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Orientations of point groups—phase choices in the Racah–Wigner algebra

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Abstract. The SO_3-SO_2-$3jm$'s (the '$3j$ symbols' of angular momentum) are known to incorporate no information about the orientation of axes and may be calculated from a knowledge of character theory alone, together with some freedom of choice of phases. For many point-group embeddings, at least once in every finite-group basis of SO_3, an extra phase choice arises in the $3jm$ calculation. We show that choosing this phase corresponds to choosing the orientation of the symmetry axes of the groups.

1. Introduction

Elementary applications of group theory in physics and chemistry yield qualitative information such as degeneracies and selection rules. To produce quantitative results requires the use of the Wigner–Eckart theorem and therefore the calculation of jm factors and j symbols (equivalently coupling and recoupling coefficients).

Most calculations proceed from an explicit definition of the symmetry axes or the generators of the group (e.g. Harnung and Schäffer 1972, Kibler and Grenet 1977, Kramer 1968). It has been shown that the j symbols and jm factors for arbitrary compact groups may be calculated from a knowledge of character theory alone and a methodology has been developed along these lines. It has been applied to SO_3, the embedding $SO_3 \supset SO_2$, the point groups T and C_3, the Lie groups in the chain $E_7 \supset SU_6 \times SU_3 \supset SU_2 \times SU_3 \times SU_3$ and the dihedral and cyclic groups. See Butler (1975, 1976, 1979), Donini (1979, pp 123–77), Butler and Wybourne (1976a, b), Butler *et al* (1978, 1979), Butler and Reid (1979) and Prasad and Bharathi (1980).

Several questions remain unanswered. Butler and Wybourne (1976a) were unable to demonstrate the completeness of their equations for all groups. Furthermore, in applications involving point groups it may be necessary to know where the symmetry axes lie. These calculations appear to contain no such information.

Within the Racah–Wigner algebra one may freely choose certain coupling and basis phases (Butler 1975, Butler and Wybourne 1976a). We shall show that for many point-group embeddings an extra phase choice (in addition to the above) must be made. This special phase choice affects the orientation of the symmetry axes of the group and we shall therefore refer to it as an orientation phase.

The embedding $D_3 \supset C_3$ is discussed in § 4 as an example. We show that the choice of orientation phase determines whether C_{2y} or C_{2x} (or neither) is in D_3. In § 5 orientation phases for other point groups are discussed. We show how the orientation of the symmetry axes may be determined once the $3jm$ factors have been calculated.

All finite group bases of SO_3 involve at least one orientation phase. This corresponds to the freedom one has when choosing axes for point groups and is largely overlooked in calculations which fix the axes before calculating $3jm$'s. It has been noted by Boyle and Schäffer (1974) that different axis choices for the icosahedron are not equivalent. This is a special example of the phenomenon we discuss here.

We restrict ourselves to pure rotation groups in what follows. The properties of reflection–rotation and reflection–inversion groups are similar (but not trivially so—see Butler 1980).

2. Free phases in the Racah–Wigner algebra

The free phases which appear in the calculation of j symbols and jm factors were discussed by Butler (1975). Butler and Wybourne (1976a) gave a method of calculation which was based on building up from any chosen faithful irrep, called the primitive irrep. They proved that all $3jm$'s and $6j$'s could be calculated recursively once those containing the primitive irrep were known, but were unable to give a complete method for calculating primitive $6j$'s and $3jm$'s.

The reader is referred to the above for notation and definitions and for a discussion of the free phases involved in the calculation of j symbols. Here we shall be concerned only with jm factors which, unlike the j symbols, contain basis information, being dependent on the branching of the irreps of a group to its chosen subgroup. For example, the SO_3–SO_2-$3jm$ factors, the '$3j$ symbols' of angular momentum, depend on the SO_3-$6j$ symbols, and on the SO_3-SO_2-branching rules and nothing else (Butler 1976). In building up a set of primitive $3jm$ factors, certain branching multiplicity separations and choices of phase must be made. These choices are choices of the relationship among the partners of an irrep, and as such correspond to choices of the form of the irrep matrices (Butler 1975, equation (11.6)). We make these choices in the sequence used in Butler and Wybourne (1976a, § 6) and Butler and Reid (1979). The $2jm$ factors are first chosen, real and of a sign such that as many $3jm$ factors as possible are real. This action fixes the relationship between each pair of complex conjugate kets. Then for each (non-primitive) pair there is one free phase, which is fixed when the ket first arises in the $3jm$ calculation. In addition there may be orientation phases. We give examples in § 4 and § 5.

3. Transformation of basis

In the following sections we shall need to consider transformations between bases. Let the kets $|\lambda i\rangle$ form a $G \supset H \supset K$ basis and $|\lambda l\rangle'$ form a $G \supset H' \supset K$ basis. The transformation coefficients between the bases may be calculated by rewriting equation (11.6) of Butler (1975) as

$$\langle \lambda i | \lambda l\rangle' = \sum_{\substack{i_1 i_2 \\ l_1 l_2}} |\lambda| \begin{pmatrix} \lambda_1 & \lambda_2 & \lambda \\ i_1 & i_2 & i \end{pmatrix}^{*r} \langle \lambda_1 i_1 | \lambda_1 l_1\rangle'^* \langle \lambda_2 i_1 | \lambda_2 l_2\rangle'^* \begin{pmatrix} \lambda_1 & \lambda_2 & \lambda \\ l_1 & l_2 & l \end{pmatrix}'^r . \tag{3.1}$$

If, in this equation, λ_1 is chosen to be the primitive irrep we have a recursion relation for all transformation coefficients in terms of primitive G-H-K-$3jm$'s, primitive G-H′-K-$3jm$'s and the primitive transformation coefficients.

We label the identity and primitive irreps of point groups by 0 and $\frac{1}{2}$ respectively. The basis labels (i and l in (3.1)) may in practice be several point-group labels, depending on which group chain is used. For example, the partners of the irrep $\frac{1}{2}$ of SO_3 are $|\frac{1}{2}\frac{1}{2}\rangle$ and $|\frac{1}{2}-\frac{1}{2}\rangle$ in the JM basis. In the SO_3-D_∞-D_6-D_3-C_3 basis discussed in § 5 they are $|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\rangle$ and $|\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}\text{-}\frac{1}{2}\rangle$.

The primitive transformation coefficients are not all independent. Because of our $2jm$ choices ($\binom{0}{0} = \binom{\frac{1}{2}}{\frac{1}{2}} = 1$ for all embeddings) one may deduce from equation (3.1) that

$$\langle 00|00\rangle' = 1$$

$$\langle \tfrac{1}{2}\tfrac{1}{2}|\tfrac{1}{2}\tfrac{1}{2}\rangle' = A = \langle \tfrac{1}{2}-\tfrac{1}{2}|\tfrac{1}{2}-\tfrac{1}{2}\rangle'^* \qquad \langle \tfrac{1}{2}-\tfrac{1}{2}|\tfrac{1}{2}\tfrac{1}{2}\rangle' = B = -\langle \tfrac{1}{2}\tfrac{1}{2}|\tfrac{1}{2}-\tfrac{1}{2}\rangle'^* \tag{3.2}$$

or equivalently

$$|\tfrac{1}{2}\tfrac{1}{2}\rangle' = |\tfrac{1}{2}\tfrac{1}{2}\rangle A + |\tfrac{1}{2}-\tfrac{1}{2}\rangle B \qquad |\tfrac{1}{2}-\tfrac{1}{2}\rangle' = |\tfrac{1}{2}\tfrac{1}{2}\rangle(-B^*) + |\tfrac{1}{2}-\tfrac{1}{2}\rangle A^*.$$

These restrictions are just those for having the primed kets related to the unprimed by a rotation $R(\alpha, \beta, \gamma)$ described by the Euler angles α, β, γ (see Messiah 1965, appendix C), where

$$A = \mathrm{e}^{-\mathrm{i}\alpha/2} \cos \tfrac{1}{2}\beta \, \mathrm{e}^{-\mathrm{i}\gamma/2} \qquad B = \mathrm{e}^{\mathrm{i}\alpha/2} \sin \tfrac{1}{2}\beta \, \mathrm{e}^{-\mathrm{i}\gamma/2}. \tag{3.3}$$

The point-group basis of SO_3 described by a given set of $3jm$ symbols may be transformed to the JM basis by using a particular A, B in equation (3.1). This is the converse of the approach of many other authors who first calculate the transformation coefficients in order to be able to calculate $3jm$ symbols. See for example Dobosh (1972), Golding and Newmarch (1977), Harnung and Schäffer (1972), Kibler and Grenet (1977) and Kramer (1968).

4. Example of $D_3 \supset C_3$

The j symbols and jm factors of all dihedral and cyclic groups were discussed by Butler and Reid (1979) and a possible choice of phases was suggested. In this section we shall analyse the repercussions of the orientation phase choices which occur in the embeddings $D_n \supset C_n$ and $D_{odd} \supset C_2$ by considering the embedding $D_3 \supset C_3$ in detail.

The above paper introduced a notation which used integers and half integers to label true and spin irreps respectively, in analogy to SO_3 and SO_2. The character table (table 1) gives the correspondence between our notation and those of some other authors.

The branching rules for $D_3 \supset C_3$ are

$$0 \to 0 \qquad \tilde{0} \to 0 \qquad \tfrac{1}{2} \to \tfrac{1}{2} + -\tfrac{1}{2} \qquad \tfrac{3}{2} \to \tfrac{3}{2} \qquad -\tfrac{3}{2} \to \tfrac{3}{2}. \tag{4.1}$$

We noted in § 2 that all phase choices in the $3jm$ calculation are contained in the $2jm$'s and primitive $3jm$'s. The $2jm$'s are chosen in such a way that as many $3jm$'s as possible may be real. The set

$$\begin{pmatrix}0\\0\end{pmatrix} = 1, \quad \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\end{pmatrix} = 1, \quad \begin{pmatrix}\frac{1}{2}\\-\frac{1}{2}\end{pmatrix} = -1, \quad \begin{pmatrix}\tilde{0}\\0\end{pmatrix} = -1,$$

$$\begin{pmatrix}1\\1\end{pmatrix} = 1, \quad \begin{pmatrix}1\\-1\end{pmatrix} = 1, \quad \begin{pmatrix}\frac{3}{2}\\\frac{3}{2}\end{pmatrix} = 1, \quad \begin{pmatrix}-\frac{3}{2}\\\frac{3}{2}\end{pmatrix} = -1 \tag{4.2}$$

Table 1. Character table for D_3. D_3 consists of: C_3: three-fold rotations about some axis; C_2': two-fold rotations about three axes perpendicular to the three-fold axis. Our irrep labels are shown, also those of Griffith (1961), Ballhausen (1962) and Koster *et al* (1963). We follow Lax (1974) in using the active convention for rotations.

Griffith, Ballhausen	Koster *et al*		E	$\bar{E}$	$2C_3$	$2\bar{C}_3$	$3C_2'$	$3\bar{C}_2'$
A_1	Γ_1	0	1	1	1	1	1	1
E'	Γ_4	$\frac{1}{2}$	2	−2	1	−1	0	0
A_2	Γ_2	$\tilde{0}$	1	1	1	1	−1	−1
E	Γ_3	1	2	2	−1	−1	0	0
E''	Γ_5	$\frac{3}{2}$	1	−1	−1	1	−i	i
	Γ_6	$-\frac{3}{2}$	1	−1	−1	1	i	−i

is suitable. There are only four inequivalent non-trivial primitive D_3-C_3-$3jm$ factors:

$$\begin{pmatrix} \tilde{0} & \frac{1}{2} & \frac{1}{2} \\ 1 & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{4.3}$$

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ 1 & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \tag{4.4}$$

$$\begin{pmatrix} \frac{3}{2} & 1 & \frac{1}{2} \\ \frac{3}{2} & 1 & \frac{1}{2} \end{pmatrix} \tag{4.5}$$

$$\begin{pmatrix} \frac{3}{2} & 1 & \frac{1}{2} \\ \frac{3}{2} & -1 & -\frac{1}{2} \end{pmatrix}. \tag{4.6}$$

The orthogonality relations (Butler and Wybourne 1976a, equations (35) and (36)) show that all have a norm of $1/\sqrt{2}$.

There is a free phase for each ket. However the phases of $|\frac{1}{2}-\frac{1}{2}\rangle$, $|1-1\rangle$ and $|\frac{3}{2}-\frac{3}{2}\rangle$ are related by the $2jm$ choices to their complex conjugates:

$$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} = \sqrt{2}\langle \tfrac{1}{2}\tfrac{1}{2}, \tfrac{1}{2}-\tfrac{1}{2}|00\rangle \qquad \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \sqrt{2}\langle 11, 1-1|00\rangle \qquad \begin{pmatrix} \frac{3}{2} \\ \frac{3}{2} \end{pmatrix} = \langle \tfrac{3}{2}\tfrac{3}{2}, -\tfrac{3}{2}\tfrac{3}{2}|00\rangle \tag{4.7}$$

(Butler and Wybourne 1976a, equation (29)). Furthermore, because the $3jm$'s involve only relative phase information, the primitive ket $|\frac{1}{2}\frac{1}{2}\rangle$ does not contribute a freedom to the algebra. Therefore there are only three primitive $3jm$'s which have this kind of phase freedom associated with them. Because $|\tilde{0}0\rangle$ is a real ket its choice is merely a sign. This corresponds to the fact that (4.3) is restricted to being real by the complex conjugation and column interchange symmetries (Butler and Wybourne 1976a, equations (37) and (38)). For (4.4) and (4.5) the choice is an arbitrary phase, corresponding to the kets $|11\rangle$ and $|\frac{3}{2}\frac{3}{2}\rangle$. We choose (4.3)–(4.5) as $1/\sqrt{2}$. At this stage there appear to be no free phases left and we would expect the calculation of all other $3jm$'s to be straightforward. However, none of the equations (Butler and Wybourne 1976a, § 6–§ 8) tells us the phase of (4.6). This counters the speculation at the end of § 7 of Butler and Wybourne (1976a).

Let the phase of (4.6) relative to (4.3)–(4.5) be $e^{i\theta}$. We shall show that $e^{i\theta}$ is indeed free, but that it has an effect on the orientation of the group.

In order to do this we consider the transformation from the point-group basis $SO_3 \supset D_\infty \supset D_6 \supset D_3 \supset C_3$ to the JM basis, as discussed in § 2. We use the phase choices of Butler and Reid (1979) for the SO_3-D_∞-D_6-D_3 chain and we use the standard SO_3-SO_2-$3jm$'s. Taking $A = 1$, $B = 0$ in (3.2) and then using (3.1) recursively gives the $SO_3 \supset D_\infty \supset D_6 \supset D_3 \supset C_3$ kets (primed) in terms of the JM kets:

$$|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\rangle' = |\tfrac{3}{2}\tfrac{3}{2}\rangle\, e^{i\theta}/\sqrt{2} + |\tfrac{3}{2}-\tfrac{3}{2}\rangle(-1\sqrt{2}) \qquad |\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}-\tfrac{3}{2}\tfrac{3}{2}\rangle' = |\tfrac{3}{2}\tfrac{3}{2}\rangle 1/\sqrt{2} + |\tfrac{3}{2}-\tfrac{3}{2}\rangle\, e^{-i\theta}/\sqrt{2}. \tag{4.8}$$

Rotation by an angle $\frac{2}{3}\pi$ about the z axis (Messiah 1965, equation (C63)) shows that the z axis is the three-fold axis:

$$R(\tfrac{2}{3}\pi, z)|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\rangle' = -|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\rangle' \tag{4.9}$$

(see figure 1). The two-fold axes are therefore in the xy plane.

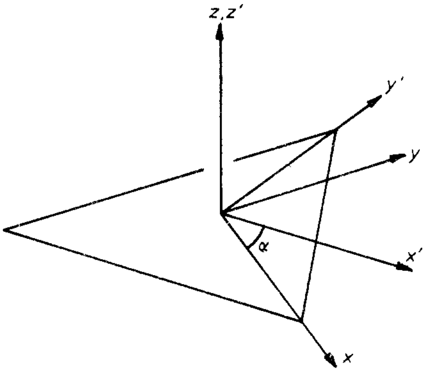

Figure 1. Axes for D_3. The unprimed and primed axes refer to equations (4.10) and (4.11) respectively. $\alpha = \pi/6$ corresponds to $\theta = \pi/2$ in (4.14).

If $\theta = 0$ in (4.8), then

$$R(\pi, x)|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\rangle' = -i|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\rangle' \qquad R(\pi, y)|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\rangle' = -|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}-\tfrac{3}{2}\tfrac{3}{2}\rangle' \tag{4.10}$$

(Messiah 1965, equations (C61) and (C62)). In this case the operator $R(\pi, x)$ is contained in the group while $R(\pi, y)$ is not. If $\theta = \frac{1}{2}\pi$ then

$$R(\pi, x)|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\rangle' = -|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}-\tfrac{3}{2}\tfrac{3}{2}\rangle' \qquad R(\pi, y)|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\rangle' = -i|\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\rangle'. \tag{4.11}$$

$R(\pi, y)$ is now in the group (see figure 1). (For other choices of the phase $e^{i\theta}$ neither $R(\pi, x)$ nor $R(\pi, y)$ is in the group.)

Of the phase choices of (4.3)–(4.6), only the phase of (4.6) relative to (4.5) affects the orientation of the two-fold axes. This may be seen by repeating the above arguments with arbitrary phases for (4.3)–(4.6).

Now consider two sets of $3jm$'s for $D_3 \supset C_3$ for which the phase of (4.6) has been chosen differently (but (4.3)–(4.5) are identical):

$$\begin{pmatrix} \frac{3}{2} & 1 & \frac{1}{2} \\ \frac{3}{2} & -1 & -\frac{1}{2} \end{pmatrix}' = e^{i\theta} \begin{pmatrix} \frac{3}{2} & 1 & \frac{1}{2} \\ \frac{3}{2} & -1 & -\frac{1}{2} \end{pmatrix}. \tag{4.12}$$

We may transform between two SO_3-D_∞-D_6-D_3-C_3 bases, one with the unprimed and the other the primed choice, and also rotate the primed basis by an angle $\alpha/2$ about the z

axis by choosing $A = \mathrm{e}^{-\mathrm{i}\alpha/2}$, $B = 0$ in (3.3). The relationship between the $J = \frac{3}{2}$ kets is then:

$$\begin{aligned} \langle \tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2} | \tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2} \rangle' &= \tfrac{1}{2}(\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{e}^{-3\mathrm{i}\alpha/2} + \mathrm{e}^{3\mathrm{i}\alpha/2}) \\ \langle \tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2} - \tfrac{3}{2}\tfrac{3}{2} | \tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2} \rangle' &= \tfrac{1}{2}(\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{e}^{-3\mathrm{i}\alpha/2} - \mathrm{e}^{3\mathrm{i}\alpha/2}). \end{aligned} \tag{4.13}$$

If the unprimed and the primed D_3 irreps are not to be mixed, then one requires

$$\mathrm{e}^{\mathrm{i}\theta} = \mathrm{e}^{3\mathrm{i}\alpha}. \tag{4.14}$$

Thus if $\alpha = 0$, $\mathrm{e}^{\mathrm{i}\theta} = 1$ only, while if $\theta = 0$ then α must be a multiple of $\frac{2}{3}\pi$. Observe that a $\frac{2}{3}\pi$ rotation about the z axis is a symmetry operation of D_3. See figure 1.

We have shown that a special orientation phase choice exists which changes the orientation of the group D_3 in the C_3 basis. (4.14) proves that it is equivalent to a rotation about the z axis. In the next section we shall discuss similar phase choices for other groups.

5. Orientation phases in the other point groups

In § 4 we showed that for $D_3 \supset C_3$ there was a phase choice which was equivalent to a rotation about the z axis. For all $D_n \supset C_n$, $D_{\mathrm{odd}} \supset C_2$ and $T \supset C_3$ a similar orientation phase choice exists. For many embeddings, e.g. $SO_3 \supset SO_2$, $SO_3 \supset O$, $D_{mn} \supset D_n$, $O \supset D_4$ and $O \supset T$, no such choice exists. For $O \supset D_3$, $T \supset D_2$, $K \supset T$ and $K \supset D_5$ we must choose between a pair of double roots. In the double root cases the choice is still equivalent to a rotation about the z axis but now there are only two possible orientations.

As an example of the double root case we consider $T \supset D_2$. Butler (1979) proved that some $3jm$ factors of $T \supset D_2$ must be complex. In the calculation of $T \supset D_2$ $3jm$'s by the methods described in § 4, a similar problem arises—once all the phases are fixed. The real part and the magnitude of

$$\begin{pmatrix} \frac{3}{2} & 1 & \frac{1}{2} \\ \frac{1}{2} & 1 & \frac{1}{2} \end{pmatrix}^{\mathrm{T}}_{D_2} = \frac{-1}{2\sqrt{3}} \pm \frac{\mathrm{i}}{2} \tag{5.1}$$

may be calculated, but not the sign of the imaginary part (table 2 gives the correspondence between our notation and some others). As in § 4 the choice affects the orientation of the tetrahedron and corresponds to the two distinct ways of orienting a tetrahedron about D_2 axes (see figure 2).

The two phase choices, like the figures, are related by a $\frac{1}{2}\pi$ rotation. Table 3 shows a transformation between the $O \supset T \supset D_2 \supset C_2$ bases with two root choices in which a rotation of $\frac{1}{2}\pi$ about the z axis has been used to bring the two tetrahedra into coincidence. (The fact that $D_2 \supset C_2$ contains an orientation phase is irrelevant because it is the same in both schemes.) Note that the rotation mixes the irreps of D_2 but not O. This is because a $\frac{1}{2}\pi$ rotation about the z axis is an octahedral operation (with this orientation), but not a tetrahedral or D_2 operation. In tables 3, 4 and 5 kets in one basis are written as a sum of kets in another basis in the format: $|$ket in one basis$\rangle = \Sigma_{\mathrm{basis}}\,|$ket in the other basis$\rangle \times$ (transformation coefficient). In table 3 the labels on both sides of the equations are irrep labels for the groups O, T, D_2 and C_2 (see table 2).

Table 2. Correspondence between our notation and that of Koster *et al* (1963) and Griffith (1961).

Cyclic Group C_2								
	0	$\frac{1}{2}$	$-\frac{1}{2}$	1				
Koster *et al*	Γ_1	Γ_3	Γ_4	Γ_2				
Dihedral Group D_2								
	0	$\frac{1}{2}$	$\tilde{0}$	1	$\tilde{1}$			
Koster *et al*	Γ_1	Γ_5	Γ_3	Γ_2	Γ_4			
Griffith	A_1	E'	B_1	B_2	B_3			
Cyclic Group C_4								
	0	$\frac{1}{2}$	$-\frac{1}{2}$	1	-1	$\frac{3}{2}$	$-\frac{3}{2}$	2
Koster *et al*	Γ_1	Γ_5	Γ_6	Γ_3	Γ_4	Γ_8	Γ_7	Γ_2
Dihedral Group D_4								
	0	$\frac{1}{2}$	$\tilde{0}$	1	$\frac{3}{2}$	2	$\tilde{2}$	
Koster *et al*	Γ_1	Γ_6	Γ_2	Γ_5	Γ_7	Γ_3	Γ_4	
Griffith	A_1	E'	A_2	E	E''	B_1	B_2	
Tetrahedral Group T								
	0	$\frac{1}{2}$	1	$\frac{3}{2}$	$-\frac{3}{2}$	2	-2	
Koster *et al*	Γ_1	Γ_5	Γ_4	Γ_6	Γ_7	Γ_2	Γ_3	
Griffith	A_1	E'	T	E''	E'''	E		
Octahedral Group O								
	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\tilde{1}$	$\tilde{\frac{1}{2}}$	$\tilde{0}$
Koster *et al*	Γ_1	Γ_6	Γ_4	Γ_8	Γ_3	Γ_5	Γ_7	Γ_2
Griffith	A_1	E'	T_1	U'	E	T_2	E''	A_2

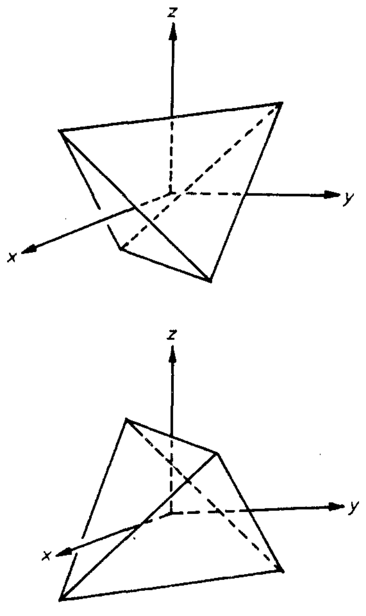

Figure 2. Orientations of a tetrahedron about D_2 axes.

Table 3. Transformation between two $O \supset T \supset D_2 \supset C_2$ bases. The format is: $|$ket with +ve root choice in equation (5.1)$\rangle$ = $|$ket with −ve choice$\rangle \times$ (transformation coefficient). The labels are O, T, D_2 and C_2 irrep labels (see table 2).

$$
\begin{aligned}
&|\,0\ 0\ 0\ 0> \;=\; |\,0\ 0\ 0\ 0>+1\\[6pt]
&|\,\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \;=\; |\,\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}>+1/\sqrt{2}-i/\sqrt{2}\\
&|\,\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \;=\; |\,\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}>+1/\sqrt{2}+i/\sqrt{2}\\[6pt]
&|\,1\ 1\ \tilde{0}\ 0> \;=\; |\,1\ 1\ \tilde{0}\ 0>+1\\
&|\,1\ 1\ 1\ 1> \;=\; |\,1\ 1\ \tilde{1}\ 1>+i\\
&|\,1\ 1\ \tilde{1}\ 1> \;=\; |\,1\ 1\ 1\ 1>+i\\[6pt]
&|\,\tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \;=\; |\,\tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}>+1/\sqrt{2}-i/\sqrt{2}\\
&|\,\tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \;=\; |\,\tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}>+1/\sqrt{2}+i/\sqrt{2}\\
&|\,\tfrac{3}{2}\text{-}\tfrac{3}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \;=\; |\,\tfrac{3}{2}\text{-}\tfrac{3}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}>+1/\sqrt{2}-i/\sqrt{2}\\
&|\,\tfrac{3}{2}\text{-}\tfrac{3}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \;=\; |\,\tfrac{3}{2}\text{-}\tfrac{3}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}>+1/\sqrt{2}+i/\sqrt{2}\\[6pt]
&|\,2\ 2\ 0\ 0> \;=\; |\,2\ 2\ 0\ 0>+1\\
&|\,2\text{-}2\ 0\ 0> \;=\; |\,2\text{-}2\ 0\ 0>+1\\[6pt]
&|\,\tilde{1}\ 1\ \tilde{0}\ 0> \;=\; |\,\tilde{1}\ 1\ \tilde{0}\ 0>+1\\
&|\,\tilde{1}\ 1\ 1\ 1> \;=\; |\,\tilde{1}\ 1\ \tilde{1}\ 1>+i\\
&|\,\tilde{1}\ 1\ \tilde{1}\ 1> \;=\; |\,\tilde{1}\ 1\ 1\ 1>+i\\[6pt]
&|\,\tilde{\tfrac{1}{2}}\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \;=\; |\,\tilde{\tfrac{1}{2}}\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}>+1/\sqrt{2}-i/\sqrt{2}\\
&|\,\tilde{\tfrac{1}{2}}\ \tfrac{1}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \;=\; |\,\tilde{\tfrac{1}{2}}\ \tfrac{1}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}>+1/\sqrt{2}+i/\sqrt{2}\\[6pt]
&|\,\tilde{0}\ 0\ 0\ 0> \;=\; |\,\tilde{0}\ 0\ 0\ 0>+1
\end{aligned}
$$

Table 4. Transformation of $SO_3 \supset O \supset D_4 \supset C_4$ to the JM basis with the $D_4 \supset C_4$ orientation phase choice of equation (5.2). The format is: $|SO_3OD_4C_4\ \text{ket}\rangle = \Sigma_M\ |\text{JM ket}\rangle \times$ (transformation coefficient).

$$
\begin{aligned}
&|\,0\ 0\ 0\ 0> \;=\; |\,0\ 0>+1\\[6pt]
&|\,\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \;=\; |\,\tfrac{1}{2}\ \tfrac{1}{2}>+1\\
&|\,\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \;=\; |\,\tfrac{1}{2}\text{-}\tfrac{1}{2}>+1\\[6pt]
&|\,1\ 1\ \tilde{0}\ 0> \;=\; |\,1\ 0>+1\\
&|\,1\ 1\ 1\ 1> \;=\; |\,1\ 1>-1\\
&|\,1\ 1\ 1\text{-}1> \;=\; |\,1\text{-}1>-1\\[6pt]
&|\,\tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \;=\; |\,\tfrac{3}{2}\ \tfrac{1}{2}>+1\\
&|\,\tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \;=\; |\,\tfrac{3}{2}\text{-}\tfrac{1}{2}>-1\\
&|\,\tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}> \;=\; |\,\tfrac{3}{2}\ \tfrac{3}{2}>+1\\
&|\,\tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\text{-}\tfrac{3}{2}> \;=\; |\,\tfrac{3}{2}\text{-}\tfrac{3}{2}>+1
\end{aligned}
$$

Table 4.—continued.

$|\ 2\ 2\ 0\ 0> \ = \ |\ 2\ 0> -1$

$|\ 2\ 2\ 2\ 2> \ = \ |\ 2\ 2> -1/\sqrt{2} \ + \ |\ 2\text{-}2> -1/\sqrt{2}$

$|\ 2\ \tilde{1}\ 1\ 1> \ = \ |\ 2\ 1> -1$

$|\ 2\ \tilde{1}\ 1\text{-}1> \ = \ |\ 2\text{-}1> +1$

$|\ 2\ \tilde{1}\ \tilde{2}\ 2> \ = \ |\ 2\ 2> +1/\sqrt{2} \ + \ |\ 2\text{-}2> -1/\sqrt{2}$

$|\ \tfrac{5}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \ = \ |\ \tfrac{5}{2}\ \tfrac{1}{2}> +1$

$|\ \tfrac{5}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \ = \ |\ \tfrac{5}{2}\text{-}\tfrac{1}{2}> +1$

$|\ \tfrac{5}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}> \ = \ |\ \tfrac{5}{2}\ \tfrac{3}{2}> -1/\sqrt{2.3} \ + \ |\ \tfrac{5}{2}\text{-}\tfrac{5}{2}> -\sqrt{5}/\sqrt{2.3}$

$|\ \tfrac{5}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\text{-}\tfrac{3}{2}> \ = \ |\ \tfrac{5}{2}\ \tfrac{5}{2}> +\sqrt{5}/\sqrt{2.3} \ + \ |\ \tfrac{5}{2}\text{-}\tfrac{3}{2}> +1/\sqrt{2.3}$

$|\ \tfrac{5}{2}\ \widetilde{\tfrac{1}{2}}\ \tfrac{3}{2}\ \tfrac{3}{2}> \ = \ |\ \tfrac{5}{2}\ \tfrac{3}{2}> +\sqrt{5}/\sqrt{2.3} \ + \ |\ \tfrac{5}{2}\text{-}\tfrac{5}{2}> -1/\sqrt{2.3}$

$|\ \tfrac{5}{2}\ \widetilde{\tfrac{1}{2}}\ \tfrac{3}{2}\text{-}\tfrac{3}{2}> \ = \ |\ \tfrac{5}{2}\ \tfrac{5}{2}> +1/\sqrt{2.3} \ + \ |\ \tfrac{5}{2}\text{-}\tfrac{3}{2}> -\sqrt{5}/\sqrt{2.3}$

$|\ 3\ 1\ \tilde{0}\ 0> \ = \ |\ 3\ 0> -1$

$|\ 3\ 1\ 1\ 1> \ = \ |\ 3\ 1> -\sqrt{3}/2\sqrt{2} \ + \ |\ 3\text{-}3> -\sqrt{5}/2\sqrt{2}$

$|\ 3\ 1\ 1\text{-}1> \ = \ |\ 3\ 3> -\sqrt{5}/2\sqrt{2} \ + \ |\ 3\text{-}1> -\sqrt{3}/2\sqrt{2}$

$|\ 3\ \tilde{1}\ 1\ 1> \ = \ |\ 3\ 1> -\sqrt{5}/2\sqrt{2} \ + \ |\ 3\text{-}3> +\sqrt{3}/2\sqrt{2}$

$|\ 3\ \tilde{1}\ 1\text{-}1> \ = \ |\ 3\ 3> +\sqrt{3}/2\sqrt{2} \ + \ |\ 3\text{-}1> -\sqrt{5}/2\sqrt{2}$

$|\ 3\ \tilde{1}\ \tilde{2}\ 2> \ = \ |\ 3\ 2> -1/\sqrt{2} \ + \ |\ 3\text{-}2> -1/\sqrt{2}$

$|\ 3\ \tilde{0}\ 2\ 2> \ = \ |\ 3\ 2> -1/\sqrt{2} \ + \ |\ 3\text{-}2> +1/\sqrt{2}$

$|\ \tfrac{7}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \ = \ |\ \tfrac{7}{2}\ \tfrac{1}{2}> -\sqrt{7}/2\sqrt{3} \ + \ |\ \tfrac{7}{2}\text{-}\tfrac{7}{2}> -\sqrt{5}/2\sqrt{3}$

$|\ \tfrac{7}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \ = \ |\ \tfrac{7}{2}\ \tfrac{7}{2}> +\sqrt{5}/2\sqrt{3} \ + \ |\ \tfrac{7}{2}\text{-}\tfrac{1}{2}> +\sqrt{7}/2\sqrt{3}$

$|\ \tfrac{7}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \ = \ |\ \tfrac{7}{2}\ \tfrac{1}{2}> -\sqrt{5}/2\sqrt{3} \ + \ |\ \tfrac{7}{2}\text{-}\tfrac{7}{2}> +\sqrt{7}/2\sqrt{3}$

$|\ \tfrac{7}{2}\ \tfrac{3}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \ = \ |\ \tfrac{7}{2}\ \tfrac{7}{2}> -\sqrt{7}/2\sqrt{3} \ + \ |\ \tfrac{7}{2}\text{-}\tfrac{1}{2}> +\sqrt{5}/2\sqrt{3}$

$|\ \tfrac{7}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}> \ = \ |\ \tfrac{7}{2}\ \tfrac{3}{2}> +\sqrt{3}/2 \ + \ |\ \tfrac{7}{2}\text{-}\tfrac{5}{2}> +1/2$

$|\ \tfrac{7}{2}\ \tfrac{3}{2}\ \tfrac{3}{2}\text{-}\tfrac{3}{2}> \ = \ |\ \tfrac{7}{2}\ \tfrac{5}{2}> +1/2 \ + \ |\ \tfrac{7}{2}\text{-}\tfrac{3}{2}> +\sqrt{3}/2$

$|\ \tfrac{7}{2}\ \widetilde{\tfrac{1}{2}}\ \tfrac{3}{2}\ \tfrac{3}{2}> \ = \ |\ \tfrac{7}{2}\ \tfrac{3}{2}> +1/2 \ + \ |\ \tfrac{7}{2}\text{-}\tfrac{5}{2}> -\sqrt{3}/2$

$|\ \tfrac{7}{2}\ \widetilde{\tfrac{1}{2}}\ \tfrac{3}{2}\text{-}\tfrac{3}{2}> \ = \ |\ \tfrac{7}{2}\ \tfrac{5}{2}> -\sqrt{3}/2 \ + \ |\ \tfrac{7}{2}\text{-}\tfrac{3}{2}> +1/2$

$|\ 4\ 0\ 0\ 0> \ = \ |\ 4\ 4> +\sqrt{5}/2\sqrt{2.3} \ + \ |\ 4\ 0> +\sqrt{7}/2\sqrt{3} \ + \ |\ 4\text{-}4> +\sqrt{5}/2\sqrt{2.3}$

$|\ 4\ 1\ \tilde{0}\ 0> \ = \ |\ 4\ 4> +1/\sqrt{2} \ + \ |\ 4\text{-}4> -1/\sqrt{2}$

$|\ 4\ 1\ 1\ 1> \ = \ |\ 4\ 1> +\sqrt{7}/2\sqrt{2} \ + \ |\ 4\text{-}3> +1/2\sqrt{2}$

$|\ 4\ 1\ 1\text{-}1> \ = \ |\ 4\ 3> -1/2\sqrt{2} \ + \ |\ 4\text{-}1> -\sqrt{7}/2\sqrt{2}$

$|\ 4\ 2\ 0\ 0> \ = \ |\ 4\ 4> -\sqrt{7}/2\sqrt{2.3} \ + \ |\ 4\ 0> +\sqrt{5}/2\sqrt{3} \ + \ |\ 4\text{-}4> -\sqrt{7}/2\sqrt{2.3}$

$|\ 4\ 2\ 2\ 2> \ = \ |\ 4\ 2> -1/\sqrt{2} \ + \ |\ 4\text{-}2> -1/\sqrt{2}$

$|\ 4\ \tilde{1}\ 1\ 1> \ = \ |\ 4\ 1> +1/2\sqrt{2} \ + \ |\ 4\text{-}3> -\sqrt{7}/2\sqrt{2}$

$|\ 4\ \tilde{1}\ 1\text{-}1> \ = \ |\ 4\ 3> +\sqrt{7}/2\sqrt{2} \ + \ |\ 4\text{-}1> -1/2\sqrt{2}$

$|\ 4\ \tilde{1}\ \tilde{2}\ 2> \ = \ |\ 4\ 2> +1/\sqrt{2} \ + \ |\ 4\text{-}2> -1/\sqrt{2}$

Table 5. Transformation of $SO_3 \supset O \supset D_4 \supset C_4$ to the JM basis with the orientation phase choice of equation (5.3). The format is: $|SO_3OD_4C_4\ \text{ket}\rangle = \Sigma_M\ |JM\ \text{ket}\rangle \times$ (transformation coefficient).

$|\ 0\ 0\ 0\ 0> \ = \ |\ 0\ 0> +1$

$|\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}> \ = \ |\ \tfrac{1}{2}\ \tfrac{1}{2}> +1$

$|\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> \ = \ |\ \tfrac{1}{2}\text{-}\tfrac{1}{2}> +1$

Table 5.—continued

$|\,1\ 1\ \tilde{0}\ 0\rangle = |\,1\ 0\rangle + 1$
$|\,1\ 1\ 1\ 1\rangle = |\,1\ 1\rangle - 1$
$|\,1\ 1\ 1\,\text{-}1\rangle = |\,1\,\text{-}1\rangle - 1$

$|\,\frac{3}{2}\ \frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\rangle = |\,\frac{3}{2}\ \frac{1}{2}\rangle + 1$
$|\,\frac{3}{2}\ \frac{3}{2}\ \frac{1}{2}\,\text{-}\frac{1}{2}\rangle = |\,\frac{3}{2}\,\text{-}\frac{1}{2}\rangle - 1$
$|\,\frac{3}{2}\ \frac{3}{2}\ \frac{3}{2}\ \frac{3}{2}\rangle = |\,\frac{3}{2}\ \frac{3}{2}\rangle + 1$
$|\,\frac{3}{2}\ \frac{3}{2}\ \frac{3}{2}\,\text{-}\frac{3}{2}\rangle = |\,\frac{3}{2}\,\text{-}\frac{3}{2}\rangle + 1$

$|\,2\ 2\ 0\ 0\rangle = |\,2\ 0\rangle - 1$
$|\,2\ 2\ 2\ 2\rangle = |\,2\ 2\rangle + i/\sqrt{2} \ + \ |\,2\,\text{-}2\rangle - i/\sqrt{2}$
$|\,2\ \tilde{1}\ 1\ 1\rangle = |\,2\ 1\rangle - 1$
$|\,2\ \tilde{1}\ 1\,\text{-}1\rangle = |\,2\,\text{-}1\rangle + 1$
$|\,2\ \tilde{1}\ \tilde{2}\ 2\rangle = |\,2\ 2\rangle - i/\sqrt{2} \ + \ |\,2\,\text{-}2\rangle - i/\sqrt{2}$

$|\,\frac{5}{2}\ \frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\rangle = |\,\frac{5}{2}\ \frac{1}{2}\rangle + 1$
$|\,\frac{5}{2}\ \frac{3}{2}\ \frac{1}{2}\,\text{-}\frac{1}{2}\rangle = |\,\frac{5}{2}\,\text{-}\frac{1}{2}\rangle + 1$
$|\,\frac{5}{2}\ \frac{3}{2}\ \frac{3}{2}\ \frac{3}{2}\rangle = |\,\frac{5}{2}\ \frac{3}{2}\rangle - 1/\sqrt{2.3} \ + \ |\,\frac{5}{2}\,\text{-}\frac{5}{2}\rangle + \sqrt{5}/\sqrt{2.3}$
$|\,\frac{5}{2}\ \frac{3}{2}\ \frac{3}{2}\,\text{-}\frac{3}{2}\rangle = |\,\frac{5}{2}\ \frac{5}{2}\rangle - \sqrt{5}/\sqrt{2.3} \ + \ |\,\frac{5}{2}\,\text{-}\frac{3}{2}\rangle + 1/\sqrt{2.3}$
$|\,\frac{5}{2}\ \tilde{\frac{1}{2}}\ \frac{3}{2}\ \frac{3}{2}\rangle = |\,\frac{5}{2}\ \frac{3}{2}\rangle + \sqrt{5}/\sqrt{2.3} \ + \ |\,\frac{5}{2}\,\text{-}\frac{5}{2}\rangle + 1/\sqrt{2.3}$
$|\,\frac{5}{2}\ \tilde{\frac{1}{2}}\ \frac{3}{2}\,\text{-}\frac{3}{2}\rangle = |\,\frac{5}{2}\ \frac{5}{2}\rangle - 1/\sqrt{2.3} \ + \ |\,\frac{5}{2}\,\text{-}\frac{3}{2}\rangle - \sqrt{5}/\sqrt{2.3}$

$|\,3\ 1\ \tilde{0}\ 0\rangle = |\,3\ 0\rangle - 1$
$|\,3\ 1\ 1\ 1\rangle = |\,3\ 1\rangle - \sqrt{3}/2\sqrt{2} \ + \ |\,3\,\text{-}3\rangle + \sqrt{5}/2\sqrt{2}$
$|\,3\ 1\ 1\,\text{-}1\rangle = |\,3\ 3\rangle + \sqrt{5}/2\sqrt{2} \ + \ |\,3\,\text{-}1\rangle - \sqrt{3}/2\sqrt{2}$
$|\,3\ \tilde{1}\ 1\ 1\rangle = |\,3\ 1\rangle - \sqrt{5}/2\sqrt{2} \ + \ |\,3\,\text{-}3\rangle - \sqrt{3}/2\sqrt{2}$
$|\,3\ \tilde{1}\ 1\,\text{-}1\rangle = |\,3\ 3\rangle - \sqrt{3}/2\sqrt{2} \ + \ |\,3\,\text{-}1\rangle - \sqrt{5}/2\sqrt{2}$
$|\,3\ \tilde{1}\ \tilde{2}\ 2\rangle = |\,3\ 2\rangle + i/\sqrt{2} \ + \ |\,3\,\text{-}2\rangle - i/\sqrt{2}$
$|\,3\ \tilde{0}\ 2\ 2\rangle = |\,3\ 2\rangle + i/\sqrt{2} \ + \ |\,3\,\text{-}2\rangle + i/\sqrt{2}$

$|\,\frac{7}{2}\ \frac{1}{2}\ \frac{1}{2}\ \frac{1}{2}\rangle = |\,\frac{7}{2}\ \frac{1}{2}\rangle - \sqrt{7}/2\sqrt{3} \ + \ |\,\frac{7}{2}\,\text{-}\frac{7}{2}\rangle + \sqrt{5}/2\sqrt{3}$
$|\,\frac{7}{2}\ \frac{1}{2}\ \frac{1}{2}\,\text{-}\frac{1}{2}\rangle = |\,\frac{7}{2}\ \frac{7}{2}\rangle - \sqrt{5}/2\sqrt{3} \ + \ |\,\frac{7}{2}\,\text{-}\frac{1}{2}\rangle + \sqrt{7}/2\sqrt{3}$
$|\,\frac{7}{2}\ \frac{3}{2}\ \frac{1}{2}\ \frac{1}{2}\rangle = |\,\frac{7}{2}\ \frac{1}{2}\rangle - \sqrt{5}/2\sqrt{3} \ + \ |\,\frac{7}{2}\,\text{-}\frac{7}{2}\rangle - \sqrt{7}/2\sqrt{3}$
$|\,\frac{7}{2}\ \frac{3}{2}\ \frac{1}{2}\,\text{-}\frac{1}{2}\rangle = |\,\frac{7}{2}\ \frac{7}{2}\rangle + \sqrt{7}/2\sqrt{3} \ + \ |\,\frac{7}{2}\,\text{-}\frac{1}{2}\rangle + \sqrt{5}/2\sqrt{3}$
$|\,\frac{7}{2}\ \frac{3}{2}\ \frac{3}{2}\ \frac{3}{2}\rangle = |\,\frac{7}{2}\ \frac{3}{2}\rangle + \sqrt{3}/2 \ + \ |\,\frac{7}{2}\,\text{-}\frac{5}{2}\rangle - 1/2$
$|\,\frac{7}{2}\ \frac{3}{2}\ \frac{3}{2}\,\text{-}\frac{3}{2}\rangle = |\,\frac{7}{2}\ \frac{5}{2}\rangle - 1/2 \ + \ |\,\frac{7}{2}\,\text{-}\frac{3}{2}\rangle + \sqrt{3}/2$
$|\,\frac{7}{2}\ \tilde{\frac{1}{2}}\ \frac{3}{2}\ \frac{3}{2}\rangle = |\,\frac{7}{2}\ \frac{3}{2}\rangle + 1/2 \ + \ |\,\frac{7}{2}\,\text{-}\frac{5}{2}\rangle + \sqrt{3}/2$
$|\,\frac{7}{2}\ \tilde{\frac{1}{2}}\ \frac{3}{2}\,\text{-}\frac{3}{2}\rangle = |\,\frac{7}{2}\ \frac{5}{2}\rangle + \sqrt{3}/2 \ + \ |\,\frac{7}{2}\,\text{-}\frac{3}{2}\rangle + 1/2$

$|\,4\ 0\ 0\ 0\rangle = |\,4\ 4\rangle - \sqrt{5}/2\sqrt{2.3} \ + \ |\,4\ 0\rangle + \sqrt{7}/2\sqrt{3} \ + \ |\,4\,\text{-}4\rangle - \sqrt{5}/2\sqrt{2.3}$
$|\,4\ 1\ \tilde{0}\ 0\rangle = |\,4\ 4\rangle - 1/\sqrt{2} \ + \ |\,4\,\text{-}4\rangle + 1/\sqrt{2}$
$|\,4\ 1\ 1\ 1\rangle = |\,4\ 1\rangle + \sqrt{7}/2\sqrt{2} \ + \ |\,4\,\text{-}3\rangle - 1/2\sqrt{2}$
$|\,4\ 1\ 1\,\text{-}1\rangle = |\,4\ 3\rangle + 1/2\sqrt{2} \ + \ |\,4\,\text{-}1\rangle - \sqrt{7}/2\sqrt{2}$
$|\,4\ 2\ 0\ 0\rangle = |\,4\ 4\rangle + \sqrt{7}/2\sqrt{2.3} \ + \ |\,4\ 0\rangle + \sqrt{5}/2\sqrt{3} \ + \ |\,4\,\text{-}4\rangle + \sqrt{7}/2\sqrt{2.3}$
$|\,4\ 2\ 2\ 2\rangle = |\,4\ 2\rangle + i/\sqrt{2} \ + \ |\,4\,\text{-}2\rangle - i/\sqrt{2}$
$|\,4\ \tilde{1}\ 1\ 1\rangle = |\,4\ 1\rangle + 1/2\sqrt{2} \ + \ |\,4\,\text{-}3\rangle + \sqrt{7}/2\sqrt{2}$
$|\,4\ \tilde{1}\ 1\,\text{-}1\rangle = |\,4\ 3\rangle - \sqrt{7}/2\sqrt{2} \ + \ |\,4\,\text{-}1\rangle - 1/2\sqrt{2}$
$|\,4\ \tilde{1}\ \tilde{2}\ 2\rangle = |\,4\ 2\rangle - i/\sqrt{2} \ + \ |\,4\,\text{-}2\rangle - i/\sqrt{2}$

Boyle and Schäffer (1974) showed that orientations of the icosahedron unrelated by icosahedral operations ($\pi/2$ apart) gave distinct icosahedral tensors. Their two orientations correspond to the scheme $K \supset T \supset D_2 \supset C_2$ with the two choices of root for $T \supset D_2$.

Since all finite group bases of SO_3 contain an embedding of a cyclic group in a dihedral group or the embedding $T \supset C_3$ (Koster *et al* 1963), any application of such bases involves an orientation phase. This corresponds to the freedom one has to choose the orientation of the x and y axes, the z axis being determined, up to group operations, by the choice of groups. For $SO_3 \supset O \supset D_3 \supset C_3$ the z axis is three-fold, through a corner of the cube; for $SO_3 \supset O \supset D_4 \supset C_4$ the z axis is four-fold, through a face of the cube.

Consider $SO_3 \supset O \supset D_4 \supset C_4$. Tables 4 and 5 show the transformation of this basis to the JM basis for two particular choices of orientation phase for $D_4 \supset C_4$:

$$\begin{pmatrix} 2 & \frac{3}{2} & \frac{1}{2} \\ 2 & \frac{3}{2} & \frac{1}{2} \end{pmatrix}^{D_4}_{C_4} = \frac{+1}{\sqrt{2}} \tag{5.2}$$

$$\begin{pmatrix} 2 & \frac{3}{2} & \frac{1}{2} \\ 2 & \frac{3}{2} & \frac{1}{2} \end{pmatrix}^{D_4}_{C_4} = \frac{i}{\sqrt{2}}. \tag{5.3}$$

A calculation of the character of the irrep $\tilde{0}$ of O under a two-fold rotation about the y axis (see § 4) shows that the choice (5.2) corresponds to having the x and y axes through the faces of the cube and (5.3) to having the x and y axes through the edges. See figure 3 and the character tables of Koster *et al* (1963). In the former case the rotation matrices (Messiah 1965, appendix C) may be used to show that the 111 axis is a three-fold axis of O. In the latter the 101 and 110 axes are three-fold.

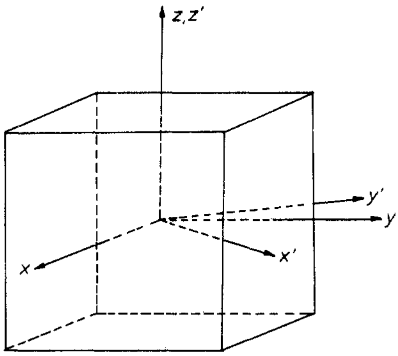

Figure 3. Axes of a cube. The unprimed and primed axes correspond to the choices (5.2) and (5.3) respectively.

The fourth-order scalar operator for octahedral symmetry with a four-fold z axis is commonly written

$$C^4 = C^4_0 + \sqrt{5/14}(C^4_4 + C^4_{-4}) \tag{5.4}$$

(e.g. Hutchings 1964). This corresponds to table 4—in table 5 the first sign in (5.4) is changed. Table 4 is similar to the table of Ballhausen (1962, p 95), the differences being due to the free (non-orientation) phases for the $SO_3 \supset O \supset D_4 \supset C_4$ kets.

6. Branching rules

The orientation phase problem must not be confused with another problem—the existence of several sets of valid branching rules for some point-group embeddings. Branching rules depend on the labelling of classes, for this determines which operations are to be discarded on going from the group to the subgroup.

An extreme case is the embedding $D_2 \supset C_2$. There are, in addition to the identity, three one-dimensional irreps of D_2: $\tilde{0}$, 1 and $\tilde{1}$. These irreps are not distinguished by the product rules of D_2, and three different $D_2 \supset C_2$ branching rules are possible since any one of these one-dimensional irreps of D_2 may reduce to the identity irrep of C_2. The usual branching (Koster *et al* 1963) is $\tilde{0} \to 0$; the others correspond to relabelling the x, y and z axes of D_2 (Koster's C_2 axis is z).

7. Conclusions

The existence of the orientation phases clarifies the speculations of Butler and Wybourne (1976a). The phase choices discussed there have no effect on the orientation of the group—changing them merely changes the phases of the partners. (In the presence of branching multiplicity this phase becomes a unitary matrix.) Equation (4.13) shows that a change in orientation phase mixes irreps of the group, i.e. the groups are no longer identical, merely isomorphic. Properties of transformations between bases chosen with respect to isomorphic subgroups of a symmetric group have been studied by Sullivan (1978).

In some applications it is important to know where the symmetry axes lie for the given set of point-group j and jm symbols. Sections 4 and 5 showed how to find such axes, and, further, indicated how these may be rotated, either by changing the orientation phase, or by rotating all partners.

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