}^{4} = \tfrac{1}{5}P^{\mu}C_{2,5}P^{\bar{\mu}}, \qquad (18a)$$
$$\phi_{\mu}^{1} = (1/5^{1/2})P^{\mu}, \quad \phi_{\mu}^{2} = (1/5^{1/2})P^{\mu}C_{2,8}. \qquad (18b)$$

It is seen that there are altogether $5+5+25+25=60$ linearly independent basis vectors in (18), which is just the order of the group I.

Using the same procedure as detailed in Chen & Fan (1998*a*) and the multiplication table of the group I in Fan *et al.* (1999), from (3) and (18), we can find the representation matrix $M \equiv M(\mu, \bar{\mu})$ of the CSCO in the double-induced representation,

$$M = 2\begin{bmatrix} c_{\mu}\delta_{\mu\bar{\mu}} & 0 & 0 & 5^{1/2}c_{2\mu}\delta_{\mu\bar{\mu}} \\ 0 & c_{\mu}\delta_{\mu-\bar{\mu}} & 5^{1/2}c_{2\mu}\delta_{\mu-\bar{\mu}} & 0 \\ 0 & 5^{1/2}c_{2\mu}\delta_{\mu-\bar{\mu}} & c_{\mu}+c_{\bar{\mu}}+c_{\mu+\bar{\mu}} & c_{2\mu+2\bar{\mu}}+c_{3\mu+2\bar{\mu}} \\ 5^{1/2}c_{2\mu}\delta_{\mu\bar{\mu}} & 0 & c_{2\mu+2\bar{\mu}}+c_{3\mu+2\bar{\mu}} & c_{\bar{\mu}}+c_{\mu}+c_{\mu-\bar{\mu}} \end{bmatrix}. \qquad (19)$$

The eigenvectors of the matrix M will be obtained separately in four cases:

Case (i). $\mu = \bar{\mu} = 0$ ($\rho = \bar{\rho} = 1$). M is simplified as

$$M = \begin{pmatrix} 2 & 0 & 0 & 2(5)^{1/2} \\ 0 & 2 & 2(5)^{1/2} & 0 \\ 0 & 2(5)^{1/2} & 6 & 4 \\ 2(5)^{1/2} & 0 & 4 & 6 \end{pmatrix}. \qquad (20a)$$

The eigenvalues are found as

$$\lambda = 12, \quad -8c_{2}, \quad -8c_{4}, \quad 0. \qquad (20b)$$

Solving the homogeneous linear equations $(M - \lambda\mathbf{I})\mathbf{u} = 0$, we get the eigenvectors

$$\mathcal{P}_{0}^{(\lambda)0} = N_{\lambda}\Big[\phi_{0}^{1} + \Big(\frac{\lambda-6}{4} - \frac{5}{\lambda-2}\Big)\phi_{0}^{2} + \frac{\lambda^{2}-8\lambda-8}{8(5)^{1/2}}\phi_{00}^{3} + \frac{\lambda-2}{2(5)^{1/2}}\phi_{00}^{4}\Big]. \qquad (20c)$$

Equation (20*c*) gives the algebraic expression of the projection operators as a function of λ. This expression is very elegant if the quantum number λ is used as the irrep label. Unfortunately, people are not familiar with this new labeling scheme, and it is more convenient to change back to the Mulliken notation. From (20*b*), (20*c*) and Table 3, we obtain the projection operators in a more explicit but less compact form,

$$\begin{cases} \mathcal{P}_{0}^{(A)0} = [1/(12)^{1/2}](\phi_{0}^{1} + \phi_{0}^{2} + 5^{1/2}\phi_{00}^{3} + 5^{1/2}\phi_{00}^{4}), \\ \mathcal{P}_{0}^{(F_1)0} = \frac{1}{2}(\phi_{0}^{1} - \phi_{0}^{2} - \phi_{00}^{3} + \phi_{00}^{4}), \\ \mathcal{P}_{0}^{(F_2)0} = \frac{1}{2}(\phi_{0}^{1} - \phi_{0}^{2} + \phi_{00}^{3} - \phi_{00}^{4}), \\ \mathcal{P}_{0}^{(H)0} = [1/(12)^{1/2}](5^{1/2}\phi_{0}^{1} + 5^{1/2}\phi_{0}^{2} - \phi_{00}^{3} - \phi_{00}^{4}). \end{cases} \qquad (20d)$$

Case (ii). $\mu = \bar{\mu} = \pm 1, \pm 2$ ($\rho = \bar{\rho} \neq$ real). In this case, the matrix M becomes three-dimensional. In the basis ϕ_{μ}^{1}, $\phi_{\mu\mu}^{3}$ and $\phi_{\mu\mu}^{4}$,

$$M = 2\begin{bmatrix} c_{\mu} & 0 & 5^{1/2}c_{2\mu} \\ 0 & 2c_{\mu}+c_{2\mu} & c_{\mu}+1 \\ 5^{1/2}c_{2\mu} & c_{\mu}+1 & 2c_{\mu}+1 \end{bmatrix} \qquad (21a)$$

and its eigenvectors are

$$\mathcal{P}_{\mu}^{(\lambda)\mu} = N_{\lambda}\Big[\phi_{\mu}^{1} + \frac{(\lambda-2c_{\mu})(2c_{\mu}+2)}{5^{1/2}(\rho_{\mu}^{2}+\rho_{\mu}^{*2})(\lambda-4c_{\mu}-2c_{2\mu})}\phi_{\mu\mu}^{3} + \frac{\lambda-2c_{\mu}}{5^{1/2}(\rho_{\mu}^{2}+\rho_{\mu}^{*2})}\phi_{\mu\mu}^{4}\Big]. \qquad (21b)$$

The eigenvalue is found as $\lambda = 0, -3, -8c_{2\mu}$. Substituting it into (21*b*), we obtain the projection operators,

$$\begin{cases} \mathcal{P}_\mu^{(H)\mu} = [1/(12)^{1/2}](5^{1/2}\phi_\mu^1 + 4c_{2\mu}^2\phi_{\mu\mu}^3 + 4c_\mu^2\phi_{\mu\mu}^4), \\ \mathcal{P}_\mu^{(G)\mu} = (1/3^{1/2})[\phi_\mu^1 + (-1)^\mu\phi_{\mu\mu}^3 - (-1)^\mu\phi_{\mu\mu}^4], \\ \mathcal{P}_\mu^{(F_{|\mu|})\mu} = \frac{1}{2}[\phi_\mu^1 + (-1)^\mu 2c_\mu\phi_{\mu\mu}^3 - (-1)^\mu 2c_{2\mu}\phi_{\mu\mu}^4], \\ \qquad\qquad \mu = \pm 1, \pm 2. \end{cases} \tag{21c}$$

Case (iii). $\mu = -\bar{\mu} = \pm 1, \pm 2$ ($\rho = \bar{\rho}^* \neq$ real). The matrix M is again three dimensional. In the basis ϕ_μ^2, $\phi_{\mu-\mu}^3$ and $\phi_{\mu-\mu}^4$,

$$M = 2\begin{bmatrix} c_\mu & 5^{1/2}c_{2\mu} & 0 \\ 5^{1/2}c_{2\mu} & 2c_\mu + 1 & c_\mu + 1 \\ 0 & c_\mu + 1 & 2c_\mu + c_{2\mu} \end{bmatrix}. \tag{22a}$$

The eigenvalues are the same as for case (ii), while the eigenvectors are

$$\mathcal{P}_\mu^{(\lambda)-\mu} = N_\lambda\Bigg[\phi_\mu^2 + \frac{\lambda - 2c_\mu}{5^{1/2}(\rho_\mu^{*2} + \rho_\mu^2)}\phi_{\mu-\mu}^3 + \frac{(\lambda - 2c_\mu)(2c_\mu + 2)}{5^{1/2}(\rho_\mu^{*2} + \rho_\mu^2)(\lambda - 4c_\mu - 2c_{2\mu})}\phi_{\mu-\mu}^4\Bigg]. \tag{22b}$$

The projection operators are

$$\begin{cases} \mathcal{P}_\mu^{(H)-\mu} = [1/(12)^{1/2}](5^{1/2}\phi_\mu^2 + 4c_\mu^2\phi_{\mu-\mu}^3 + 4c_{2\mu}^2\phi_{\mu-\mu}^4), \\ \mathcal{P}_\mu^{(G)-\mu} = (1/3^{1/2})[\phi_\mu^2 - (-1)^\mu\phi_{\mu-\mu}^3 + (-1)^\mu\phi_{\mu-\mu}^4], \\ \mathcal{P}_\mu^{(E_{|\mu|})-\mu} = \frac{1}{2}[\phi_\mu^2 - (-1)^\mu 2c_{2\mu}\phi_{\mu-\mu}^3 + (-1)^\mu 2c_\mu\phi_{\mu-\mu}^4], \\ \qquad\qquad \mu = \pm 1, \pm 2. \end{cases} \tag{22c}$$

Case (iv). $\mu \neq -\mu \neq \bar{\mu}$ ($\rho \neq \rho^* \neq \bar{\rho}$). Now $\phi^1 = \phi^2 \equiv 0$ and the double-induced representation becomes two dimensional. In the basis $(\phi_{\mu\bar{\mu}}^3, \phi_{\mu\bar{\mu}}^4)$, the matrix M is simplified as

$$M = 2\begin{bmatrix} c_{\bar{\mu}} + c_\mu + c_{\mu+\bar{\mu}}, & c_{2\mu+2\bar{\mu}} + c_{3\mu+2\bar{\mu}} \\ c_{2\mu+2\bar{\mu}} + c_{3\mu+2\bar{\mu}}, & c_\mu + c_{\bar{\mu}} + c_{\mu-\bar{\mu}} \end{bmatrix}, \tag{23a}$$

which has nondegenerate eigenvalues in the following cases:

$$\lambda = \begin{cases} 0, & (\mu : \bar{\mu}) = (0, \pm 1), (0, \pm 2), (\pm 1, \pm 2), \\ -8c_{2\mu}, & (\mu : \bar{\mu}) = (0, \pm 1), (0, \pm 2), \\ -3, & (\mu : \bar{\mu}) = (\pm 1, \pm 2). \end{cases} \tag{23b}$$

Since the ranges of μ and $\bar{\mu}$ are exactly the same, for simplicity we always use the convention:

$$(\mu : \bar{\mu}) \quad \text{means} \quad (\mu, \bar{\mu}) \quad \text{or} \quad (\bar{\mu}, \mu).$$

The eigenvectors of M are

$$\mathcal{P}_\mu^{(\lambda)\bar{\mu}} = N_\lambda\Bigg[\phi_{\mu\bar{\mu}}^3 + \frac{\lambda - 2c_\mu - 2c_{\bar{\mu}} - 2c_{\mu+\bar{\mu}}}{2c_{2\mu+2\bar{\mu}} + 2c_{3\mu+2\bar{\mu}}}\phi_{\mu\bar{\mu}}^4\Bigg]. \tag{23c}$$

Combining (23*b*) and (23*c*), we obtain the projection operators

$$\begin{cases} \mathcal{P}_\mu^{(H)\bar{\mu}} = (1/2^{1/2})(\phi_{\mu\bar{\mu}}^3 + \phi_{\mu\bar{\mu}}^4), \\ \mathcal{P}_\mu^{(F_{|\mu+\bar{\mu}|})\bar{\mu}} = (1/2^{1/2})(\phi_{\mu\bar{\mu}}^3 - \phi_{\mu\bar{\mu}}^4), \\ \qquad\qquad (\mu : \bar{\mu}) = (0, \pm 1), (0, \pm 2), \\ \mathcal{P}_\mu^{(H)\bar{\mu}} = (2/3^{1/2})(c_{\mu-\bar{\mu}}\phi_{\mu\bar{\mu}}^3 + c_{\mu+\bar{\mu}}\phi_{\mu\bar{\mu}}^4), \\ \mathcal{P}_\mu^{(G)\bar{\mu}} = (2/3^{1/2})(c_{\mu+\bar{\mu}}\phi_{\mu\bar{\mu}}^3 - c_{\mu-\bar{\mu}}\phi_{\mu\bar{\mu}}^4), \\ \qquad\qquad (\mu : \mu) = (\pm 1, \pm 2). \end{cases} \tag{23d}$$

5.2. *The $I \supset C_5$ reduced projection operators*

Substituting (18*a*) into (20*d*), (21*c*), (22*c*) and (23*d*), we get the projection operators $\mathcal{P}_\mu^{(\lambda)\bar{\mu}}$ in terms of $P^\mu\hat{\beta}_i P^{\bar{\mu}}$. By deleting the factor $(h_\lambda/60)^{1/2}P^\mu P^{\bar{\mu}}$, we obtain the following reduced projection operators

$$\wp_0^{(A)0} = \tfrac{1}{5}(e + \hat{\beta}_2) + \hat{\beta}_3 + \hat{\beta}_4, \tag{24a}$$

$$\begin{cases} \wp_0^{(F_1)0} = \frac{1}{5}(e - \hat{\beta}_2) - (1/5^{1/2})(\hat{\beta}_3 - \hat{\beta}_4), \\ \wp_\mu^{(F_1)\mu} = \frac{1}{5}e - (2/5^{1/2})(c_1\hat{\beta}_3 - c_2\hat{\beta}_4), \\ \wp_\mu^{(F_1)-\mu} = \frac{1}{5}\hat{\beta}_2 + (2/5^{1/2})(c_2\hat{\beta}_3 - c_1\hat{\beta}_4), \qquad \mu = \pm 1, \\ \wp_\mu^{(F_1)\bar{\mu}} = (2/5)^{1/2}\theta_{\mu\bar{\mu}}(\hat{\beta}_3 - \hat{\beta}_4), \quad (\mu : \bar{\mu}) = (0, \pm 1), \end{cases} \tag{24b}$$

where $\theta_{\mu\bar{\mu}}$ are one except $\theta_{10} = \theta_{01} = -1$.

$$\begin{cases} \wp_0^{(F_2)0} = \frac{1}{5}(e - \hat{\beta}_2) + (1/5^{1/2})(\hat{\beta}_3 - \hat{\beta}_4), \\ \wp_\mu^{(F_2)\mu} = \frac{1}{5}e + (2/5^{1/2})(c_2\hat{\beta}_3 - c_1\hat{\beta}_4), \\ \wp_\mu^{(F_2)-\mu} = -\frac{1}{5}\hat{\beta}_2 + (2/5^{1/2})(c_1\hat{\beta}_3 - c_2\hat{\beta}_4), \qquad \mu = \pm 2, \\ \wp_\mu^{(F_2)\bar{\mu}} = -(2/5)^{1/2}(\hat{\beta}_3 - \hat{\beta}_4), \qquad (\mu : \bar{\mu}) = (0, \pm 2), \end{cases} \tag{24c}$$

$$\begin{cases} \wp_\mu^{(G)\mu} = \frac{1}{5}e + (1/5^{1/2})(-1)^\mu(\hat{\beta}_3 - \hat{\beta}_4), \\ \wp_\mu^{(G)-\mu} = (-1)^{|\mu|-1}[(\frac{1}{5}\hat{\beta}_2) - (-1)^\mu(1/5^{1/2})(\hat{\beta}_3 - \hat{\beta}_4)], \\ \qquad\qquad \mu = \pm 1, \pm 2, \\ \wp_\mu^{(G)\bar{\mu}} = (2/5^{1/2})\theta_{\mu\bar{\mu}}(c_{\mu+\bar{\mu}}\hat{\beta}_3 - c_{\mu-\bar{\mu}}\hat{\beta}_4), \\ \qquad\qquad (\mu : \bar{\mu}) = (\pm 1, \pm 2), \end{cases} \tag{24d}$$

where $\theta_{\mu\bar{\mu}} = \theta_{\bar{\mu},\mu}$ are one except $\theta_{-12} = \theta_{-1-2} = -1$.

$$\begin{cases} \wp_0^{(H)0} = \frac{1}{5}(e + \hat{\beta}_2 - \hat{\beta}_3 - \hat{\beta}_4), \\ \wp_\mu^{(H)\mu} = \frac{1}{5}e + \frac{4}{5}(c_{2\mu}^2\hat{\beta}_3 + c_\mu^2\hat{\beta}_4), \\ \wp_\mu^{(H)-\mu} = (-1)^{|\mu|}[(\frac{1}{5}\hat{\beta}_2) + \frac{4}{5}(c_\mu^2\hat{\beta}_3 + c_{2\mu}^2\hat{\beta}_4)], \\ \qquad\qquad \mu = \pm 1, \pm 2, \\ \wp_\mu^{(H)\bar{\mu}} = (6^{1/2}/5)\theta_{\mu\bar{\mu}}(\hat{\beta}_3 + \hat{\beta}_4), \\ \qquad\qquad (\mu : \bar{\mu}) = (0, \pm 1), (0, \pm 2), \\ \wp_\mu^{(H)\bar{\mu}} = \frac{4}{5}\theta_{\mu\bar{\mu}}(c_{\mu-\bar{\mu}}\hat{\beta}_3 + c_{\mu+\bar{\mu}}\hat{\beta}_4), \\ \qquad\qquad (\mu : \bar{\mu}) = (\pm 1, \pm 2), \end{cases} \tag{24e}$$

where $\theta_{\mu\bar{\mu}} = \theta_{\bar{\mu}\mu} = 1$ except $\theta_{0-1} = \theta_{-12} = \theta_{-1-2} = -1$.

Table 4. *The elements of double cosets*

j	0	1	2	3	4					
$C_{5,6}^{j}$	**1**	**2**	**14**	**15**	**3**					
$C_{5,6}^{j} \cdot \mathbf{53}$	**53**	**54**	**49**	**59**	**47**					
(j,k)	(0,0)	(0,1)	(0,2)	(0,3)	(0,4)	(1,0)	(1,1)	(1,2)	(1,3)	(1,4)
$C_{5,6}^{j} \cdot \mathbf{58} \cdot C_{5,6}^{k}$	**58**	**21**	**30**	**28**	**16**	**17**	**42**	**32**	**24**	**52**
$C_{5,6}^{j} \cdot \mathbf{50} \cdot C_{5,6}^{k}$	**50**	**35**	**13**	**6**	**44**	**45**	**11**	**8**	**41**	**56**
(j,k)	(2,0)	(2,1)	(2,2)	(2,3)	(2,4)	(3,0)	(3,1)	(3,2)	(3,3)	(3,4)
$C_{5,6}^{j} \cdot \mathbf{58} \cdot C_{5,6}^{k}$	**7**	**4**	**36**	**57**	**40**	**12**	**26**	**46**	**37**	**9**
$C_{5,6}^{j} \cdot \mathbf{50} \cdot C_{5,6}^{k}$	**29**	**39**	**22**	**55**	**25**	**31**	**18**	**60**	**23**	**33**
(j,k)	(4,0)	(4,1)	(4,2)	(4,3)	(4,4)					
$C_{5,6}^{j} \cdot \mathbf{58} \cdot C_{5,6}^{k}$	**20**	**48**	**19**	**38**	**43**					
$C_{5,6}^{j} \cdot \mathbf{50} \cdot C_{5,6}^{k}$	**34**	**51**	**27**	**5**	**10**					

It is seen that the reduced projection operators of the group I are only functions of the quantum numbers λ (or the irrep label), μ and $\bar{\mu}$.

6. The $I \supset C_5$ irreducible matrices

The algebraic expressions of the reduced projection operators are merely functions of the quantum numbers λ, μ, $\bar{\mu}$ and thus are very concise, yet they contain essentially all the information about the irreducible matrix elements. For constructing the SAF's a knowledge of the reduced projection operators is sufficient. However, if one needs to find the CG coefficients, a knowledge of the irreducible matrices of the coset generators is also required, which can be found in the following way.

Since the operator $C_{5,6} = C_{5z}$ is diagonalized in the $I \supset C_5$ basis, its irreducible matrix is $D^{(\lambda)}_{\mu\bar{\mu}}(C_{5,6}) = \rho_\mu \delta_{\mu\bar{\mu}}$. On the other hand, according to (14*b*), the coefficients in front of the coset generator $\hat{\beta}_i/M_i$ in the reduced projection operators are just the complex conjugate of the matrix elements of $\hat{\beta}_i$. Therefore, from (24), we can read off the irreducible matrices of the double coset generator $\hat{\beta}_2, \hat{\beta}_3, \hat{\beta}_4$ directly.

$$
\begin{aligned}
D^{(F_1)}(C_{5,6}) &= \begin{bmatrix} \rho_1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \rho_{-1} \end{bmatrix}, \\
D^{(F_1)}(\hat{\beta}_2) &= \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \\
D^{(F_1)}(\hat{\beta}_3) &= (1/5^{1/2}) \begin{bmatrix} -2c_1 & -2^{1/2} & 2c_2 \\ -2^{1/2} & -1 & 2^{1/2} \\ 2c_2 & 2^{1/2} & -2c_1 \end{bmatrix}, \\
D^{(F_1)}(\hat{\beta}_4) &= (1/5^{1/2}) \begin{bmatrix} 2c_2 & 2^{1/2} & -2c_1 \\ 2^{1/2} & 1 & -2^{1/2} \\ -2c_1 & -2^{1/2} & 2c_2 \end{bmatrix}.
\end{aligned} \tag{25a}
$$

$$
\begin{aligned}
D^{(F_2)}(C_{5,6}) &= \begin{bmatrix} \rho_2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \rho_{-2} \end{bmatrix}, \\
D^{(F_2)}(\hat{\beta}_2) &= \begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \\
D^{(F_2)}(\hat{\beta}_3) &= (1/5^{1/2}) \begin{bmatrix} 2c_2 & -2^{1/2} & 2c_1 \\ -2^{1/2} & 1 & -2^{1/2} \\ 2c_1 & -2^{1/2} & 2c_2 \end{bmatrix}, \\
D^{(F_2)}(\hat{\beta}_4) &= (1/5^{1/2}) \begin{bmatrix} -2c_1 & 2^{1/2} & -2c_2 \\ 2^{1/2} & -1 & 2^{1/2} \\ -2c_2 & 2^{1/2} & -2c_1 \end{bmatrix}.
\end{aligned} \tag{25b}
$$

$$
\begin{aligned}
D^{(G)}(C_{5,6}) &= \begin{bmatrix} \rho_2 & 0 & 0 & 0 \\ 0 & \rho_1 & 0 & 0 \\ 0 & 0 & \rho_{-1} & 0 \\ 0 & 0 & 0 & \rho_{-2} \end{bmatrix}, \\
D^{(G)}(\hat{\beta}_2) &= \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}, \\
D^{(G)}(\hat{\beta}_3) &= (1/5^{1/2}) \begin{bmatrix} 1 & 2c_2 & -2c_1 & 1 \\ 2c_2 & -1 & 1 & 2c_1 \\ -2c_1 & 1 & -1 & -2c_2 \\ 1 & 2c_1 & -2c_2 & 1 \end{bmatrix}, \\
D^{(G)}(\hat{\beta}_4) &= (1/5^{1/2}) \begin{bmatrix} -1 & -2c_1 & 2c_2 & -1 \\ -2c_1 & 1 & -1 & -2c_2 \\ 2c_2 & -1 & 1 & 2c_1 \\ -1 & -2c_2 & 2c_1 & -1 \end{bmatrix}.
\end{aligned} \tag{25c}
$$

$$D^{(H)}(C_{5,6}) = \{\rho_2, \rho_1, 1, \rho_{-1}, \rho_{-2}\}_{\text{diag}},$$
$$D^{(H)}(\hat{\beta}_2) = \{1, -1, 1, -1, 1\}_{\text{antidiag}},$$
$$D^{(H)}(\hat{\beta}_3) = \tfrac{1}{5}\begin{bmatrix} 4c_1^2 & 4c_1 & 6^{1/2} & -4c_2 & 4c_2^2 \\ 4c_1 & 4c_2^2 & 6^{1/2} & -4c_1^2 & 4c_2 \\ 6^{1/2} & 6^{1/2} & -1 & -6^{1/2} & 6^{1/2} \\ -4c_2 & -4c_1^2 & -6^{1/2} & 4c_2^2 & -4c_1 \\ 4c_2^2 & 4c_2 & 6^{1/2} & -4c_1 & 4c_1^2 \end{bmatrix},$$
$$D^{(H)}(\hat{\beta}_4) = \tfrac{1}{5}\begin{bmatrix} 4c_2^2 & 4c_2 & 6^{1/2} & -4c_1 & 4c_1^2 \\ 4c_2 & 4c_1^2 & 6^{1/2} & -4c_2^2 & 4c_1 \\ 6^{1/2} & 6^{1/2} & -1 & -6^{1/2} & 6^{1/2} \\ -4c_1 & -4c_2^2 & -6^{1/2} & 4c_1^2 & -4c_2 \\ 4c_1^2 & 4c_1 & 6^{1/2} & -4c_2 & 4c_2^2 \end{bmatrix}, \tag{25d}$$

where $c_1 = c_4$, $c_2 = c_3$ and $c_{-\mu} = c_\mu$ are used.

It is shown in Chen & Fan (1998*b*) that to calculate the CG coefficients with the reduced projection operator only the irreducible matrices of the above double-coset generators are required. If one needs the irreducible matrices of other elements, they can be obtained by the following simple formulas:

$$\begin{aligned} D^{(\lambda)}_{\mu\bar{\mu}}(C^j_{5,6}\hat{\beta}_2) &= \rho^j d^{(\lambda)}_{\mu\bar{\mu}}(\hat{\beta}_2), \\ D^{(\lambda)}_{\mu\bar{\mu}}(C^j_{5,6}\hat{\beta}_3 C^k_{5,6}) &= \rho^j d^{(\lambda)}_{\mu\bar{\mu}}(\hat{\beta}_3)\bar{\rho}^k, \\ D^{(\lambda)}_{\mu\bar{\mu}}(C^j_{5,6}\hat{\beta}_4 C^k_{5,6}) &= \rho^j d^{(\lambda)}_{\mu\bar{\mu}}(\hat{\beta}_4)\bar{\rho}^k, \end{aligned} \tag{26}$$

where $\rho \equiv \rho_\mu$. Using the group table of I in Fan *et al.* (1999), we can obtain the pair of indices (j, k) for each element of I, as shown in Table 4.

Equations (25) and (26) give the algebraic expressions for the irreducible matrix elements.

7. The $I \supset C_5$ SAF's

7.1. *The algebraic expressions for the SAF's*

Now we derive the algebraic expressions for the SAF's, which are functions of the angular momentum l, the quantum numbers λ, μ and the multiplicity label $\bar{m}$. To construct the SAF's, for each irrep, we need only one set of the reduced projection operators with a specific intrinsic quantum number $\bar{\mu}$. The intrinsic quantum number can be chosen according to convenience. For example, from (24), it is seen that the projection operators of the irreps F_1, F_2 and H associated with $\bar{\mu} = 0$ are the simplest and can be chosen as the projection operators, while for the irrep G we can choose $\wp^{(G)\bar{\mu}=1}_\mu$ as the projection operator. In other words, for constructing the SAF's, only the following projection operators are needed:

$$\begin{aligned} \wp_0^{(A)0} &= \tfrac{1}{5}(e + \hat{\beta}_2) + \hat{\beta}_3 + \hat{\beta}_4, \\ \wp_0^{(F_\sigma)0} &= \tfrac{1}{5}(e - \hat{\beta}_2) + (-1)^\sigma(1/5^{1/2})(\hat{\beta}_3 - \hat{\beta}_4), \quad \sigma = 1, 2, \\ \wp_\mu^{(F_\sigma)0} &= (-1)^{\sigma+1}(2/5)^{1/2}(\hat{\beta}_3 - \hat{\beta}_4), \quad \mu = \pm\sigma, \\ \wp_\mu^{(G)1} &= \tfrac{1}{5}\hat{\beta}_\mu + (1/5^{1/2})(-1)^{(1+\mu)/2}(\hat{\beta}_3 - \hat{\beta}_4), \\ &\qquad \mu = \pm 1, \hat{\beta}_{-1} \equiv \hat{\beta}_2, \\ \wp_\mu^{(G)1} &= (2/5^{1/2})(c_{\mu+1}\hat{\beta}_3 - c_{\mu-1}\hat{\beta}_4), \quad \mu = \pm 2, \\ \wp_0^{(H)0} &= \tfrac{1}{5}(e + \hat{\beta}_2 - \hat{\beta}_3 - \hat{\beta}_4), \\ \wp_\mu^{(H)0} &= (6^{1/2}/5)(\hat{\beta}_3 + \hat{\beta}_4), \quad \mu = \pm 1, \pm 2. \end{aligned} \tag{27}$$

Compared with the original form [equation (1)] of the projection operator, the simplicity of (27) is quite impressive.

To obtain the SAF's, we also need to introduce the coordinate system that is shown in Fig. 1. Using Rose's (1957) expression for the $d^l_{m\bar{m}}(\beta)$ and the Euler angles for the coset generators listed in Table 2, we have

$$\begin{aligned} \hat{\beta}_2|l\bar{m}\rangle &= (-1)^{l-\bar{m}}|l - \bar{m}\rangle, \\ \hat{\beta}_3|l\bar{m}\rangle &= \sum_m \exp(-i\bar{m}\pi) d^l_{m\bar{m}}(\beta_3)|lm\rangle, \\ \hat{\beta}_4|l\bar{m}\rangle &= \sum_m \exp(-im\pi) d^l_{m\bar{m}}(\beta_4)|jm\rangle, \end{aligned} \tag{28}$$

where $\beta_3 = \pi - \beta_4$, $\beta_4 = \cos^{-1}(1/5)^{1/2}$.

Applying (27) to the trial state $|l\bar{m}\rangle$, using (28) and the magnetic quantum-number conservation rule, we immediately obtain the $I \supset C_5$ unnormalized SAF's $\psi^{(\lambda)\bar{m}}_\mu = \wp^{(\lambda)\bar{\mu}}_\mu |l\bar{m}\rangle$.

7.1.1. *One-dimensional irreps.*

$$\psi^{(A)\bar{m}} = |l\bar{m}\rangle + (-1)^{l+\bar{m}}|l - \bar{m}\rangle + 5\sum_{m \doteq 0}[(-1)^{\bar{m}} d^{(l)}_{m\bar{m}}(\beta_3) + (-1)^m d^{(l)}_{m\bar{m}}(\beta_4)]|lm\rangle, \tag{29a}$$

where $\bar{m} = 0 \,(\text{mod } 5)$.

7.1.2. *Three-dimensional irreps.*

$$\begin{aligned} \psi_0^{(F_\sigma)\bar{m}} &= |l\bar{m}\rangle - (-1)^{l+\bar{m}}|l - \bar{m}\rangle + (-1)^\sigma(5)^{1/2} \times \sum_{m \doteq 0}[(-1)^{\bar{m}} d^{(l)}_{m\bar{m}}(\beta_3) - (-1)^m d^{(l)}_{m\bar{m}}(\beta_4)]|lm\rangle, \\ \psi_\mu^{(F_\sigma)\bar{m}} &= \theta_{\sigma\mu}\sum_{m \doteq \mu}[(-1)^{\bar{m}+1} d^{(l)}_{m\bar{m}}(\beta_3) + (-1)^m d^{(l)}_{m\bar{m}}(\beta_4)]|lm\rangle, \\ &\qquad \mu = \pm\sigma, \end{aligned} \tag{29b}$$

with $\theta_{\sigma\mu} = \mu$ and 1 for $\sigma = 1$ and 2, respectively, and $\bar{m} = 0 \,(\text{mod } 5)$.

7.1.3. *Four-dimensional irreps.*

$$\begin{aligned}
\psi_1^{(G)\bar{m}} &= |l\bar{m}\rangle - (5)^{1/2} \sum_{m \doteq 1} [(-1)^{\bar{m}} d^{(l)}_{m\bar{m}}(\beta_3) \\
&\quad - (-1)^m d^{(l)}_{m\bar{m}}(\beta_4)]|lm\rangle, \\
\psi_{-1}^{(G)\bar{m}} &= (-1)^{l+\bar{m}}|l-\bar{m}\rangle + (5)^{1/2} \sum_{m \doteq -1} [(-1)^{\bar{m}} d^{(l)}_{m\bar{m}}(\beta_3) \\
&\quad - (-1)^m d^{(l)}_{m\bar{m}}(\beta_4)]|lm\rangle, \\
\psi_\mu^{(G)\bar{m}} &= \sum_{m \doteq \mu} [(-1)^{\bar{m}} c_{\mu+1} d^{l}_{m\bar{m}}(\beta_3) \\
&\quad - (-1)^m c_{\mu-1} d^{l}_{m\bar{m}}(\beta_4)]|lm\rangle, \quad \mu = \pm 2,
\end{aligned} \tag{29c}$$

where $\bar{m} = 1 \,(\mathrm{mod}\, 5)$.

7.1.4. *Five-dimensional irreps.*

$$\begin{aligned}
\psi_\mu^{(H)\bar{m}} &= (|l\bar{m}\rangle + (-1)^{l+\bar{m}}|l-\bar{m}\rangle)\delta_{\mu,0} \\
&\quad + \theta_\mu \sum_{m \doteq \mu} [(-1)^{\bar{m}} d^{(l)}_{m\bar{m}}(\beta_3) + (-1)^m d^{(l)}_{m\bar{m}}(\beta_4)]|lm\rangle,
\end{aligned} \tag{29d}$$

where $\bar{m} = 0 \,(\mathrm{mod}\, 5)$, while $\theta_\mu = -1$ for $\mu = 0, -1$ and $\theta_\mu = 1$ for $\mu = 1, \pm 2$.

7.2. *The symmetry of the SAF's*

From (29) and using the property of $d^l_{m\bar{m}}(\beta) = (-1)^{l-\bar{m}} d^l_{-m\bar{m}}(\pi - \beta)$ (Rose, 1957), we can derive the following symmetries for the SAF's:

$$\begin{aligned}
\langle lm|\psi^{(A)\bar{m}}\rangle &= (-1)^{l+m}\langle l-m|\psi^{(A)\bar{m}}\rangle \\
\langle lm|\psi_\mu^{(F_1)\bar{m}}\rangle &= (-1)^{l+m+\mu+1}\langle l-m|\psi_{-\mu}^{(F_1)\bar{m}}\rangle, \quad \mu = 0, 1, \\
\langle lm|\psi_\mu^{(F_2)\bar{m}}\rangle &= (-1)^{l+m+1}\langle l-m|\psi_{-\mu}^{(F_2)\bar{m}}\rangle, \quad \mu = 0, 2, \\
\langle lm|\psi_\mu^{(G)\bar{m}}\rangle &= (-1)^{l+m+\mu+1}\langle l-m|\psi_{-\mu}^{(G)\bar{m}}\rangle, \quad \mu = 1, 2, \\
\langle lm|\psi_\mu^{(H)\bar{m}}\rangle &= (-1)^{l+m+\mu}\langle l-m|\psi_{-\mu}^{(H)\bar{m}}\rangle, \quad \mu = 0, 1, 2.
\end{aligned} \tag{30}$$

It is interesting to note that the symmetry of the SAF's is independent of the intrinsic quantum number $\bar{m}$.

7.3. *The multiplicity problem*

In (29), it is seen that the quantum $\bar{m}$ serves naturally as the multiplicity label and the SAF's are functions of l, λ, μ and the multiplicity label $\bar{m}$. The construction of linearly independent SAF's for the multiplicity not-free case is troublesome in the conventional projection-operator method or the recursive method (Prandl *et al.*, 1996). In Altmann & Herzig (1994), the SAF's symmetry adapted to the group chain $I \supset T \supset C_2$ are obtained by using the conventional projection-operator method and the multiplicity problem is solved *numerically* by using the trial-and-error method, *i.e.* by trying to use the projection operators [which are denoted as W^i_{np} in Altmann & Herzig (1994)] with different column index p and different trial state $|l\bar{m}\rangle$ in each case. In contrast, we chose a fixed 'column' index, *i.e.* the intrinsic quantum number $\bar{\mu}$, in the projection operator $\wp_\mu^{(\lambda)\bar{\mu}}$, which is zero for all irrepss except for the irrep G, for which $\bar{\mu} = 1$ and the multiplicity label $\bar{m}$ are determined by the magnetic quantum-number conservation rule $\bar{m} \doteq \bar{\mu}$ and the subduction rule from the irrep l of O_3 to the irrep λ of group I. When an irrep λ occurs only once in D^l, $\bar{m}$ may take any permissible value. The results with different $\bar{m}$ differ at most by an overall phase. When the irrep λ occurs τ times, we need to take τ different values for $\bar{m}$. In general, the SAF's $\psi_\mu^{(\lambda)\bar{m}}$ with different $\bar{m}$ may be neither orthogonal nor linearly independent. To find numerical results from the algebraic expressions, the multiplicity τ^l_λ for the occurrence of the irrep λ of I in the subduced representation $l \downarrow \lambda$ is calculated first by using the character theory and is used as a control parameter for the calculation. The linear independence of the SAF's $\psi_\mu^{(\lambda)\bar{m}}$ with different $\bar{m}$ is checked in each step. No orthogonal procedure is included for keeping the simplicity of the algebraic expressions of the SAF's.

With the algebraic expressions, it is easy to find the exact numerical expressions of the SAF's $\psi_\mu^{(\lambda)\bar{m}}$ for any l with the help of some software, say the Maple software. It takes only minutes to calculate the SAF's with $l = 100$. The code in Maple is available upon request. Part of the SAF's is listed in Table 5.

8. The relation between the double-induced representation and the symmetrized boson representation

The point-group symmetrized boson representation (SBR) introduced by Chen & Ping (1997) is a powerful technique for constructing algebraic expressions of the symmetry-adapted basis and is particularly useful for describing vibrations of large molecules and for high overtones. The advantages of the SBR are that its basis vectors have a clear physical picture and symmetry-adapted bases for any concrete cases can be constructed in algebraic form once for all for a given point group without any projection procedure. However, the derivation in Chen & Ping (1997) is rather involved. In this section, we show that, using the algebraic expressions of the single-valued projection operators, we can obtain the results of Chen & Ping (1997) easily.

We begin with a brief review of the SBR. Let us consider the stretching vibration of an icosahedral molecule $C_{12}H_{12}$ with $I_h = (I \otimes \hat{\mathcal{I}})$ symmetry, where $\hat{\mathcal{I}}$ is the inversion group. The 12 C—H bonds are indexed as shown in Fig. 1. Since symmetry adaptation to the inversion group is trivial, in the following we only consider the group I. A state in which the bonds 1, 2, 3, 4, 5, 6, 1′, 2′, 3′, 4′, 5′, 6′ have respectively a, b, c, d, e, f, α, β, γ, δ, ε, ϕ vibrational quanta is denoted by

Table 5. *The $I \supset C_5$ SAF's*

The superscript is the multiplicity label.

$l = 1$ $\bar{m} = 0$ $|F_1\mu\rangle = |1\mu\rangle, \mu = 0, \pm 1$

$l = 2$ $\bar{m} = 0$ $|H\mu\rangle = |2\mu\rangle, \mu = 0, \pm 1, \pm 2$

$l = 3$ $\bar{m} = 0$ $|F_2 2\rangle = -(2/5)^{1/2}|3-3\rangle + (3/5)^{1/2}|32\rangle, \quad |F_2 0\rangle = |30\rangle, \quad |F_2 - 2\rangle = (3/5)^{1/2}|3-2\rangle + (2/5)^{1/2}|33\rangle$

$\bar{m} = 1$ $|G2\rangle = (3/5)^{1/2}|3-3\rangle + (2/5)^{1/2}|32\rangle, \quad |G1\rangle = |31\rangle, \quad |G-1\rangle = |3-1\rangle, \quad |G-2\rangle = (2/5)^{1/2}|3-2\rangle - (3/5)^{1/2}|33\rangle$

$l = 6$ $\bar{m} = -5$ $|A\rangle = (7^{1/2}/5)|6-5\rangle - (11^{1/2}/5)|60\rangle - (7^{1/2}/5)|65\rangle$

$l = 8$

$$|H2\rangle^1 = \{(2\times 11\times 7^{1/2}/[5^2(3\times 5)^{1/2}]\}|8-8\rangle + [19(13)^{1/2}/2\times 5^2 5^{1/2}]|8-3\rangle - [(11\times 13)^{1/2}/5^2(2\times 3\times 5)^{1/2}]|82\rangle$$
$$-\{37\times 7^{1/2}/[2\times 5^2(3\times 5)^{1/2}]\}|87\rangle$$

$\bar{m} = -5$

$$|H1\rangle^1 = -[2^3(13)^{1/2}/5^2 3^{1/2}]|8-4\rangle - [(7\times 11\times 13)^{1/2}/5^2 3^{1/2}]|81\rangle - [(2\times 7)^{1/2}/5^2]|86\rangle$$
$$|H0\rangle^1 = (1/2^{1/2})|8-5\rangle - (1/2^{1/2})|85\rangle$$
$$|H-1\rangle^1 = [(2\times 7)^{1/2}/5^2]|8-6\rangle - [(7\times 11\times 13)^{1/2}/5^2 3^{1/2}]|8-1\rangle + [2^3(13)^{1/2}/5^2 3^{1/2}]|84\rangle$$
$$|H-2\rangle^1 = [37\times 7^{1/2}/2\times 5^2(3\times 5)^{1/2}]|8-7\rangle - [(11\times 13)^{1/2}/5^2(2\times 3\times 5)^{1/2}]|8-2\rangle$$
$$-[19(13)^{1/2}/2\times 5^2 5^{1/2}]|83\rangle + [2\times 11\times 7^{1/2}/5^2(3\times 5)^{1/2}]|88\rangle$$

$\bar{m} = 0$

$$|H2\rangle^2 = [(3\times 11\times 13)^{1/2}/5^2 5^{1/2}]|8-8\rangle + [2(7\times 11)^{1/2}/5^2 5^{1/2}]|8-3\rangle$$
$$+[2^2(2\times 3\times 7)^{1/2}/5^2 5^{1/2}]|82\rangle + [2(3\times 11\times 13)^{1/2}/5^2 5^{1/2}]|87\rangle$$
$$|H1\rangle^2 = -[(3\times 7\times 11)^{1/2}/5^2]|8-4\rangle + [2\times 3\times 3^{1/2}/5^2]|81\rangle + [(2\times 11\times 13)^{1/2}/5^2]|86\rangle$$
$$|H0\rangle^2 = |80\rangle$$
$$|H-1\rangle^2 = -[(2\times 11\times 13)^{1/2}/5^2]|8-6\rangle + [2\times 3\times 3^{1/2}/5^2]|8-1\rangle + [(3\times 7\times 11)^{1/2}/5^2]|84\rangle$$
$$|H-2\rangle^2 = -[2(3\times 11\times 13)^{1/2}/5^2 5^{1/2}]|8-7\rangle + [2^2(2\times 3\times 7)^{1/2}/5^2 5^{1/2}]|8-2\rangle$$
$$-[2(7\times 11)^{1/2}/5^2 5^{1/2}]|83\rangle + [(3\times 11\times 13)^{1/2}/5^2 5^{1/2}]|88\rangle$$

$l = 9$

$$|G2\rangle^1 = [29(2\times 3\times 61)^{1/2}/3\times 5^2\times 61]|9-8\rangle + [2(7\times 13\times 17\times 61)^{1/2}/5^2\times 61]|9-3\rangle$$
$$-[2^4(3\times 13\times 17\times 61)^{1/2}/3\times 5^2\times 61]|92\rangle + [47(3\times 17\times 61)^{1/2}/3\times 5^2\times 61]|97\rangle$$

$\bar{m} = -9$

$$|G1\rangle^1 = [(3\times 61)^{1/2}/5^2]|9-9\rangle - [2\times 7(2\times 3\times 7\times 17\times 61)^{1/2}/3\times 5^2\times 61]|9-4\rangle$$
$$+[(2\times 3\times 11\times 13\times 17\times 61)^{1/2}/3\times 5^2\times 61]|91\rangle - [2^3\times 3(17\times 61)^{1/2}/5^2\times 61]|96\rangle$$
$$|G-1\rangle^1 = [2^3\times 3(17\times 61)^{1/2}/5^2\times 61]|9-6\rangle + [(2\times 3\times 11\times 13\times 17\times 61)^{1/2}/3\times 5^2\times 61]|9-1\rangle$$
$$+[2\times 7(2\times 3\times 7\times 17\times 61)^{1/2}/3\times 5^2\times 61]|94\rangle + [(3\times 61)^{1/2}/5^2]|99\rangle$$
$$|G-2\rangle^1 = -[47(3\times 17\times 61)^{1/2}/3\times 5^2\times 61]|9-7\rangle - [2^4(3\times 13\times 17\times 61)^{1/2}/3\times 5^2\times 61]|9-2\rangle$$
$$-[2(7\times 13\times 17\times 61)^{1/2}/5^2\times 61]|93\rangle + [29(2\times 3\times 61)^{1/2}/3\times 5^2\times 61]|98\rangle$$

$\bar{m} = -4$

$$|G2\rangle^2 = [2^2(2\times 3\times 7\times 17\times 409)^{1/2}/3\times 5^2\times 409]|9-8\rangle - [2\times 31(13\times 409)^{1/2}/5^2\times 409]|9-3\rangle$$
$$+[53(3\times 7\times 13\times 409)^{1/2}/3\times 5^2\times 409]|92\rangle - [2\times 113(3\times 7\times 409)^{1/2}/3\times 5^2\times 409]|97\rangle$$
$$|G1\rangle^2 = -[2\times 7(3\times 7\times 17\times 409)^{1/2}/5^2\times 409]|9-9\rangle + [(2\times 3\times 409)^{1/2}/3\times 5^2]|9-4\rangle$$
$$-[2^3(2\times 3\times 7\times 11\times 13\times 409)^{1/2}/3\times 5^2\times 409]|91\rangle + [67(7\times 409)^{1/2}/5^2\times 409]|96\rangle$$
$$|G-1\rangle^2 = -[67(7\times 409)^{1/2}/5^2\times 409]|9-6\rangle - [2^3(2\times 3\times 7\times 11\times 13\times 409)^{1/2}/3\times 5^2\times 409]|9-1\rangle$$
$$-[(2\times 3\times 409)^{1/2}/3\times 5^2]|94\rangle - [2\times 7(3\times 7\times 17\times 409)^{1/2}/5^2\times 409]|99\rangle$$
$$|G-2\rangle^2 = [2\times 113(3\times 7\times 409)^{1/2}/3\times 5^2\times 409]|9-7\rangle + [53(3\times 7\times 13\times 409)^{1/2}/3\times 5^2\times 409]|9-2\rangle$$
$$+[2\times 31(13\times 409)^{1/2}/5^2\times 409]|93\rangle + [2^2(2\times 3\times 7\times 17\times 409)^{1/2}/3\times 5^2\times 409]|98\rangle$$

$l = 11$

$$|F_1 1\rangle^1 = -[347(5\times 7)^{1/2}/2^3\times 3\times 5^3]|11\ -9\rangle + [17(5\times 17\times 19)^{1/2}/2^2\times 3\times 5^3]|11\ -4\rangle$$
$$-[(2\times 3\times 5\times 7\times 13\times 17\times 19)^{1/2}/2^3\times 3\times 5^3]|11\,1\rangle - [7(2\times 3\times 5\times 7\times 19)^{1/2}/2^3\times 5^3]|11\,6\rangle$$
$$+[41(3\times 5\times 11)^{1/2}/2^3\times 3\times 5^3]|11\,11\rangle$$

$\bar{m} = -10$

$$|F_1 0\rangle^1 = [2^2\times 3(3\times 5)^{1/2}/5^3]|11\ -10\rangle - [(2\times 5\times 7\times 17\times 19)^{1/2}/2^3\times 3\times 5^3]|11\ -5\rangle$$
$$\times[(5\times 7\times 11\times 13\times 17\times 19)^{1/2}/2^2\times 3\times 5^3]|11\,0\rangle + [(2\times 5\times 7\times 17\times 19)^{1/2}/2^3\times 3\times 5^3]|11\,5\rangle$$
$$+[2^2\times 3(3\times 5)^{1/2}/5^3]|11\,10\rangle$$
$$|F_1 - 1\rangle^1 = [41(3\times 5\times 11)^{1/2}/2^3\times 3\times 5^3]|11\ -11\rangle + [7(2\times 3\times 5\times 7\times 19)^{1/2}/2^3\times 5^3]|11\ -6\rangle$$
$$-[(2\times 3\times 5\times 7\times 13\times 17\times 19)^{1/2}/2^3\times 3\times 5^3]|11\ -1\rangle - [17(5\times 17\times 19)^{1/2}/2^2\times 3\times 5^3]|11\,4\rangle$$
$$-[347(5\times 7)^{1/2}/2^3\times 3\times 5^3]|11\,9\rangle$$

$\bar{m} = -5$

$$|F_1 1\rangle^2 = [3\times 47(5\times 17\times 19\times 3119)^{1/2}/2\times 5^3\times 3119]|11\ -9\rangle + [2\times 43(5\times 7\times 3119)^{1/2}/5^3\times 3119]|11\ -4\rangle$$
$$+[3^2\times 41(2\times 3\times 5\times 13\times 3119)^{1/2}/2\times 5^3\times 3119]|11\,1\rangle - [353(2\times 3\times 5\times 17\times 3119)^{1/2}/2\times 5^3\times 3119]|11\,6\rangle$$
$$+[11(3\times 5\times 7\times 11\times 17\times 19\times 3119)^{1/2}/2\times 5^3\times 3119]|11\,11\rangle$$
$$|F_1 0\rangle^2 = -[(3\times 5\times 7\times 17\times 19\times 3119)^{1/2}/5^3\times 3119]|11\ -10\rangle + [(2\times 5\times 3119)^{1/2}/2\times 5^3]|11\ -5\rangle$$
$$+[2\times 3(5\times 11\times 13\times 3119)^{1/2}/5^3\times 3119]|11\,0\rangle - [(2\times 5\times 3119)^{1/2}/2\times 5^3]|11\,5\rangle$$
$$-[(3\times 5\times 7\times 17\times 19\times 3119)^{1/2}/5^3\times 3119]|11\,10\rangle$$
$$|F_1 - 1\rangle^2 = [11(3\times 5\times 7\times 11\times 17\times 19\times 3119)^{1/2}/2\times 5^3\times 3119]|11\ -11\rangle$$
$$+[353(2\times 3\times 5\times 17\times 3119)^{1/2}/2\times 5^3\times 3119]|11\ -6\rangle$$
$$+[3^2\times 41(2\times 3\times 5\times 13\times 3119)^{1/2}/2\times 5^3\times 3119]|11\ -1\rangle - [2\times 43(5\times 7\times 3119)^{1/2}/5^3\times 3119]|11\,4\rangle$$
$$+[3\times 47(5\times 17\times 19\times 3119)^{1/2}/2\times 5^3\times 3119]|11\,9\rangle$$

$$\begin{aligned}\varphi_0 &\equiv |abcdef)) \\ &\equiv |abcde\alpha\beta\gamma\delta\varepsilon f\phi) \\ &\equiv |1^a2^b3^c4^d5^e1'^\alpha2'^\beta3'^\gamma4'^\delta5'^\varepsilon6^f6'^\phi). \end{aligned} \tag{31}$$

The state (31) is said to be nonsymmetry adapted and is called the normal order state or a reference state.

Applying the operator $\phi^1_\mu = (1/5)^{1/2}P^\mu$ in (18*b*) to the reference state φ_0 and noticing that the operator C_{5z} induces a cyclic permutation of the bonds as $C_{5z} = \{12345\} \equiv (12345)(1'2'3'4'5')$, we get

$$\begin{aligned}\phi^1_\mu|_{\rm SBR} &\equiv \phi^1_\mu\varphi_0 \\ &= (1/5^{1/2})P^\mu\varphi_0 \\ &= (1/5^{1/2})|abcde; f\rangle\rangle_\rho \\ &\equiv (1/5^{1/2})[|abcdef)) + \rho|bcdeaf)) + \rho^2|cdeabf)) \\ &\quad + \rho^3|deabcf)) + \rho^4|eabcdf))], \end{aligned} \tag{32}$$

where we use a semicolon to denote symmetrization with respect to the horizontal bonds 1–5 and 1′–5′.

The states $\phi^1_\mu|_{\rm SBR} = (1/5^{1/2})|abcde; f\rangle\rangle_\rho$ is a basis vector in the so-called C_5-symmetrized boson representation. Notice that the bond indices are symmetrized and hidden in $|abcde; f\rangle\rangle_\rho$. Instead of specifying how many vibrational quanta are in each bond, we only need to specify that there are $a, b, c, d, e, f, \alpha, \beta, \gamma, \delta, \varepsilon, \phi$ quanta distributed over the 12 bonds with cyclic symmetry ρ. In analogy with the second quantization formalism which makes the particle labels meaningless, here the symmetry boson representation makes the bond indices meaningless, resulting in great simplicity. The basis vectors $|abcde; f\rangle\rangle$ have the symmetry:

$$\begin{aligned}|abcde; f\rangle\rangle_\rho &= \rho|bcdea; f\rangle\rangle_\rho \\ &= \rho^2|cdeab; f\rangle\rangle_\rho \\ &= \rho^3|deabc; f\rangle\rangle_\rho \\ &= \rho^4|eabcd; f\rangle\rangle_\rho. \end{aligned} \tag{33}$$

Similarly, applying the operators $\phi^2_\mu = (1/5)^{1/2}P^\mu\hat\beta_2$ in (18*b*) and $\phi^3_{\mu,\bar\mu}$, $\phi^4_{\mu,\bar\mu}$ in (18*a*) to the reference state φ_0 and noticing that $\hat\beta_2$, $\hat\beta_3$, and $\hat\beta_4$ interchange the bond indices as $\hat\beta_2 = \{15'\}\{24'\}(33')(66')$, $\hat\beta_3 = \{15\}\{36'\}(22')(44')$ and $\hat\beta_4 = \{24\}\{36\}(11')(55')$ (see Fig. 1), we obtain

$$\phi^2_\mu|_{\rm SBR} \equiv \phi^2_\mu\varphi_0 = (1/5^{1/2})|\varepsilon\delta\gamma\beta\alpha; \phi\rangle\rangle_\rho \tag{34}$$

$$\begin{aligned}\phi^3_{\mu,\bar\mu}|_{\rm SBR} &\equiv \phi^3_{\mu,\bar\mu}\varphi_0 \\ &= \tfrac{1}{5}P^\mu\hat\beta_3[|abcdef)) + \bar\rho|bcdeaf)) + \bar\rho^2|cdeabf)) \\ &\quad + \bar\rho^3|deabcf)) + \bar\rho^4|eabcdf))] \\ &= \tfrac{1}{5}P^\mu[|e\beta\phi\delta a\gamma)) + \bar\rho|a\gamma\phi\varepsilon b\delta)) + \bar\rho^2|b\delta\phi\alpha c\varepsilon)) \\ &\quad + \bar\rho^3|c\varepsilon\phi\beta d\alpha)) + \bar\rho^4|d\alpha\phi\gamma e\beta))] \\ &= \tfrac{1}{5}[|e\beta\phi\delta a; \gamma\rangle\rangle_\rho + \bar\rho|a\gamma\phi\varepsilon b; \delta\rangle\rangle_\rho \\ &\quad + \bar\rho^2|b\delta\phi\alpha c; \varepsilon\rangle\rangle_\rho + \bar\rho^3|c\varepsilon\phi\beta d; \alpha\rangle\rangle_\rho \\ &\quad + \bar\rho^4|d\alpha\phi\gamma e; \beta\rangle\rangle_\rho] \\ \phi^4_{\mu,\bar\mu}|_{\rm SBR} &= \phi^4_{\mu,\bar\mu}\varphi_0 \\ &= \tfrac{1}{5}P^\mu\hat\beta_4[|abcdef)) + \bar\rho|bcdeaf)) + \bar\rho^2|cdeabf)) \\ &\quad + \bar\rho^3|deabcf)) + \bar\rho^4|eabcdf))] \\ &= \tfrac{1}{5}P^\mu[|\alpha dfb\varepsilon c)) + \bar\rho|\beta efc\alpha d)) + \bar\rho^2|\gamma afd\beta e)) \\ &\quad + \bar\rho^3|\delta bfe\gamma a)) + \bar\rho^4|\varepsilon cfa\delta b))] \\ &= \tfrac{1}{5}[|\alpha dfb\varepsilon; c\rangle\rangle_\rho + \bar\rho|\beta efc\alpha; d\rangle\rangle_\rho \\ &\quad + \bar\rho^2|\gamma afd\beta; e\rangle\rangle_\rho + \bar\rho^3|\delta bfe\gamma; a\rangle\rangle_\rho \\ &\quad + \bar\rho^4|\varepsilon cfa\delta; b\rangle\rangle_\rho]. \end{aligned}$$

From (32) and (34), we know that the irreducible basis vectors in the SBR are readily obtained by adding the suffix SBR to the basis ϕ^1_μ, ϕ^2_μ, $\phi^3_{\mu\bar\mu}$ and $\phi^4_{\mu\bar\mu}$ in (20*d*), (21*c*), (22*c*) and (23*d*). For comparing the results with the those in Chen & Ping (1997), we only list the principal components in the following:

$$\begin{aligned}\Psi^A &= [1/(12)^{1/2}](\phi^1_0|_{\rm SBR} + \phi^2_0|_{\rm SBR} + 5^{1/2}\phi^3_{00}|_{\rm SBR} \\ &\quad + 5^{1/2}\phi^4_{00}|_{\rm SBR}), \\ \Psi^{(F_1)0}_0 &= \tfrac{1}{2}(\phi^1_0|_{\rm SBR} - \phi^2_0|_{\rm SBR} - \phi^3_{00}|_{\rm SBR} + \phi^4_{00}|_{\rm SBR}), \\ \Psi^{(F_1)\bar\mu}_0 &= (1/2^{1/2})(\phi^3_{0\bar\mu}|_{\rm SBR} + \phi^4_{0\bar\mu}|_{\rm SBR}), \quad \bar\mu = \pm1, \\ \Psi^{(F_2)0}_0 &= \tfrac{1}{2}(\phi^1_0|_{\rm SBR} - \phi^2_0|_{\rm SBR} + \phi^3_{00}|_{\rm SBR} - \phi^4_{00}|_{\rm SBR}), \\ \Psi^{(F_2)\bar\mu}_0 &= (1/2^{1/2})(\phi^3_{0\bar\mu}|_{\rm SBR} + \phi^4_{0\bar\mu}|_{\rm SBR}), \quad \bar\mu = \pm2, \\ \Psi^{(G)2}_2 &= (1/3^{1/2})(\phi^1_2|_{\rm SBR} + \phi^3_{22}|_{\rm SBR} - \phi^4_{22}|_{\rm SBR}), \\ \Psi^{(G)-2}_2 &= (1/3^{1/2})(\phi^2_2|_{\rm SBR} - \phi^3_{22}|_{\rm SBR} + \phi^4_{22}|_{\rm SBR}), \\ \Psi^{(G)\bar\mu}_2 &= (2/3^{1/2})(c_{2+\bar\mu}\phi^3_{2\bar\mu}|_{\rm SBR} - c_{2-\bar\mu}\phi^4_{2\bar\mu}|_{\rm SBR}), \\ &\qquad \bar\mu = \pm1, \\ \Psi^{(H)0}_0 &= [1/(12)^{1/2}](5^{1/2}\phi^1_0|_{\rm SBR} + 5^{1/2}\phi^2_0|_{\rm SBR} - \phi^3_{00}|_{\rm SBR} \\ &\quad - \phi^4_{00}|_{\rm SBR}), \\ \Psi^{(H)\bar\mu}_0 &= (1/2^{1/2})(\phi^3_{0\bar\mu}|_{\rm SBR} + \phi^4_{0\bar\mu}|_{\rm SBR}), \quad \bar\mu = \pm1, \pm2. \end{aligned} \tag{35}$$

Using the symmetry (33), it can be shown that $\phi^1_\mu|_{\rm SBR}$, $\phi^2_\mu|_{\rm SBR}$, $\phi^3_{\mu\bar\mu}|_{\rm SBR}$ and $\phi^4_{\mu\bar\mu}|_{\rm SBR}$ are related to the corresponding basis vectors φ^1_ρ, φ^2_ρ, $\varphi^3_{\rho\bar\rho}$ and $\varphi^4_{\rho\bar\rho}$ in (27), (29) and (30) of Chen & Ping (1997) as

$$\begin{aligned}\phi^1_\mu|_{\rm SBR} &= \varphi^1_\rho, & \phi^2_\mu|_{\rm SBR} &= \varphi^2_\rho, \\ \phi^3_{\mu,\bar\mu}|_{\rm SBR} &= \bar\rho^2\rho^*\varphi^4_{\rho,\bar\rho}, & \phi^4_{\mu,\bar\mu}|_{\rm SBR} &= \bar\rho^2\rho\varphi^3_{\rho,\bar\rho}. \end{aligned} \tag{36}$$

Owing to (36), (35) are identical with the corresponding equations (45)–(46) in Chen & Ping (1997) except for the difference of the phase factors. To be more specific, the relations between the irreducible bases are

$$
\begin{aligned}
\Psi^{A} &= A, \\
\Psi_0^{F_{|\bar{\mu}|}0} &= F^0_{|\bar{\mu}|,0}, \\
\Psi_0^{F_{|\bar{\mu}|}\bar{\mu}} &= \rho^2_{\bar{\mu}}(-1)^{\bar{\mu}+1}F^{\bar{\mu}}_{|\bar{\mu}|,0}, \\
\Psi_2^{(G)2} &= G_2^2, \quad \Psi_2^{(G)-2} = \varepsilon G_2^{-2}, \quad \varepsilon = \exp(-\pi i/5) \\
\Psi_2^{(G)1} &= -\varepsilon^* G_2^1, \quad \Psi_2^{(G)-1} = \varepsilon^2 G_2^{-1}, \\
\Psi_0^{(H)0} &= H_0^0, \quad \Psi_0^{(H)\bar{\mu}} = \rho^2_{\bar{\mu}}(-1)^{\bar{\mu}} H_0^{\bar{\mu}},
\end{aligned} \tag{37}
$$

where $\bar{\mu} = \pm 1, \pm 2$, and the symbols $\lambda_\mu^{\bar{\mu}}$ on the right-hand side are notations used in Chen & Ping (1997) for the irreducible bases $\Psi_\mu^{(\lambda)\bar{\mu}}$. Since only the principal components are calculated in Chen & Ping (1997), the difference in phase is irrelevant. From the above, it is seen that once the projection operators are known it is trivial to get the irreducible basis in SBR.

9. Discussion and summary

For multiplicity-free cases, the $I \supset C_5$ SAF's obtained in this paper are identical with the tables given by Damhus *et al.* (1984, p. 439) for $j = 0$–5, and are different to those given by Butler (1981) in phase factors (owing to different choices of coordinate axes). The SAF's are all real in this paper and Butler (1981), while the SAF's in McLellian (1961) are complex.

McLellian (1961) gives the $SO_3 \downarrow I$ irreducible matrices of the element C, *i.e.* our generator $\hat{\beta}_4 = C_{2,5}$. Notice that McLellian used $\rho_{\mu'} = \exp[(2\pi\mu'/5)i]$, and his quantum number μ' is equivalent to our $-\mu$. The relationship between the $SO_3 \downarrow I$ irreducible matrix in McLellian (1961), denoted as $D^{(\lambda)'}(R_a)$, and our $D^{(\lambda)}(R_a)$ is

$$
D^{(\lambda)}(R_a) = U^{-1} D^{(\lambda)'}(R_a) U, \tag{38}
$$

where

$$
\begin{aligned}
U^{F_1} &= \{\,1 \quad -1 \quad -1\,\}_{\text{diag}}, \\
U^{F_2} &= \{\,1 \quad 1 \quad 1\,\}_{\text{diag}}, \\
U^{G} &= \{\,1 \quad 1 \quad -1 \quad 1\,\}_{\text{diag}}, \\
U^{H} &= \{\,1 \quad -1 \quad 1 \quad 1 \quad 1\,\}_{\text{diag}}\,.
\end{aligned} \tag{39}
$$

The corresponding SAF's, denoted by $\psi'^{(\lambda)}_\mu$, are given by

$$
\psi'^{(\lambda)}_\mu = \sum_\sigma U^*_{\mu\sigma} \psi^{(\lambda)}_\sigma. \tag{40}
$$

However, the $\psi'^{(\lambda)}_\mu$ differ from the McLellian SAF's by phase factors due to the different choice of the coordinate axes.

Prandl *et al.* (1996) have calculated the SAF's for the identity irrep of the group I by a recursive method. The SAF's obtained by the recursive procedure are also not orthogonal in the multiplicity label but they used the Schmidt procedure to orthogonalize them. It is found that, by rotating our coordinate system around the z axis through $\pi/5$, our results for $l < 30$ (multiplicity-free cases) are different to those in Prandl *et al.* (1996) in overall phase factors, while for $l = 30$ the relation between the two is

$$
\begin{aligned}
\psi_2 &= \psi^{(A)'\bar{m}=-30}, \\
\psi_1 &= [\alpha\psi^{(A)'\bar{m}=-30} - \psi^{(A)'\bar{m}=-25}]/N, \\
\alpha &= 0.041\,587\,724\,606, \\
N &= 0.999\,134\,856\,344,
\end{aligned}
$$

where $\psi^{(A)'\bar{m}}$ are our SAF's in the rotated coordinate system, while ψ_1 and ψ_2 are the basis vectors 30–1 and 30–2 in Prandl *et al.* (1996). It should be pointed out that only the SAF's for even l are calculated by Prandl *et al.* and their symmetry equation (4) applies only to the SAF's with even l. Besides, there is a misprint in their Table 1: the factor 2^2 in coefficient $-2^2 \times 3 \times (2 \times 5 \times 13 \times 29 \times 41 \times 47)^{1/2}$ of $L = 28$, $M = \pm 20$ should be 2, otherwise the normalization will be 0.651 203 434 3 instead of 1.

In summary, the algebraic expressions (24) for the reduced projection operators and equation (29) for the SAF's in the group chain $I \supset C_5$ are derived by the double-induced technique in an *ab initio* way. The algebraic expressions for the former are functions of only the quantum numbers $(\lambda, \mu, \bar{\mu})$, and those for the latter are functions of only the quantum numbers $(l, \lambda, \mu, \bar{m})$ with $\bar{m}$ serving as the multiplicity label. With the algebraic expression for the SAF's available, the symmetries of the SAF's are found, which are otherwise hidden in the numerical tables.

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