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SYMMETRY AND MOLECULAR ORBITALS OF C_{60}

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Abstract

The symmetry and energy levels of icosahedral C_{60} are studied. Explicit matrix representations of the icosahedral group are constructed. Projection operators are obtained to simplify eigenvalue problem. We summarize role of the group theory to specify energy levels of C_{60}.

1. INTRODUCTION

Many spectroscopic problems require the computation of projection operators. To calculate these operators, matrix representations of a point group, in appropriate dimension must be carried out. The software packages, Mathematica and GAP are much more versatile for this purpose. We demonstrate with a specific example how Mathematica and GAP are useful for computing matrix representations of a point group and projection operators of molecular system.

It is well known that molecular and crystallographic point groups can be constructed by breaking symmetries of Special Orthogonal Group SO(3)[1]. There are a number of interesting work about construction of crystallographic and molecular point groups[2]. Symmetry breaking method is a simple way for Mathametica and GAP users to construct these point groups.

Group theory has been applied in many different fields of physics, such as, classification of eigenfunctions, analysis of different types of phase transitions in solids, classification of energy levels of atomic, molecular, solid state and nuclear systems. In many cases, these applications require matrix representations of corresponding group[3,4].

In recent years, there have been some reports on calculation of the energy levels of icosahedral C_{60} and its various compounds[5]. Since C_{60} has high symmetry with symmetric group I_h ,the computations are based on group theoretical analysis. Many quasicrystals have icosahedral structure, and crystallographic description of I_h quasicrystals is purely mathematical.

The purpose of this paper is threefold. Firstly, we develop a systematic method to construct matrix representation of a point group. Secondly we compute projection

operators of icosahedral point group which has great interest for physicists who study C_{60} molecule or quasicrystals. Lastly, we demonstrate a specific example.

2. FINITE SUBGROUPS OF SO(3)

The irreducible representation of SO(3) are all real. SO(3) is a subgroup of SU(2) and generators of SU(2) can be written as $e^{i\vec{\omega}.\vec{J}}$, where J are angular momentum operator and closed under commutation

$$[J_1, J_2] = iJ_3 \quad [J_2, J_3] = iJ_1 \quad [J_3, J_1] = iJ_2 \quad . \tag{1}$$

To obtain the standard form of the commutation relationship of SO(3) algebra, we can write

$$J_{\pm} = \frac{1}{\sqrt{2}}(J_1 \pm iJ_2) \tag{2}$$

with the relation

$$[J_+, J_-] = J_3 \quad [J_3, J_{\pm}] = \pm J_{\pm} \tag{3}$$

Table 1. Generators and generation relations of the polyhedral subgroups of SO(3)

Finite subgroups of SO(3)	Generators	Generation relations
C_n (Cyclic)	$A = \mathrm{Exp}\left(\frac{i\pi J_3}{n}\right)$	$A^n=1$
D_n (Dihedral)	$A = \mathrm{Exp}\left(\frac{i2\pi J_3}{n}\right)$ $B = \mathrm{Exp}(i\pi J_1)$	$A^n=B^2=C^2=1$
T (Tetrahedral)	$A = \mathrm{Exp}\left(\frac{i2\pi(J_1+J_2+J_3)}{3\sqrt{3}}\right)$ $C = \mathrm{Exp}(i\pi J_1)$	$A^3=B^3=(AB)^2=1$, $B=A^2C$
O (Octahedral)	$A = \mathrm{Exp}\left(\frac{i\pi J_3}{2}\right)$ $B = \mathrm{Exp}\left(\frac{i2\pi(J_1+J_2+J_3)}{3\sqrt{3}}\right)$	$A^4=B^3=(AB)^2=1$
I (Icosahedral)	$A = \mathrm{Exp}\left(\frac{i2\pi(\sigma J_1+J_3)}{5\sqrt{2+\sigma}}\right)$ $B = \mathrm{Exp}\left(\frac{i2\pi(-\sigma J_2+\tau J_3)}{3}\right)$ $\sigma = \frac{1}{2}(1-\sqrt{5}), \quad \tau = \frac{1}{2}(1+\sqrt{5})$	$A^5=B^3=C^2=1$, $C=AB$

The operators J_+, J_- and J_3 act on a basic vector $\phi(jm)$ such as

$$J_{\pm}\phi(jm) = \sqrt{(j \mp m)(j \pm m + 1)}\,\phi(jm \pm 1)$$
$$J_3\phi(jm) = m\phi(jm) \tag{4}$$

since the range of m is bounded from j to -j, the unitary representations of SO(3) has dimension 2j+1, when j takes integer values. The generation relations of the finite subgroups of SO(3) are given in the last column of Table 1.

The molecular and/or crystallographic point groups can be classified as cyclic groups C_n, dihedral groups D_n, tetrahedral group T, octahedral group O, icosahedral group I. In the following table, we list the generators and generation relations of finite subgroups of SO(3).

Detailed description of the groups C_n, D_n, T, and O were studied in previously[1]. Since we are dealing with icosahedral group I, we construct irreducible matrix representations of the corresponding group. Icosahedral group has five irreducible representations with dimensions 1, 3, 4, and 5. It is obvious that one dimensional matrix representations of the J's are obtained from Eqn(4) for the values of j=0.

2.1 Construction of 3 and 5 dimensional matrix representations of I group

The breaking of SO(3) to icosahedral group is made by finding vacuum expectation values for ϕ. In a mathematical point of view the icosahedral group generators can be obtained by choosing the w and J's in the form of Table 1. To obtain 3×3 matrix representations of icosahedral group j, are taken as 1. From Eqn(4), we obtain J's and from last row of the table, we find the generators A and B which are complex matrices. These are transformed to a real base by choosing the field $\chi = T\phi$.

$$\chi_1 = \frac{i}{\sqrt{2}}(\phi(11) + \phi(1-1))$$
$$\chi_2 = \frac{i}{\sqrt{2}}(\phi(11) - \phi(1-1)) \tag{5}$$
$$\chi_3 = \phi(10)$$

that transforms 3 dimensional representation to real field. The other 3×3 representation of I group can be obtained by replacing σ and τ in Table 1 and transforming to a real field with the $\chi = T\phi$ given in Eqn(5). The representations are given in Appendix 1.

In this case, 5×5 matrix generator are carried out for j=2 as in j=1 case. The 5 dimensional generators are transformed to real base by choosing the base vectors which transforms 5×5 matrix representations that are given in Appendix 1, into real field. The diagonal generator in Appendix 1 are obtained by multiplying A and B at the last column of Table 1.

$$\chi_1 = \frac{1}{\sqrt{2}}(\phi(22) + \phi(2-2))$$
$$\chi_2 = \frac{i}{\sqrt{2}}(\phi(22) - \phi(2-2))$$
$$\chi_3 = \frac{1}{\sqrt{2}}(\phi(21) - \phi(2-1)) \qquad (6)$$
$$\chi_4 = \frac{i}{\sqrt{2}}(\phi(21) + \phi(2-1))$$
$$\chi_5 = \phi(20)$$

2.3. Construction of 4 dimensional matrix representations of I group

Even dimensional representations of the group cannot be obtained as odd dimensional representations, because 2j+1 always give odd dimension for integer values of j. Four dimensional representations are obtained by taking j=6 which gives 13×13 generators of SO(3). The conjugate classes of 13 dimensional representation are given in Table 2 and we have checked that this representation can be decomposed as

$$\underline{13} = \underline{1} + \underline{3} + \underline{4} + \underline{5}. \qquad (7)$$

The choice of the basis given in Eqn (8) transform these matrices to real matrices. After a few attempts 13 dimension generators are blockdiogonalized and 4 dimensional matrix representations given in Appendix 1 are obtained.

$$\chi_1 = \frac{1}{\sqrt{2}}(\phi(66) + \phi(6-6)) \qquad \chi_7 = \frac{1}{\sqrt{2}}(\phi(63) + \phi(6-3))$$
$$\chi_2 = \frac{i}{\sqrt{2}}(\phi(66) - \phi(6-6)) \qquad \chi_8 = \frac{1}{\sqrt{2}}(\phi(63) + \phi(6-3))$$
$$\chi_3 = \frac{1}{\sqrt{2}}(\phi(65) - \phi(6-5)) \qquad \chi_9 = \frac{1}{\sqrt{2}}(\phi(62) + \phi(6-2))$$
$$\chi_4 = \frac{i}{\sqrt{2}}(\phi(65) + \phi(6-5)) \qquad \chi_{10} = \frac{1}{\sqrt{2}}(\phi(61) + \phi(6-1)) \qquad (8)$$
$$\chi_5 = \frac{1}{\sqrt{2}}(\phi(64) - \phi(6-4)) \qquad \chi_{11} = \frac{1}{\sqrt{2}}(\phi(61) + \phi(6-1))$$
$$\chi_6 = \frac{i}{\sqrt{2}}(\phi(64) + \phi(6-4)) \qquad \chi_{12} = \frac{i}{\sqrt{2}}(\phi(61) + \phi(6-1))$$
$$\chi_{13} = \phi(60)$$

All these calculations are easily made by preparing a simple program in Mathematica.

3. PROJECTION OPERATORS AND MOLECULAR ORBITALS

The frequently used method for establishing permissible quantum states for a molecule involved use of projection operators[6]. Projection operators based on the group representations are often used for formulating appropriate linear combinations of a set of basis functions. The operator for the k^{th} irreducible representation of dimension n_k belonging to a group of order h is defined as

$$P_{ij}^{\alpha} = \frac{n_\alpha}{g} \sum_R D_{ij}^{\alpha}(R_1) R_1 \qquad (9)$$

where D_{ij} represents the irreducible matrix form , R_i is the symmetry operations, n_α is the dimension of the irreducible representation and g is the order of the group. In this section, we develop a method to obtain projection operators for C_{60} molecule. It is well known that Hückel molecular orbital theory is very useful for large carbon systems. For large carbon systems Hückel determinant must be block diagonal form. This can be done by projection operators.

Table 2. Character table for the full icosahedral group I_h. The last two row demonstrates the characters of site symmetry matrices and the characters of 13×13 matrices.

I_h	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	I	$12S_{10}$	$12S_{10}^3$	$20S_6$	15σ	
A_g	1	1	1	1	1	1	1	1	1	1	
F_{1g}	3	τ	$-\sigma$	0	-1	3	$-\sigma$	τ	0	-1	R_x,R_y,R_z
F_{2g}	3	$-\sigma$	τ	0	-1	3	τ	$-\sigma$	0	-1	
G_g	4	-1	-1	1	0	4	-1	-1	1	0	
H_g	5	0	0	-1	1	5	0	0	-1	1	
A_u	1	1	1	1	1	-1	-1	-1	-1	-1	
F_{1u}	3	τ	$-\sigma$	0	-1	-3	σ	$-\tau$	0	1	x,y,z
F_{2u}	3	$-\sigma$	τ	0	-1	-3	$-\tau$	σ	0	1	
G_u	4	-1	-1	1	0	-4	1	1	-1	0	
H_u	5	0	0	-1	1	-5	0	0	1	-1	
χ_{site}	60	0	0	0	0	0	0	0	0	4	
χ_{13}	13	σ	τ	1	1	-13	$-\sigma$	$-\tau$	-1	-1	

Icosahedral C_{60} molecule includes sixty carbon atoms in a site. The position vectors from the center of molecule to the i^{th} atom in a site can be found by choosing a radial vector r_1 for an atom and the other vectors are obtained from

$$\vec{r}_i = g_i \vec{r}_1 \qquad (10)$$

where g_i are 3 dimensional group elements and are given in Appendix 1. Site symmetry matrix generators (60x60) of I_h are constructed by transforming each position vector using

3x3 generators.

$$\begin{aligned} D_{ij} &= g_1 \vec{r}_i \rightarrow \vec{r}_j \\ F_{ij} &= g_2 \vec{r}_i \rightarrow \vec{r}_j \end{aligned} \qquad i, j=1,2...60 \tag{11}$$

where D and F are 60 dimension matrix generators of the group and the characters χ_{site} are presented in Table 2. Decomposition of χ_{site} in terms of irreducible representations are given

$$\chi_{site} = A_g + T_{1g} + T_{2g} + 2G_g + 3H_g + 2T_{1u} + 2T_{2u} + 2G_u + 2H_u \tag{12}$$

We now want to obtain projection operators which blockdiagonalize Hückel Hamiltonian matrix in the form of the Eqn(12). We carried out all elements of the group in GAP and from Eqn(9), we obtained projection operators.

The molecular orbitals of I_h site are formed by following a simple way. We choose a basis vector ϕ_1 and the wave vectors of each atom ψ_{ij}^k are written in terms of base vectors ϕ_i are

$$\psi_{ij}^k = P_{ij}^k \phi_1 . \tag{13}$$

The molecular orbital for I_h site obtained from Eqn(13) are given in Appendix 2.

4. AN APPLICATION: ENERGY LEVELS OF C_{60}

In previous section, we have classified the atomic orbitals and wave functions according to the irreducible representations of I_h. In this section, we will find the energy eigenvalues of C_{60} molecule. It is known that energy expectation value of i^{th} state of a molecule is given by

$$\begin{aligned} E_i &= \langle \psi_i | H | \psi_i \rangle \\ &= N_i^2 \left[C_i^2 \langle \phi_j | H | \phi_j \rangle + C_{ij} C_{ik} \langle \phi_j | H | \phi_k \rangle \right] \\ &= \alpha + 2N_i^2 C_{ij} C_{ik} \langle \phi_j | H | \phi_k \rangle \end{aligned} \tag{14}$$

where $\alpha = \langle \phi_j | H | \phi_j \rangle$ and N_i, C_{ij} are scalar coefficients. According to the Hückel approximation, in evaluating E_i we can neglect any integral form $\langle \phi_j | H | \phi_k \rangle$ in Eqn(14), if ϕ_j and ϕ_k refer to non-adjacent atoms. For C_{60} molecule each atom are bonded to three neighborhood atom with two single bond and one double bond. In this case , we neglect the interaction between further atoms and we can write

$$\langle \phi_j | H | \phi_k \rangle = \begin{cases} \beta_1 & \text{for double bond} \\ \beta_2 & \text{for single bond} \end{cases} \tag{15}$$

To simplify our problem we can make another approximation. Since β_1 and β_2 are double and single bonds respectively, one can choose $\beta_1 = 2\beta_2$. We have taken α=0 in

our calculations according to the Hückel approximation. The Hamiltonian matrix is computed from Eqn(14), for each representation of I_h group and eigenvalues of these matrices are given in Appendix 2. As shown from Figure 1, there are antibonding and bonding energy levels. Eigenvalues of block diagonalized Hamiltonian matrices give two different energy levels which correspond to one irreducible representation (T_{1u},G_g, etc..) Larger energy represents antibonding energies, smaller energy represents bonding energies of an electron in an atom.

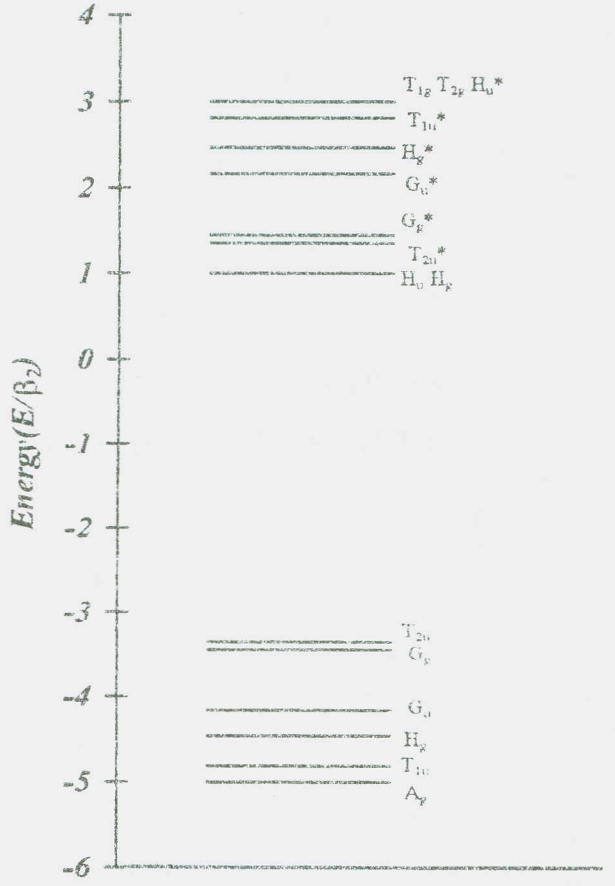

Figure 1. Molecular Energy levels of C_{60}

4. DISCUSSION

The paper presents a systematic way to construct the molecular orbitals and energy eigenvalues of C_{60} molecule. The projection operators are also used to simplify vibrational energy problem, by taking direct product of P_i's by 3×3 matrix representations. The energy values of C_{60} are classified according to their symmetry.

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APPENDIX 1

IRREDUCIBLE MATRIX GENERATORS OF ICOSEHEDRAL GROUP

$$g_1(3)=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}\quad g_1(3)=\frac{1}{2}\begin{pmatrix}-\tau&\sigma&1\\-\sigma&1&\tau\\-1&\tau&\sigma\end{pmatrix}$$

$$g_1(4)=\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix}\quad g_2(4)=\frac{1}{6}\begin{pmatrix}-1&3\sqrt{3}&\sqrt{5}&-\sqrt{3}\\-\sqrt{3}&-3&\sqrt{5}&-3\\-2\sqrt{5}&0&1&\sqrt{5}\\-2\sqrt{3}&0&-\sqrt{5}&-3\end{pmatrix}$$

$$g_1(5)=\begin{pmatrix}1&0&0&0&0\\0&1&0&0&0\\0&0&1&0&0\\0&0&0&-1&0\\0&0&0&0&-1\end{pmatrix}$$

$$g_2(5)=\frac{1}{8}\begin{pmatrix}1&3-\sqrt{5}&-\sqrt{5}&3+\sqrt{5}&-2\sqrt{5}\\-3+\sqrt{5}&-4&-\sqrt{3}(1+\sqrt{5})&0&4\\-\sqrt{15}&\sqrt{3}(1+\sqrt{5})&-1&\sqrt{3}(-1+\sqrt{5})&2\sqrt{3}\\3+\sqrt{5}&0&\sqrt{3}(-1+\sqrt{5})&4&4\\2\sqrt{5}&4&-2\sqrt{3}&-4&0\end{pmatrix}$$

APPENDIX 2

ENERGY MATRICES AND ENERGY EIGENVALUES OF C_{60}

$$H_{A_g} = 2\beta_1 + \beta_2 \qquad H_{T_{1g}} = \begin{pmatrix} -\lambda & 0 & 0 \\ 0 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix} \qquad H_{T_{2g}} = \begin{pmatrix} -\lambda & 0 & 0 \\ 0 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix}$$

$$H_{G_g} = \begin{pmatrix} \delta & 0 & 0 & 0 & \rho & 0 & 0 & 0 \\ 0 & \delta & 0 & 0 & 0 & \rho & 0 & 0 \\ 0 & 0 & \delta & 0 & 0 & 0 & \rho & 0 \\ 0 & 0 & 0 & \delta & 0 & 0 & 0 & \rho \\ \rho & 0 & 0 & 0 & \delta & 0 & 0 & 0 \\ 0 & \rho & 0 & 0 & 0 & \delta & 0 & 0 \\ 0 & 0 & \rho & 0 & 0 & 0 & \delta & 0 \\ 0 & 0 & 0 & \rho & 0 & 0 & 0 & \delta \end{pmatrix}$$

$$H_{H_g} = \frac{1}{4}\begin{pmatrix} \varepsilon & 0 & 0 & 0 & 0 & \omega & 0 & 0 & 0 & 0 & \mu & 0 & 0 & 0 & 0 \\ 0 & \varepsilon & 0 & 0 & 0 & 0 & \omega & 0 & 0 & 0 & 0 & \mu & 0 & 0 & 0 \\ 0 & 0 & \varepsilon & 0 & 0 & 0 & 0 & \omega & 0 & 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & \varepsilon & 0 & 0 & 0 & 0 & \omega & 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & \varepsilon & 0 & 0 & 0 & 0 & \omega & 0 & 0 & 0 & 0 & \mu \\ \omega & 0 & 0 & 0 & 0 & -\beta_2 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 \\ 0 & \omega & 0 & 0 & 0 & 0 & -\beta_2 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 \\ 0 & 0 & \omega & 0 & 0 & 0 & 0 & -\beta_2 & 0 & 0 & 0 & 0 & \alpha & 0 & 0 \\ 0 & 0 & 0 & \omega & 0 & 0 & 0 & 0 & -\beta_2 & 0 & 0 & 0 & 0 & \alpha & 0 \\ 0 & 0 & 0 & 0 & \omega & 0 & 0 & 0 & 0 & -\beta_2 & 0 & 0 & 0 & 0 & \alpha \\ \mu & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & \kappa & 0 & 0 & 0 & 0 \\ 0 & \mu & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & \kappa & 0 & 0 & 0 \\ 0 & 0 & \mu & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & \kappa & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & \kappa & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 & \kappa \end{pmatrix}$$

$$H_{T_{1u}} = \begin{pmatrix} \xi & 0 & 0 & -\beta_1 & 0 & 0 \\ 0 & \xi & 0 & 0 & -\beta_1 & 0 \\ 0 & 0 & \xi & 0 & 0 & -\beta_1 \\ -\beta_1 & 0 & 0 & \zeta & 0 & 0 \\ 0 & -\beta_1 & 0 & 0 & \zeta & 0 \\ 0 & 0 & -\beta_1 & 0 & 0 & \zeta \end{pmatrix}$$

$$H_{T_{2u}} = \begin{pmatrix} \tau\beta_1 - \beta_2 & 0 & 0 & \beta_2 & 0 & 0 \\ 0 & \tau\beta_1 - \beta_2 & 0 & 0 & \beta_2 & 0 \\ 0 & 0 & \tau\beta_1 - \beta_2 & 0 & 0 & \beta_2 \\ \beta_2 & 0 & 0 & \sigma\beta_1 + \beta_2 & 0 & 0 \\ 0 & \beta_2 & 0 & 0 & \sigma\beta_1 + \beta_2 & 0 \\ 0 & 0 & \beta_2 & 0 & 0 & \sigma\beta_1 + \beta_2 \end{pmatrix}$$

$$H_{G_u} = \begin{pmatrix} -\beta_1 & 0 & 0 & 0 & \beta_2 & 0 & 0 & 0 \\ 0 & -\beta_1 & 0 & 0 & 0 & \beta_2 & 0 & 0 \\ 0 & 0 & -\beta_1 & 0 & 0 & 0 & \beta_2 & 0 \\ 0 & 0 & 0 & -\beta_1 & 0 & 0 & 0 & \beta_2 \\ \beta_2 & 0 & 0 & 0 & 2\beta_1 & 0 & 0 & 0 \\ 0 & \beta_2 & 0 & 0 & 0 & 2\beta_1 & 0 & 0 \\ 0 & 0 & \beta_2 & 0 & 0 & 0 & 2\beta_1 & 0 \\ 0 & 0 & 0 & \beta_2 & 0 & 0 & 0 & 2\beta_1 \end{pmatrix}$$

$$H_{H_u} = \begin{pmatrix} -\lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\lambda & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \nu & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \nu & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \nu \end{pmatrix}$$

$$\delta = -\beta_1 + \frac{2\beta_2}{3},\ \varepsilon = -\delta\beta_1 + 4\beta_2,\ \kappa = \delta\beta_1 + 4\beta_2,\ \omega = -2\beta_1,\ \alpha = 2\sqrt{3\sigma}\beta_1,\ \mu = \sqrt{3\tau}\beta_1,$$

$$\nu = -\beta_1 + \beta_2,\ \rho = \frac{\sqrt{5}\beta_2}{3},\ \lambda = \beta_1 + \beta_2,\ \xi = \sigma\beta_1 - \beta_2,\ \zeta = \tau\beta_1 + \beta_2$$

$$E_{A_g}: \{2\beta_1 + \beta_2\} \quad E_{T_{1g}}: \{-\beta_1 - \beta_2\} \quad E_{T_{2g}}: \{-\beta_1 - \beta_2\}$$

$$E_{G_g}: \begin{Bmatrix} \frac{1}{2}\left[\beta_1 + \sqrt{9\beta_1^2 - 8\beta_1\beta_2 + 4\beta_2^2}\right] \\ \frac{1}{2}\left[\beta_1 - \sqrt{9\beta_1^2 - 8\beta_1\beta_2 + 4\beta_2^2}\right] \end{Bmatrix} \quad E_{H_g}: \begin{Bmatrix} \frac{1}{2}\left[\beta_1 - \sqrt{9\beta_1^2 + 4\beta_1\beta_2 + 4\beta_2^2}\right] \\ \frac{1}{2}\left[\beta_1 + \sqrt{9\beta_1^2 + 4\beta_1\beta_2 + 4\beta_2^2}\right] \\ -\beta_1 + \beta_2 \end{Bmatrix}$$

$$E_{T_{1u}}: \begin{Bmatrix} \frac{1}{2}\left[\beta_1 - \sqrt{9\beta_1^2 + 4\sqrt{5}\beta_1\beta_2 + 4\beta_2^2}\right] \\ \frac{1}{2}\left[\beta_1 + \sqrt{9\beta_1^2 + 4\sqrt{5}\beta_1\beta_2 + 4\beta_2^2}\right] \end{Bmatrix} \quad E_{T_{2u}}: \begin{Bmatrix} \frac{1}{2}\left[\beta_1 - \sqrt{9\beta_1^2 - 4\sqrt{5}\beta_1\beta_2 + 4\beta_2^2}\right] \\ \frac{1}{2}\left[\beta_1 + \sqrt{9\beta_1^2 - 4\sqrt{5}\beta_1\beta_2 + 4\beta_2^2}\right] \end{Bmatrix}$$

$$E_{G_u}: \begin{Bmatrix} \frac{1}{2}\left[\beta_1 - \sqrt{9\beta_1^2 + 4\beta_2^2}\right] \\ \frac{1}{2}\left[\beta_1 + \sqrt{9\beta_1^2 + 4\beta_2^2}\right] \end{Bmatrix} \qquad E_{H_u}: \begin{Bmatrix} -\beta_1 + \beta_2 \\ -\beta_1 - \beta_2 \end{Bmatrix}$$