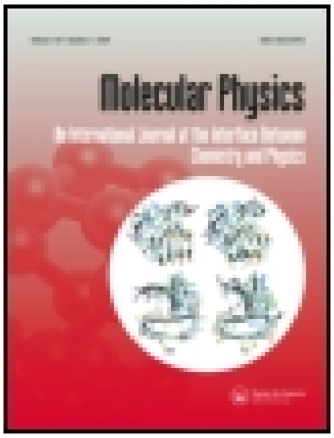

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Icosahedral symmetry adaptation of |JM⟩ bases

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Icosahedral symmetry adaptation of $|JM\rangle$ bases

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The behaviour of the orbital and spin harmonic kets $|JM\rangle$ under the icosahedral double group I^* is described by means of the irreducible icosahedral representations in a D_2 quantization. Real and complex forms are discussed. The results are listed in practical subduction tables, both for integer ($J = 1 \rightarrow 6$) and half-integer ($J = 1/2 \rightarrow 11/2$) harmonics.

1. Introduction

In the study of molecular problems with cubic or icosahedral symmetries sets of spherical harmonic functions which are adapted to the point group symmetry can render useful service. Prime examples of the construction and use of such basis sets were given by Griffith in his monumental work on the theory of transition-metal ions [1]. Griffith provided tables for the cubic forms of the spherical harmonics up to $J = 6$ and $J = 9/2$ for orbital and spin representations, respectively. The extensive research on C_{60} and its family members [2] has necessitated the provision of similar tables for icosahedral basis functions.

Damhus *et al.* published expressions for icosahedral basis functions in a pentagonal quantization scheme [3]. Similar information also including trigonal quantization is presented in Butler's book [4]. An alternative choice of quantization identifies the three Cartesian coordinate axes with three mutually perpendicular twofold axes of the icosahedron. This D_2 symmetry adaptation was advocated by Boyle and Parker, who derived generator matrices for the icosahedral symmetry representations in this scheme [5]. In subsequent works extensive tables of Clebsch–Gordan coupling coefficients for this coordinate choice were published both for orbit–orbit [6] and spin–orbit products [7]. Further information on the icosahedral group in this D_2 frame can be found in the tables of Altmann and Herzig [8]. This source also contains a description of the irreducible representations and various tables of symmetrized harmonics for integral J values. The orbit–orbit coupling tables of Fowler and Ceulemans [6] soon became a useful instrument for the investigation of C_{60} and its peculiar physical properties. They were required for the construction of the numerous new Jahn–Teller Hamiltonians which operate in the ionic and excited states of C_{60} [9–11]. Vibronic coupling problems in Buckminsterfullerene are not limited to point group symmetry but can take advantage of the spherical parent symmetry. To facilitate the combination of both symmetry levels in the treatments of C_{60}, we have chosen to complement our previous studies of the canonical D_2 frame with subduction tables for the spherical harmonics, following the chain $SO(3) \downarrow I_h \downarrow D_2$. The following section explains how these tables were derived. In the final section, we briefly illustrate how the tables can be used.

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2. Method and results

There are two ways to orient a Cartesian frame along three twofold axes of an icosahedron. The one shown in figure 1 is the standard choice of Boyle and Parker [5]. In icosahedral symmetry the symmetries of the spherical harmonics are obtained readily by group theory. It is found that

$$\begin{aligned}
J &= 0 \longrightarrow A_g,\\
J &= 1 \longrightarrow T_{1u},\\
J &= 2 \longrightarrow H_g,\\
J &= 3 \longrightarrow T_{2u} \oplus G_u,\\
J &= 4 \longrightarrow G_g \oplus H_g,\\
J &= 5 \longrightarrow T_{1u} \oplus T_{2u} \oplus H_u,\\
J &= 6 \longrightarrow A_g \oplus T_{1g} \oplus G_g \oplus H_g,\\
J &= 7 \longrightarrow \cdots
\end{aligned} \tag{1}$$

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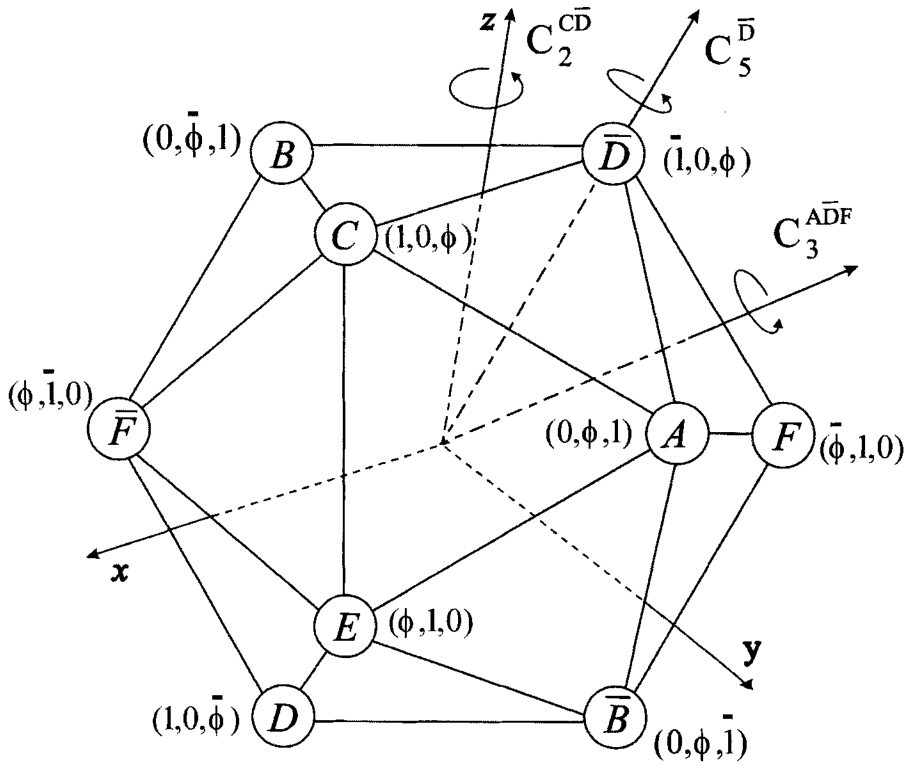

Figure 1. Icosahedron showing the coordinates of the vertices and axes of rotation.

Our derivation of the explicit expression for the symmetry adapted functions is based entirely on the correspondence between the fundamental vector representation with $J = 1$ and the icosahedral representation T_{1u} of the Cartesian functions $\{x, y, z\}$. One has

$$
\begin{aligned}
|T_{1u}x\rangle &= -\frac{1}{\sqrt{2}}(|1,1\rangle - |1,-1\rangle) \\
|T_{1u}y\rangle &= \frac{i}{\sqrt{2}}(|1,1\rangle + |1,-1\rangle) \\
|T_{1u}z\rangle &= |1,0\rangle
\end{aligned}
\tag{2}
$$

and, vice versa,

$$
\begin{aligned}
|1,1\rangle &= -\frac{1}{\sqrt{2}}(|T_{1u}x\rangle + i|T_{1u}y\rangle) \\
|1,-1\rangle &= \frac{1}{\sqrt{2}}(|T_{1u}x\rangle - i|T_{1u}y\rangle) \\
|1,0\rangle &= |T_{1u}z\rangle.
\end{aligned}
\tag{3}
$$

Once this link is established the higher harmonics can all be generated by taking appropriate powers of the basic vector representation. Consider as an example the second power of the vector both in I_h and in SO(3).

$$
\begin{aligned}
T_{1u} \otimes T_{1u} &= A_g \oplus \{T_{1g}\} \oplus H_g \\
1 \otimes 1 \quad &= 0 \;\oplus\; \{1\} \;\oplus\; 2.
\end{aligned}
\tag{4}
$$

Comparison of both products indicates that the antisymmetric product T_{1g} will match the $J = 1$ result, while the H_g product provides the icosahedral basis for $J = 2$. Proceeding along this line, we first construct the H_g components from the T_{1u} basis, using the Clebsch–Gordan coupling coefficients, e.g.

$$
\begin{aligned}
|H_g\xi\rangle &= \sum_{k,l}\langle T_{1u}kT_{1u}l|H_g\xi\rangle\, |T_{1u}k\rangle|T_{1u}l\rangle \\
&= \frac{1}{\sqrt{2}}(|T_{1u}y\rangle|T_{1u}z\rangle + |T_{1u}z\rangle|T_{1u}y\rangle),
\end{aligned}
\tag{5}
$$

which may then be converted into a coupling of $J = 1$ harmonics.

$$
\begin{aligned}
|H_g\xi\rangle = \frac{i}{2}(&|1,1\rangle|1,0\rangle + |1,-1\rangle|1,0\rangle + |1,0\rangle|1,1\rangle \\
&+ |1,0\rangle|1,-1\rangle).
\end{aligned}
\tag{6}
$$

Finally, the $|j_1m_1\rangle|j_2m_2\rangle$ states in this expression are turned into coupled $|JM\rangle$ states using the inverted form of Wigner's formula [12]:

$$|j_1m_1\rangle|j_2m_2\rangle = \sum_{jm}(-1)^{j_2-j_1-m}(2j+1)^{1/2} \times \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} |j_1j_2jm\rangle, \quad (7)$$

where $m_1 + m_2 = m$. For the present example one then obtains

$$|\mathrm{H_g}\xi\rangle = \frac{i}{\sqrt{2}}(|2,1\rangle + |2,-1\rangle). \quad (8)$$

Note that the normalization and phase conventions of the coupling conditions imply that ket combinations such as $|\mathrm{T_{1u}}x\rangle|\mathrm{T_{1u}}y\rangle$ and $|\mathrm{T_{1u}}y\rangle|\mathrm{T_{1u}}x\rangle$ should be distinguished. Similarly, a difference should be maintained between $|j_1m_1\rangle|j_2m_2\rangle$ and $|j_2m_2\rangle|j_1m_1\rangle$. In this way the combined use of icosahedral and spherical coupling coefficients will automatically lead to a normalized result. Of course the coupling procedure cannot fix the external phase factor of a representation. As an example for the $\mathrm{T_{1g}}$ basis in equation (4) we find the same expressions as in equation (2) except for a common phase factor of $-i$. In principle we could also have derived this symmetrization, at least for integral J values, directly from the tables of Altmann and Herzig [8]. The difficulty with such a derivation is that these tables are not based on the canonical choice of the icosahedral functions, which was used for the Clebsch–Gordan series in [6] and [7], and they do not provide alternative sets of icosahedral coupling coefficients.

The results of all our calculations up to $J = 6$ are listed in tables 1–6. In the tables we used the following symbols

$$\phi^{\pm 1} = \tfrac{1}{2}(\pm 1 + \sqrt{5}), \quad \beta_{\pm n,m} = \tfrac{1}{2}(\pm n + m\sqrt{5}). \quad (9)$$

For example, ϕ and ϕ^{-1} can also be written as $\beta_{1,1}$ and $\beta_{-1,1}$, respectively. A given row in a table contains the expansion coefficients describing the $|\Gamma\gamma\rangle$ row entry in

Table 1. Components of $\mathrm{T_{1u}}$ expressed as $|JM\rangle (J = 1)$.

Label	$\|1,-1\rangle$	$\|1,0\rangle$	$\|1,1\rangle$
$\|\mathrm{T_{1u}}x\rangle$	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$
$\|\mathrm{T_{1u}}y\rangle$	$\frac{i}{\sqrt{2}}$	0	$\frac{i}{\sqrt{2}}$
$\|\mathrm{T_{1u}}z\rangle$	0	1	0

Table 2. Components of $\mathrm{H_g}$ expressed as $|JM\rangle$ $(J = 2)$.

Label	$\|2,-2\rangle$	$\|2,-1\rangle$	$\|2,0\rangle$	$\|2,1\rangle$	$\|2,2\rangle$
$\|\mathrm{H_g}\theta\rangle$	$\frac{\sqrt{5}}{4}$	0	$\frac{1}{2}\sqrt{\frac{3}{2}}$	0	$\frac{\sqrt{5}}{4}$
$\|\mathrm{H_g}\epsilon\rangle$	$\frac{\sqrt{3}}{4}$	0	$-\frac{1}{2}\sqrt{\frac{5}{2}}$	0	$\frac{\sqrt{3}}{4}$
$\|\mathrm{H_g}\xi\rangle$	0	$\frac{i}{\sqrt{2}}$	0	$\frac{i}{\sqrt{2}}$	0
$\|\mathrm{H_g}\eta\rangle$	0	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	0
$\|\mathrm{H_g}\zeta\rangle$	$\frac{i}{\sqrt{2}}$	0	0	0	$-\frac{i}{\sqrt{2}}$

Table 3. Components of $\mathrm{T_{2u}}$ and $\mathrm{G_u}$ expressed as $|JM\rangle$ $(J = 3)$.

Label	$\|3,-3\rangle$	$\|3,-2\rangle$	$\|3,-1\rangle$	$\|3,0\rangle$	$\|3,1\rangle$	$\|3,2\rangle$	$\|3,3\rangle$
$\|\mathrm{T_{2u}}x\rangle$	$\frac{1}{4}\phi^{-2}$	0	$\frac{1}{4}\sqrt{3}\phi$	0	$-\frac{1}{4}\sqrt{3}\phi$	0	$-\frac{1}{4}\phi^{-2}$
$\|\mathrm{T_{2u}}y\rangle$	$\frac{i}{4}\phi^{2}$	0	$-\frac{i}{4}\sqrt{3}\phi^{-1}$	0	$-\frac{i}{4}\sqrt{3}\phi^{-1}$	0	$\frac{i}{4}\phi^{2}$
$\|\mathrm{T_{2u}}z\rangle$	0	$-\frac{1}{2}\sqrt{\frac{3}{2}}$	0	$-\frac{1}{2}$	0	$-\frac{1}{2}\sqrt{\frac{3}{2}}$	0
$\|\mathrm{G_u}a\rangle$	0	$-\frac{i}{\sqrt{2}}$	0	0	0	$\frac{i}{\sqrt{2}}$	0
$\|\mathrm{G_u}x\rangle$	$\frac{1}{4}\sqrt{3}\phi$	0	$-\frac{1}{4}\phi^{-2}$	0	$\frac{1}{4}\phi^{-2}$	0	$-\frac{1}{4}\sqrt{3}\phi$
$\|\mathrm{G_u}y\rangle$	$-\frac{i}{4}\sqrt{3}\phi^{-1}$	0	$-\frac{i}{4}\phi^{2}$	0	$-\frac{i}{4}\phi^{2}$	0	$-\frac{i}{4}\sqrt{3}\phi^{-1}$
$\|\mathrm{G_u}z\rangle$	0	$-\frac{1}{2\sqrt{2}}$	0	$\frac{1}{2}\sqrt{3}$	0	$-\frac{1}{2}\sqrt{2}$	0

Table 4. Components of G_g and H_g expressed as $|JM\rangle.(J = 4)$.

Label	$\|4,-4\rangle$	$\|4,-3\rangle$	$\|4,-2\rangle$	$\|4,-1\rangle$	$\|4,0\rangle$	$\|4,1\rangle$	$\|4,2\rangle$	$\|4,3\rangle$	$\|4,4\rangle$
$\|G_g a\rangle$	$\frac{1}{2}\sqrt{\frac{5}{6}}$	0	0	0	$\frac{1}{2}\sqrt{\frac{7}{3}}$	0	0	0	$\frac{1}{2}\sqrt{\frac{5}{6}}$
$\|G_g x\rangle$	0	$-i\frac{\beta_{-7,1}}{4\sqrt{3}}$	0	$-i\frac{\sqrt{7}\phi}{4\sqrt{3}}$	0	$-i\frac{\sqrt{7}\phi}{4\sqrt{3}}$	0	$-i\frac{\beta_{-7,1}}{4\sqrt{3}}$	0
$\|G_g y\rangle$	0	$-\frac{\beta_{7,1}}{4\sqrt{3}}$	0	$\frac{\sqrt{7}\phi^{-1}}{4\sqrt{3}}$	0	$-\frac{\sqrt{7}\phi^{-1}}{4\sqrt{3}}$	0	$\frac{\beta_{7,1}}{4\sqrt{3}}$	0
$\|G_g z\rangle$	$\frac{i}{2}\sqrt{\frac{5}{6}}$	0	$\frac{i}{2}\sqrt{\frac{7}{6}}$	0	0	0	$-\frac{i}{2}\sqrt{\frac{7}{6}}$	0	$-\frac{i}{2}\sqrt{\frac{5}{6}}$
$\|H_g\theta\rangle$	$-\frac{\sqrt{35}}{16\sqrt{3}}$	0	$\frac{3\sqrt{3}}{8}$	0	$\frac{5}{8\sqrt{6}}$	0	$\frac{3\sqrt{3}}{8}$	0	$-\frac{\sqrt{35}}{16\sqrt{3}}$
$\|H_g\epsilon\rangle$	$-\frac{3\sqrt{7}}{16}$	0	$-\frac{\sqrt{5}}{8}$	0	$\frac{3\sqrt{5}}{8\sqrt{2}}$	0	$-\frac{\sqrt{5}}{8}$	0	$-\frac{3\sqrt{7}}{16}$
$\|H_g\xi\rangle$	0	$-i\frac{\sqrt{7}\phi}{4\sqrt{3}}$	0	$i\frac{\beta_{-7,1}}{4\sqrt{3}}$	0	$i\frac{\beta_{-7,1}}{4\sqrt{3}}$	0	$-i\frac{\sqrt{7}\phi}{4\sqrt{3}}$	0
$\|H_g\eta\rangle$	0	$\frac{\sqrt{7}\phi^{-1}}{4\sqrt{3}}$	0	$\frac{\beta_{7,1}}{4\sqrt{3}}$	0	$-\frac{\beta_{7,1}}{4\sqrt{3}}$	0	$-\frac{\sqrt{7}\phi^{-1}}{4\sqrt{3}}$	0
$\|H_g\zeta\rangle$	$i\frac{\sqrt{7}}{2\sqrt{6}}$	0	$-i\frac{\sqrt{5}}{2\sqrt{6}}$	0	0	0	$i\frac{\sqrt{5}}{2\sqrt{6}}$	0	$-i\frac{\sqrt{7}}{2\sqrt{6}}$

Table 5. Components of T_{1u}, T_{2u} and H_u expressed as $|JM\rangle$ $(J = 5)$.

Label	$\|5,-5\rangle$	$\|5,-4\rangle$	$\|5,-3\rangle$	$\|5,-2\rangle$	$\|5,-1\rangle$	$\|5,0\rangle$	$\|5,1\rangle$	$\|5,2\rangle$	$\|5,3\rangle$	$\|5,4\rangle$	$\|5,5\rangle$
$\|T_{1u}x\rangle$	$-\frac{\sqrt{7}\beta_{1,3}}{16\sqrt{2}}$	0	$\frac{3\sqrt{7}\phi^{-1}}{16\sqrt{2}}$	0	$\frac{\sqrt{3}\beta_{7,1}}{16}$	0	$-\frac{\sqrt{3}\beta_{7,1}}{16}$	0	$-\frac{3\sqrt{7}\phi^{-1}}{16\sqrt{2}}$	0	$\frac{\sqrt{7}\beta_{1,3}}{16\sqrt{2}}$
$\|T_{1u}y\rangle$	$i\frac{\sqrt{7}\beta_{-1,3}}{16\sqrt{2}}$	0	$-i\frac{3\sqrt{7}\phi}{16\sqrt{2}}$	0	$i\frac{\sqrt{3}\beta_{-7,1}}{16}$	0	$i\frac{\sqrt{3}\beta_{-7,1}}{16}$	0	$-i\frac{3\sqrt{7}\phi}{16\sqrt{2}}$	0	$i\frac{\sqrt{7}\beta_{-1,3}}{16\sqrt{2}}$
$\|T_{1u}z\rangle$	0	$\frac{\sqrt{35}}{16}$	0	$\frac{\sqrt{21}}{8}$	0	$-\frac{3}{8\sqrt{2}}$	0	$\frac{\sqrt{21}}{8}$	0	$\frac{\sqrt{35}}{16}$	0
$\|T_{2u}x\rangle$	$\frac{3\phi^2}{16}$	0	$\frac{\beta_{3,5}}{16}$	0	$\frac{\sqrt{21}\phi^{-1}}{8\sqrt{2}}$	0	$-\frac{\sqrt{21}\phi^{-1}}{8\sqrt{2}}$	0	$-\frac{\beta_{3,5}}{16}$	0	$-\frac{3\phi^2}{16}$
$\|T_{2u}y\rangle$	$i\frac{3\phi^{-2}}{16}$	0	$-i\frac{\beta_{-3,5}}{16}$	0	$i\frac{\sqrt{21}\phi}{8\sqrt{2}}$	0	$i\frac{\sqrt{21}\phi}{8\sqrt{2}}$	0	$-i\frac{\beta_{-3,5}}{16}$	0	$i\frac{3\phi^{-2}}{16}$
$\|T_{2u}z\rangle$	0	$\frac{3\sqrt{5}}{8\sqrt{2}}$	0	$-\frac{\sqrt{3}}{4\sqrt{2}}$	0	$\frac{\sqrt{7}}{8}$	0	$-\frac{\sqrt{3}}{4\sqrt{2}}$	0	$\frac{3\sqrt{5}}{8\sqrt{2}}$	0
$\|H_u\theta\rangle$	0	$i\sqrt{\frac{15}{32}}$	0	$-i\frac{1}{4\sqrt{2}}$	0	0	0	$i\frac{1}{4\sqrt{2}}$	0	$-i\sqrt{\frac{15}{32}}$	0
$\|H_u\epsilon\rangle$	0	$-i\frac{1}{4\sqrt{2}}$	0	$-i\sqrt{\frac{15}{32}}$	0	0	0	$i\sqrt{\frac{15}{32}}$	0	$i\frac{1}{4\sqrt{2}}$	0
$\|H_u\xi\rangle$	$-\frac{5\sqrt{3}\phi^{-1}}{16\sqrt{2}}$	0	$\frac{\sqrt{3}\beta_{11,1}}{16\sqrt{2}}$	0	$-\frac{\sqrt{7}\phi^2}{16}$	0	$\frac{\sqrt{7}\phi^2}{16}$	0	$-\frac{\sqrt{3}\beta_{11,1}}{16\sqrt{2}}$	0	$\frac{5\sqrt{3}\phi^{-1}}{16\sqrt{2}}$
$\|H_u\eta\rangle$	$-i\frac{5\sqrt{3}\phi}{16\sqrt{2}}$	0	$i\frac{\sqrt{3}\beta_{-11,1}}{16\sqrt{2}}$	0	$-i\frac{\sqrt{7}\phi^{-2}}{16}$	0	$-i\frac{\sqrt{7}\phi^{-2}}{16}$	0	$i\frac{\sqrt{3}\beta_{-11,1}}{16\sqrt{2}}$	0	$-i\frac{5\sqrt{3}\phi}{16\sqrt{2}}$
$\|H_u\zeta\rangle$	0	$\frac{\sqrt{3}}{16}$	0	$-\frac{\sqrt{5}}{8}$	0	$-\sqrt{\frac{105}{128}}$	0	$-\frac{\sqrt{5}}{8}$	0	$\frac{\sqrt{3}}{16}$	0

Table 6. Components of A_g, T_{1g}, G_g and H_g expressed as $|JM\rangle$ $(J = 6)$.

Label	$\|6,-6\rangle$	$\|6,-5\rangle$	$\|6,-4\rangle$	$\|6,-3\rangle$	$\|6,-2\rangle$	$\|6,-1\rangle$	$\|6,0\rangle$	$\|6,1\rangle$	$\|6,2\rangle$	$\|6,3\rangle$	$\|6,4\rangle$	$\|6,5\rangle$	$\|6,6\rangle$
$\|A_g\rangle$	$-\frac{\sqrt{105}}{32}$	0	$\frac{\sqrt{77}}{16\sqrt{2}}$	0	$\frac{\sqrt{231}}{32}$	0	$-\frac{\sqrt{11}}{16}$	0	$\frac{\sqrt{231}}{32}$	0	$\frac{\sqrt{77}}{16\sqrt{2}}$	0	$-\frac{\sqrt{105}}{32}$
$\|T_{1g}x\rangle$	0	$-i\frac{\beta_{-11,3}}{16\sqrt{2}}$	0	$i\frac{\sqrt{33}\phi^2}{16\sqrt{2}}$	0	$i\frac{\sqrt{33}\phi^{-1}}{16}$	0	$i\frac{\sqrt{33}\phi^{-1}}{16}$	0	$i\frac{\sqrt{33}\phi^2}{16\sqrt{2}}$	0	$-i\frac{\beta_{-11,3}}{16\sqrt{2}}$	0
$\|T_{1g}y\rangle$	0	$-\frac{\beta_{11,3}}{16\sqrt{2}}$	0	$-\frac{\sqrt{33}\phi^{-2}}{16\sqrt{2}}$	0	$\frac{\sqrt{33}\phi}{16}$	0	$-\frac{\sqrt{33}\phi}{16}$	0	$\frac{\sqrt{33}\phi^{-2}}{16\sqrt{2}}$	0	$\frac{\beta_{11,3}}{16\sqrt{2}}$	0
$\|T_{1g}z\rangle$	$i\frac{3\sqrt{15}}{16\sqrt{2}}$	0	$-i\frac{\sqrt{11}}{8}$	0	$-i\frac{\sqrt{33}}{16\sqrt{2}}$	0	0	0	$i\frac{\sqrt{33}}{16\sqrt{2}}$	0	$i\frac{\sqrt{11}}{8}$	0	$i\frac{3\sqrt{15}}{16\sqrt{2}}$
$\|G_ga\rangle$	$-\frac{\sqrt{55}}{32}$	0	$-\frac{7\sqrt{3}}{16\sqrt{2}}$	0	$\frac{11}{32}$	0	$\frac{\sqrt{21}}{16}$	0	$\frac{11}{32}$	0	$-\frac{7\sqrt{3}}{16\sqrt{2}}$	0	$-\frac{\sqrt{55}}{32}$
$\|G_gx\rangle$	0	$i\frac{\sqrt{33}\phi^{-1}}{16}$	0	$-i\frac{\beta_{1,3}}{16}$	0	$i\frac{\beta_{3,5}}{8\sqrt{2}}$	0	$i\frac{\beta_{3,5}}{8\sqrt{2}}$	0	$-i\frac{\beta_{1,3}}{16}$	0	$i\frac{\sqrt{33}\phi^{-1}}{16}$	0
$\|G_gy\rangle$	0	$\frac{\sqrt{33}\phi}{16}$	0	$-\frac{\beta_{-1,3}}{16}$	0	$\frac{\beta_{-3,5}}{8\sqrt{2}}$	0	$-\frac{\beta_{-3,5}}{8\sqrt{2}}$	0	$\frac{\beta_{-1,3}}{16}$	0	$-\frac{\sqrt{33}\phi}{16}$	0
$\|G_gz\rangle$	$i\frac{\sqrt{55}}{16}$	0	$i\frac{1}{4}\sqrt{\frac{3}{2}}$	0	$i\frac{7}{16}$	0	0	0	$-i\frac{7}{16}$	0	$-i\frac{1}{4}\sqrt{\frac{3}{2}}$	0	$-i\frac{\sqrt{55}}{16}$
$\|H_g\theta\rangle$	$-\frac{\sqrt{55}}{32}$	0	$\frac{3}{16}\sqrt{\frac{3}{2}}$	0	$-\frac{5}{32}$	0	$\frac{3\sqrt{21}}{16}$	0	$-\frac{5}{32}$	0	$\frac{3}{16}\sqrt{\frac{3}{2}}$	0	$-\frac{\sqrt{55}}{32}$
$\|H_g\epsilon\rangle$	$\frac{3\sqrt{33}}{32}$	0	$\frac{\sqrt{5}}{16\sqrt{2}}$	0	$\frac{3\sqrt{15}}{32}$	0	$\frac{\sqrt{35}}{16}$	0	$\frac{3\sqrt{15}}{32}$	0	$\frac{\sqrt{5}}{16\sqrt{2}}$	0	$\frac{3\sqrt{33}}{32}$
$\|H_g\xi\rangle$	0	$-i\frac{\sqrt{33}\phi^2}{16\sqrt{2}}$	0	$i\frac{\sqrt{5}\phi^{-4}}{16\sqrt{2}}$	0	$i\frac{\beta_{1,3}}{16}$	0	$i\frac{\beta_{1,3}}{16}$	0	$i\frac{\sqrt{5}\phi^{-4}}{16\sqrt{2}}$	0	$-i\frac{\sqrt{33}\phi^2}{16\sqrt{2}}$	0
$\|H_g\eta\rangle$	0	$-\frac{\sqrt{33}\phi^{-2}}{16\sqrt{2}}$	0	$-\frac{\sqrt{5}\phi^4}{16\sqrt{2}}$	0	$-\frac{\beta_{-1,3}}{16}$	0	$\frac{\beta_{-1,3}}{16}$	0	$\frac{\sqrt{5}\phi^4}{16\sqrt{2}}$	0	$\frac{\sqrt{33}\phi^{-2}}{16\sqrt{2}}$	0
$\|H_g\zeta\rangle$	$i\frac{\sqrt{11}}{16\sqrt{2}}$	0	$i\frac{\sqrt{15}}{8}$	0	$-i\frac{5\sqrt{5}}{16\sqrt{2}}$	0	0	0	$i\frac{5\sqrt{5}}{16\sqrt{2}}$	0	$-i\frac{\sqrt{15}}{8}$	0	$-i\frac{\sqrt{11}}{16\sqrt{2}}$

terms of $|JM\rangle$ kets. The expansion coefficients for a given J manifold form unitary matrices. The tables can thus also be used for the inverse problem, i.e. to expand a given $|JM\rangle$ ket as a sum over the icosahedral components of the manifold. To this end one should read the tables column-wise, but not forget to apply complex conjugation which is required to invert unitary matrices, e.g.

$$|2,2\rangle = \frac{\sqrt{5}}{4}|\mathrm{H_g}\theta\rangle + \frac{\sqrt{3}}{4}|\mathrm{H_g}\epsilon\rangle + \frac{i}{\sqrt{2}}|\mathrm{H_g}\zeta\rangle. \tag{10}$$

For the purpose of calculations involving magnetic interactions, it is also convenient to rewrite the icosahedral representations in a complex form. We base our treatment here on the complex format established by Fowler and Ceulemans [7] as

$$\begin{array}{ll}
\mathrm{A} & |\mathrm{Aa}\rangle \\
\mathrm{T_1} & |\mathrm{T_1 1}\rangle = -\frac{1}{\sqrt{2}}(|\mathrm{T_1}x\rangle + i|\mathrm{T_1}y\rangle) \\
 & |\mathrm{T_1} - 1\rangle = \frac{1}{\sqrt{2}}(|\mathrm{T_1}x\rangle - i|\mathrm{T_1}y\rangle) \\
 & |\mathrm{T_1 0}\rangle = |\mathrm{T_1}z\rangle \\
\mathrm{T_2} & |\mathrm{T_2 1}\rangle = -\frac{1}{\sqrt{2}}(|\mathrm{T_2}x\rangle + i|\mathrm{T_2}y\rangle) \\
 & |\mathrm{T_2} - 1\rangle = \frac{1}{\sqrt{2}}(|\mathrm{T_2}x\rangle - i|\mathrm{T_2}y\rangle) \\
 & |\mathrm{T_2 0}\rangle = |\mathrm{T_2}z\rangle \\
\mathrm{G} & |\mathrm{G}i\rangle = i|\mathrm{Ga}\rangle \\
 & |\mathrm{G1}\rangle = -\frac{1}{\sqrt{2}}(|\mathrm{G}x\rangle + i|\mathrm{G}y\rangle) \\
 & |\mathrm{G} - 1\rangle = \frac{1}{\sqrt{2}}(|\mathrm{G}x\rangle - i|\mathrm{G}y\rangle) \\
 & |\mathrm{G0}\rangle = |\mathrm{G}z\rangle \\
\mathrm{H} & |\mathrm{H2}\rangle = \frac{1}{4}(\sqrt{5}|\mathrm{H}\theta\rangle + \sqrt{3}|\mathrm{H}\epsilon\rangle + i\sqrt{8}|\mathrm{H}\zeta\rangle) \\
 & |\mathrm{H} - 2\rangle = \frac{1}{4}(\sqrt{5}|\mathrm{H}\theta\rangle + \sqrt{3}|\mathrm{H}\epsilon\rangle - i\sqrt{8}|\mathrm{H}\zeta\rangle) \\
 & |\mathrm{H1}\rangle = -\frac{1}{\sqrt{2}}(i|\mathrm{H}\xi\rangle + |\mathrm{H}\eta\rangle) \\
 & |\mathrm{H} - 1\rangle = -\frac{1}{\sqrt{2}}(i|\mathrm{H}\xi\rangle - |\mathrm{H}\eta\rangle) \\
 & |\mathrm{H0}\rangle = \frac{1}{2\sqrt{2}}(\sqrt{3}|\mathrm{H}\theta\rangle - \sqrt{5}|\mathrm{H}\epsilon\rangle).
\end{array}$$

Combination of these expressions with the expansions of the real bases, given in tables 1–6, immediately yields expressions of the complex icosahedral functions for the J manifolds. Results for $J = 2$–4 are given in tables 7–9.

The complex form of the $\mathrm{T_{1u}}$ components, $|\mathrm{T_{1u}}, 1\rangle$, $\mathrm{T_{1u}}, 0\rangle$ and $|\mathrm{T_{1u}}, -1\rangle$ was chosen in correspondence with the $|1,1\rangle, |1,0\rangle$ and $|1,-1\rangle$ spherical harmonics, respectively. As a result the relation between $\mathrm{T_{1u}}$ and $J = 1$ is simply the unit of matrix, and similarly for $\mathrm{H_g}$ and $J = 2$ (see table 7). Also note that the choice of complex basis functions gives rise to expansion coefficients that are entirely real. This is due to the use of a fixed inner automorphism for the construction of these bases [13].

When spin is considered in a system with an odd number of particles, the symmetry will be described by the icosahedral double group which contains, in addition to the five orbital representations, four irreducible spin representations. These may conveniently be denoted by the Griffith labels [1] $\mathrm{E}', \mathrm{E}'', \mathrm{U}'$ and W'. In spherical symmetry the corresponding spin representations are characterised by half-integer J values. They can be decomposed by the icosahedral double group theory as [14]

$$\begin{aligned}
J &= 1/2 \longrightarrow \mathrm{E}', \\
J &= 3/2 \longrightarrow \mathrm{U}', \\
J &= 5/2 \longrightarrow \mathrm{W}', \\
J &= 7/2 \longrightarrow \mathrm{E}'' \oplus \mathrm{W}', \\
J &= 9/2 \longrightarrow \mathrm{U}' \oplus \mathrm{W}', \\
J &= 11/2 \longrightarrow \mathrm{E}' \oplus \mathrm{U}' \oplus \mathrm{W}', \\
J &= 13/2 \longrightarrow \mathrm{E}' \oplus \mathrm{E}'' \oplus \mathrm{U}' \oplus \mathrm{W}', \\
J &= 15/2 \longrightarrow \cdots .
\end{aligned} \tag{11}$$

Hence up to $J = 5/2$ icosahedral and spherical degeneracies coincide , while in cubic symmetry the $J = 5/2$ is already split. This observation confirms that I_h is the highest point group. The method which was used to construct subduction relations for the orbital functions

Table 7. Complex bases of H_g expressed as $|JM\rangle$ ($J = 2$).

Label	$\|2,-2\rangle$	$\|2,-1\rangle$	$\|2,0\rangle$	$\|2,1\rangle$	$\|2,2\rangle$
$\|\mathrm{H_g}-2\rangle$	1	0	0	0	0
$\|\mathrm{H_g}-1\rangle$	0	1	0	0	0
$\|\mathrm{H_g}0\rangle$	0	0	1	0	0
$\|\mathrm{H_g}1\rangle$	0	0	0	1	0
$\|\mathrm{H_g}2\rangle$	0	0	0	0	1

Table 8. The complex bases of T_{2u} and G_u expressed as $|JM\rangle$ $(J=3)$.

Label	$\|3,-3\rangle$	$\|3,-2\rangle$	$\|3,-1\rangle$	$\|3,0\rangle$	$\|3,1\rangle$	$\|3,2\rangle$	$\|3,3\rangle$
$\|T_{2u}-1\rangle$	$\frac{-3}{4\sqrt{2}}$	0	$\frac{-\sqrt{3/2}}{4}$	0	$\frac{\sqrt{15/2}}{4}$	0	$\frac{-\sqrt{5/2}}{4}$
$\|T_{2u}0\rangle$	0	$\frac{\sqrt{3/2}}{2}$	0	$\frac{1}{2}$	0	$\frac{\sqrt{3/2}}{2}$	0
$\|T_{2u}1\rangle$	$-\frac{\sqrt{5/2}}{4}$	0	$\frac{\sqrt{15/2}}{4}$	0	$\frac{-\sqrt{3/2}}{4}$	0	$\frac{-3}{4\sqrt{2}}$
$\|G_u i\rangle$	0	$-\frac{1}{\sqrt{2}}$	0	0	0	$\frac{1}{\sqrt{2}}$	0
$\|G_u-1\rangle$	$\frac{-\sqrt{3/2}}{4}$	0	$\frac{3}{4\sqrt{2}}$	0	$\frac{\sqrt{5/2}}{4}$	0	$\frac{\sqrt{15/2}}{4}$
$\|G_u0\rangle$	0	$\frac{1}{2\sqrt{2}}$	0	$\frac{-\sqrt{3}}{2}$	0	$\frac{1}{2\sqrt{2}}$	0
$\|G_u1\rangle$	$\frac{\sqrt{15/2}}{4}$	0	$\frac{\sqrt{5/2}}{4}$	0	$\frac{3}{4\sqrt{2}}$	0	$\frac{-\sqrt{3/2}}{4}$

Table 9. Complex bases of G_g and H_g expressed as $|JM\rangle$ $(J=4)$.

Label	$\|4,-4\rangle$	$\|4,-3\rangle$	$\|4,-2\rangle$	$\|4,-1\rangle$	$\|4,0\rangle$	$\|4,1\rangle$	$\|4,2\rangle$	$\|4,3\rangle$	$\|4,4\rangle$
$\|G_g i\rangle$	$\frac{\sqrt{5/6}}{2}$	0	0	0	$\frac{\sqrt{7/3}}{2}$	0	0	0	$\frac{\sqrt{5/6}}{2}$
$\|G_g-1\rangle$	0	$\frac{7}{4\sqrt{6}}$	0	$\frac{-\sqrt{35/6}}{4}$	0	$\frac{-\sqrt{7/6}}{4}$	0	$\frac{-\sqrt{5/6}}{4}$	0
$\|G_g0\rangle$	$\frac{\sqrt{5/6}}{2}$	0	$\frac{\sqrt{7/6}}{2}$	0	0	0	$\frac{-\sqrt{7/6}}{2}$	0	$\frac{-\sqrt{5/6}}{2}$
$\|G_g1\rangle$	0	$\frac{\sqrt{5/6}}{4}$	0	$\frac{\sqrt{7/6}}{4}$	0	$\frac{\sqrt{35/6}}{4}$	0	$\frac{-7}{4\sqrt{6}}$	0
$\|H_g-2\rangle$	$\frac{-\sqrt{7/3}}{32}$	0	$\frac{\sqrt{5/3}}{16}$	0	$-7\frac{\sqrt{5/6}}{16}$	0	$-7\frac{\sqrt{5/3}}{16}$	0	$\frac{5\sqrt{21}}{32}$
$\|H_g-1\rangle$	0	$\frac{\sqrt{7/6}}{4}$	0	$\frac{-\sqrt{5/6}}{4}$	0	$\frac{7}{4\sqrt{6}}$	0	$\frac{\sqrt{35/6}}{4}$	0
$\|H_g0\rangle$	$\frac{-\sqrt{35/2}}{16}$	0	$\frac{-7}{8\sqrt{2}}$	0	$\frac{5}{16}$	0	$\frac{-7}{8\sqrt{2}}$	0	$\frac{-\sqrt{35/2}}{16}$
$\|H_g1\rangle$	0	$\frac{\sqrt{35/6}}{4}$	0	$\frac{7}{4\sqrt{6}}$	0	$\frac{-\sqrt{5/6}}{4}$	0	$\frac{\sqrt{7/6}}{4}$	0
$\|H_g2\rangle$	$\frac{5\sqrt{21}}{32}$	0	$-7\frac{\sqrt{5/3}}{16}$	0	$-7\frac{\sqrt{5/6}}{16}$	0	$\frac{\sqrt{5/3}}{16}$	0	$\frac{-\sqrt{7/3}}{32}$

Table 10. Components of E″ and W′ expressed as $|JM\rangle$ $(J = 7/2)$.

Label	$\left\|\frac{7}{2},-\frac{7}{2}\right\rangle$	$\left\|\frac{7}{2},-\frac{5}{2}\right\rangle$	$\left\|\frac{7}{2},-\frac{3}{2}\right\rangle$	$\left\|\frac{7}{2},-\frac{1}{2}\right\rangle$	$\left\|\frac{7}{2},\frac{1}{2}\right\rangle$	$\left\|\frac{7}{2},\frac{3}{2}\right\rangle$	$\left\|\frac{7}{2},\frac{5}{2}\right\rangle$	$\left\|\frac{7}{2},\frac{7}{2}\right\rangle$
$\left\|\mathrm{E}''-\frac{1}{2}\right\rangle$	$\frac{-\sqrt{15}}{8}$	0	$\frac{-\sqrt{7}}{8}$	0	$\frac{-\sqrt{21}}{8}$	0	$\frac{\sqrt{21}}{8}$	0
$\left\|\mathrm{E}''\frac{1}{2}\right\rangle$	0	$\frac{-\sqrt{21}}{8}$	0	$\frac{\sqrt{21}}{8}$	0	$\frac{\sqrt{7}}{8}$	0	$\frac{\sqrt{15}}{8}$
$\left\|\mathrm{W}'-\frac{5}{2}\right\rangle$	0	$\frac{-1}{16\sqrt{2}}$	0	$\frac{7}{16\sqrt{2}}$	0	$7\,\frac{\sqrt{3/2}}{16}$	0	$-3\,\frac{\sqrt{35/2}}{16}$
$\left\|\mathrm{W}'-\frac{3}{2}\right\rangle$	$-\frac{\sqrt{7/2}}{16}$	0	$\frac{\sqrt{15/2}}{16}$	0	$-7\,\frac{\sqrt{5/2}}{16}$	0	$-7\,\frac{\sqrt{5/2}}{16}$	0
$\left\|\mathrm{W}'-\frac{1}{2}\right\rangle$	0	$\frac{7}{16}$	0	$-\frac{5}{16}$	0	$\frac{7\sqrt{3}}{16}$	0	$\frac{\sqrt{35}}{16}$
$\left\|\mathrm{W}'\frac{1}{2}\right\rangle$	$\frac{-\sqrt{35}}{16}$	0	$\frac{-7\sqrt{3}}{16}$	0	$\frac{5}{16}$	0	$-\frac{7}{16}$	0
$\left\|\mathrm{W}'\frac{3}{2}\right\rangle$	0	$7\,\frac{\sqrt{5/2}}{16}$	0	$7\,\frac{\sqrt{5/2}}{16}$	0	$-\frac{\sqrt{15/2}}{16}$	0	$\frac{\sqrt{7/2}}{16}$
$\left\|\mathrm{W}'\frac{5}{2}\right\rangle$	$3\,\frac{\sqrt{35/2}}{16}$	0	$-7\,\frac{\sqrt{3/2}}{16}$	0	$\frac{-7}{16\sqrt{2}}$	0	$\frac{1}{16\sqrt{2}}$	0

Table 11. Components of U′ and W′ expressed as $|JM\rangle$ $(J = 9/2)$.

Label	$\left\|\frac{9}{2},-\frac{9}{2}\right\rangle$	$\left\|\frac{9}{2},-\frac{7}{2}\right\rangle$	$\left\|\frac{9}{2},-\frac{5}{2}\right\rangle$	$\left\|\frac{9}{2},-\frac{3}{2}\right\rangle$	$\left\|\frac{9}{2},-\frac{1}{2}\right\rangle$	$\left\|\frac{9}{2},\frac{1}{2}\right\rangle$	$\left\|\frac{9}{2},\frac{3}{2}\right\rangle$	$\left\|\frac{9}{2},\frac{5}{2}\right\rangle$	$\left\|\frac{9}{2},\frac{7}{2}\right\rangle$	$\left\|\frac{9}{2},\frac{9}{2}\right\rangle$
$\left\|\mathrm{U}'\frac{-3}{2}\right\rangle$	0	$-\frac{\sqrt{21/5}}{16}$	0	$\frac{1}{8}$	0	$-7\,\frac{\sqrt{3/10}}{8}$	0	$\frac{-\sqrt{21}}{8}$	0	$\frac{\sqrt{105}}{16}$
$\left\|\mathrm{U}'\frac{-1}{2}\right\rangle$	$\frac{\sqrt{7}}{16}$	0	$3\,\frac{\sqrt{7/5}}{8}$	0	$\frac{-3}{8\sqrt{2}}$	0	$7\,\frac{\sqrt{3/5}}{8}$	0	$\frac{3\sqrt{7}}{16}$	0
$\left\|\mathrm{U}'\frac{1}{2}\right\rangle$	0	$\frac{-3\sqrt{7}}{16}$	0	$-7\,\frac{\sqrt{3/5}}{8}$	0	$\frac{3}{8\sqrt{2}}$	0	$-3\,\frac{\sqrt{7/5}}{8}$	0	$\frac{-\sqrt{7}}{16}$
$\left\|\mathrm{U}'\frac{3}{2}\right\rangle$	$\frac{-\sqrt{105}}{16}$	0	$\frac{\sqrt{21}}{8}$	0	$7\,\frac{\sqrt{3/10}}{8}$	0	$-\frac{1}{8}$	0	$\frac{\sqrt{21/5}}{16}$	0
$\left\|\mathrm{W}'\frac{-5}{2}\right\rangle$	$\frac{3}{32}$	0	$\frac{-\sqrt{5}}{16}$	0	$5\,\frac{\sqrt{7/2}}{16}$	0	$\frac{\sqrt{105}}{16}$	0	$\frac{-15}{32}$	0
$\left\|\mathrm{W}'\frac{-3}{2}\right\rangle$	0	$\frac{-31}{32\sqrt{5}}$	0	$\frac{\sqrt{21}}{16}$	0	$-11\,\frac{\sqrt{7/10}}{16}$	0	$\frac{-1}{16}$	0	$\frac{-9\sqrt{5}}{32}$
$\left\|\mathrm{W}'\frac{-1}{2}\right\rangle$	$\frac{9}{16\sqrt{2}}$	0	$\frac{17}{8\sqrt{10}}$	0	$\frac{-\sqrt{7}}{16}$	0	$-\frac{\sqrt{21/10}}{8}$	0	$\frac{-13}{16\sqrt{2}}$	0
$\left\|\mathrm{W}'\frac{1}{2}\right\rangle$	0	$\frac{13}{16\sqrt{2}}$	0	$\frac{\sqrt{21/10}}{8}$	0	$\frac{\sqrt{7}}{16}$	0	$\frac{-17}{8\sqrt{10}}$	0	$\frac{-9}{16\sqrt{2}}$
$\left\|W'\frac{3}{2}\right\rangle$	$\frac{9\sqrt{5}}{32}$	0	$\frac{1}{16}$	0	$11\,\frac{\sqrt{7/10}}{16}$	0	$\frac{-\sqrt{21}}{16}$	0	$\frac{31}{32\sqrt{5}}$	0
$\left\|W'\frac{5}{2}\right\rangle$	0	$\frac{15}{32}$	0	$\frac{-\sqrt{105}}{16}$	0	$-5\,\frac{\sqrt{7/2}}{16}$	0	$\frac{\sqrt{5}}{16}$	0	$\frac{-3}{32}$

Table 12. Components of E′, U′ and W′ expressed as $|JM\rangle$ $(J = 11/2)$.

Label	$\left\|\frac{11}{2},-\frac{11}{2}\right\rangle$	$\left\|\frac{11}{2},-\frac{9}{2}\right\rangle$	$\left\|\frac{11}{2},-\frac{7}{2}\right\rangle$	$\left\|\frac{11}{2},-\frac{5}{2}\right\rangle$	$\left\|\frac{11}{2},-\frac{3}{2}\right\rangle$	$\left\|\frac{11}{2},-\frac{1}{2}\right\rangle$	$\left\|\frac{11}{2},\frac{1}{2}\right\rangle$	$\left\|\frac{11}{2},\frac{3}{2}\right\rangle$	$\left\|\frac{11}{2},\frac{5}{2}\right\rangle$	$\left\|\frac{11}{2},\frac{7}{2}\right\rangle$	$\left\|\frac{11}{2},\frac{9}{2}\right\rangle$	$\left\|\frac{11}{2},\frac{11}{2}\right\rangle$
$\left\|E'-\frac{1}{2}\right\rangle$	$\frac{\sqrt{\frac{105}{2}}}{16}$	0	$-\frac{\sqrt{\frac{385}{6}}}{16}$	0	$\frac{-\sqrt{77}}{16}$	0	$\frac{\sqrt{11}}{16}$	0	$-\frac{\sqrt{\frac{77}{2}}}{16}$	0	$-\frac{\sqrt{\frac{77}{6}}}{16}$	0
$\left\|E'\frac{1}{2}\right\rangle$	0	$\frac{\sqrt{\frac{77}{6}}}{16}$	0	$\frac{\sqrt{\frac{77}{2}}}{16}$	0	$\frac{-\sqrt{11}}{16}$	0	$\frac{\sqrt{77}}{16}$	0	$\frac{\sqrt{\frac{385}{6}}}{16}$	0	$-\frac{\sqrt{\frac{105}{2}}}{16}$
$\left\|U'-\frac{3}{2}\right\rangle$	$-\frac{\sqrt{\frac{11}{2}}}{16}$	0	$\frac{-9}{16\sqrt{2}}$	0	$\frac{\sqrt{15}}{16}$	0	$\frac{-\sqrt{105}}{16}$	0	$-3\frac{\sqrt{\frac{15}{2}}}{16}$	0	$3\frac{\sqrt{\frac{5}{2}}}{16}$	0
$\left\|U'-\frac{1}{2}\right\rangle$	0	$\frac{19}{16\sqrt{6}}$	0	$\frac{13}{16\sqrt{2}}$	0	$\frac{-\sqrt{7}}{16}$	0	$\frac{1}{16}$	0	$-5\frac{\sqrt{\frac{5}{6}}}{16}$	0	$\frac{\sqrt{\frac{165}{2}}}{16}$
$\left\|U'\frac{1}{2}\right\rangle$	$\frac{\sqrt{\frac{165}{2}}}{16}$	0	$-5\frac{\sqrt{\frac{5}{6}}}{16}$	0	$\frac{1}{16}$	0	$\frac{-\sqrt{7}}{16}$	0	$\frac{13}{16\sqrt{2}}$	0	$\frac{19}{16\sqrt{6}}$	0
$\left\|U'\frac{3}{2}\right\rangle$	0	$3\frac{\sqrt{\frac{5}{2}}}{16}$	0	$-3\frac{\sqrt{\frac{15}{2}}}{16}$	0	$\frac{-\sqrt{105}}{16}$	0	$\frac{\sqrt{15}}{16}$	0	$\frac{-9}{16\sqrt{2}}$	0	$-\frac{\sqrt{\frac{11}{2}}}{16}$
$\left\|W'-\frac{5}{2}\right\rangle$	0	$\frac{3\sqrt{3}}{16}$	0	$-\frac{1}{4}$	0	$3\frac{\sqrt{\frac{7}{2}}}{8}$	0	$\frac{3}{4\sqrt{2}}$	0	$\frac{-\sqrt{15}}{16}$	0	0
$\left\|W'-\frac{3}{2}\right\rangle$	$\frac{-\sqrt{33}}{16}$	0	$\frac{-3\sqrt{3}}{8}$	0	$\frac{\sqrt{\frac{5}{2}}}{8}$	0	0	0	$\frac{3\sqrt{5}}{16}$	0	$\frac{-\sqrt{15}}{8}$	0
$\left\|W'-\frac{1}{2}\right\rangle$	0	$7\frac{\sqrt{\frac{3}{2}}}{16}$	0	$\frac{3}{16\sqrt{2}}$	0	$\frac{\sqrt{7}}{16}$	0	$-\frac{9}{16}$	0	$-\frac{\sqrt{\frac{15}{2}}}{16}$	0	$-\frac{\sqrt{\frac{165}{2}}}{16}$
$\left\|W'\frac{1}{2}\right\rangle$	$-\frac{\sqrt{\frac{165}{2}}}{16}$	0	$-\frac{\sqrt{\frac{15}{2}}}{16}$	0	$-\frac{9}{16}$	0	$\frac{\sqrt{7}}{16}$	0	$\frac{3}{16\sqrt{2}}$	0	$7\frac{\sqrt{\frac{3}{2}}}{16}$	0
$\left\|W'\frac{3}{2}\right\rangle$	0	$\frac{-\sqrt{15}}{8}$	0	$\frac{3\sqrt{5}}{16}$	0	0	0	$\frac{\sqrt{\frac{5}{2}}}{8}$	0	$\frac{-3\sqrt{3}}{8}$	0	$\frac{-\sqrt{33}}{16}$
$\left\|W'\frac{5}{2}\right\rangle$	0	0	$\frac{-\sqrt{15}}{16}$	0	$\frac{3}{4\sqrt{2}}$	0	$3\frac{\sqrt{\frac{7}{2}}}{8}$	0	$-\frac{1}{4}$	0	$\frac{3\sqrt{3}}{16}$	0

can now also be applied to the spin functions. The basis is the fundamental spin representation E', which is linked to the $J = 1/2$ spinor.

$$|\mathrm{E}'\mathrm{a}\rangle = |1/2, 1/2\rangle, \quad |\mathrm{E}'\mathrm{b}\rangle = |1/2, -1/2\rangle. \tag{12}$$

The bases of U' and W' can be obtained by $\mathrm{T}_1 \otimes \mathrm{E}'$ and $\mathrm{H} \otimes \mathrm{E}'$, respectively [7]. It is found that

$$\begin{aligned}|\mathrm{U}', -3/2\rangle &= |3/2, -3/2\rangle\\ |\mathrm{U}', -1/2\rangle &= |3/2. -1/2\rangle\\ |\mathrm{U}', 1/2\rangle &= |3/2, 1/2\rangle\\ |\mathrm{U}', 3/2\rangle &= |3/2, 3/2\rangle,\end{aligned} \tag{13}$$

and

$$\begin{aligned}|\mathrm{W}', -5/2\rangle &= |5/2, -5/2\rangle\\ |\mathrm{W}', -3/2\rangle &= |5/2, -3/2\rangle\\ |\mathrm{W}', -1/2\rangle &= |5/2, -1/2\rangle\\ |\mathrm{W}', 1/2\rangle &= |5/2, 1/2\rangle\\ |\mathrm{W}', 3/2\rangle &= |5/2, 3/2\rangle\\ |\mathrm{W}', 5/2\rangle &= |5/2, 5/2\rangle.\end{aligned} \tag{14}$$

For $J = 7/2$ to $J = 11/2$, the symmetry adaptations of the spin harmonics are listed in tables 10–12.

3. Application

Applications of the results in this paper will be directed mainly to the research areas of vibronic coupling and magnetic interactions in fullerenes. It is well known that the frontier orbitals in C_{60} can be derived from the spherical harmonic functions, corresponding to electron waves on a spherical shell [15]. The $\mathrm{H_u}$ HOMO and the $\mathrm{T_{1u}}$ LUMO are both derived from a parent $J = 5$ level. More accurate treatments even take into account small admixtures of a $J = 7$ and a $J = 1$ level for the $\mathrm{H_u}$ and $\mathrm{T_{1u}}$, respectively [16]. Similarly it has been shown that C_{60} vibrates as a hollow sphere [17], implying that its modes may also be characterized by a spherical parentage. As an example, the lowest frequency squashing mode, of $\mathrm{H_g}$ symmetry, has dominant $J = 2$ character. Spherical selection rules may thus play an important role in the physics of C_{60}. As an example, in a recent communication Anderson [18] investigated the possible role of vibronic coupling in the g value of C_{60}^{-1}. The crucial matrix element in this respect is the vibronic coupling between HOMO and LUMO via the $\mathrm{h_g}$ modes of type $\langle \mathrm{H_u}|\partial\mathcal{H}/\partial Q_{\mathrm{h_g}}|\mathrm{T_{1u}}\rangle$. Evaluation of such matrix elements in a spherical approximation involves the calculation of coupling coefficients such as $\langle \mathrm{H_u}\zeta(J=5)|\mathrm{H_g}\theta(J=2)\mathrm{T_{1u}}z(J=5)\rangle$, where we have chosen a triad $\langle\zeta|\theta z\rangle$ which has a nonzero icosahedral coupling coefficient. To evaluate the total coefficient we substitute the bra and ket parts by the respective expressions in JM bases using tables 2 and 5. The resulting expansion is in terms of standard $\langle JM|j_1m_1j_2m_2\rangle$ coefficients, which may be evaluated using the $3J$ symbols. As a result we obtain a nonzero coupling coefficient.

$$\langle 5\mathrm{H_u}\zeta|2\mathrm{H_g}\theta, 5\mathrm{T_{1u}}z\rangle = -\frac{1}{4}\sqrt{\frac{21}{13}}. \tag{15}$$

As a check we also calculated a $\langle\xi|\theta x\rangle$ component:

$$\langle 5\mathrm{H_u}\xi|2\mathrm{H_g}\theta, 5\mathrm{T_{1u}}x\rangle = \frac{1}{4\sqrt{5}}\sqrt{\frac{21}{13}}\phi^2. \tag{16}$$

The ratio of the two coefficients equals the ratio of the icosahedral coupling coefficients [6] $\langle\zeta|\theta z\rangle/\langle\xi|\theta x\rangle$, as it should be. We are thus able to confirm that spherical selection rules do not prevent vibronic coupling between HOMO and LUMO in C_{60}. This result may require that the analysis of the g tensor [18] in the anion be reopened.

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