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Orientations of reflection–rotation groups

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Abstract. We extend the work of a previous paper in which we showed that some of the phase choices in the $3jm$ factors of certain point group embeddings affect the orientation of the symmetry axes. The occurrence of such choices is unpredictable and their effect is sometimes subtle but once a set of $3jm$ factors has been calculated we can determine the orientations of the symmetry axes and mirror planes and investigate how these orientations vary with the phase choices. The properties of the reflection–rotation groups are obtained from the isomorphic pure rotation groups but care is necessary in interpreting the effects of the corresponding operations of, for example, D_3 and C_{3v}.

1. Introduction

It has been shown that the j symbols and jm factors of arbitrary compact groups may be calculated by a building up method which uses only character theory results (Butler and Wybourne 1976a). The building up method has been used to calculate j and jm symbols of finite groups (Butler and Wybourne 1976b, Donini 1979, pp 123–77, Butler and Reid 1979, Prasad and Bharathi 1980, Butler 1981) and continuous groups (Butler 1976, Butler *et al* 1978, 1979, Bickerstaff *et al* 1982). In a previous paper (Reid and Butler 1980, to be referred to as I) we showed that for certain pure rotation point group–subgroup pairs one of the phase freedoms in the $3jm$ factors corresponds to a freedom in the orientation of the symmetry axes. In this paper we shall extend these results, both to point groups containing inversions or reflections and also to continuous groups.

Several interesting results and problems have emerged from this work. There appears to be no way to determine when orientation choices occur, short of actually calculating $3jm$ factors. In addition, there are cases where the groups have the same axes and mirror planes but do not have the same 'orientation', in the sense of having unity primitive transformation coefficients.

Our discussion of groups containing reflections or inversions is related to the work of Altmann and Herzig (1981). The properties of rotation–reflection and rotation–inversion groups may be obtained from the corresponding pure rotation groups but care is necessary in interpreting the effects of corresponding operations.

2. Orientation phase choices

Many phase and multiplicity separation choices must be made in the calculation of $6j$ symbols and $3jm$ factors. For some, but not all, group–subgroup pairs an orientation phase choice arises. This phase choice is distinguished from other $3jm$ choices in that a transformation between two sets of $3jm$ factors with different orientation choices requires primitive transformation factors which are not unity (see I, equation (3.2)). There appears to be no way of ascertaining the existence of such a choice without actually calculating the $3jm$ factors.

A distinction exists between the two sorts of orientation choice discussed in I: the 'continuous' (e.g. $D_3 \supset C_3$) and 'double root' (e.g. $T \supset D_2$) choices. The former are easily seen to be a freedom of the Racah–Wigner algebra, a result of Schur's lemmas. The latter are not, and are therefore more difficult to deal with.

Butler (1981) and Bickerstaff and Wybourne (1981) have given a detailed account of the phase freedoms of the Racah–Wigner algebra. For our purposes we divide the phase and multiplicity freedoms into coupling, branching and (continuous) orientation freedoms. The coupling freedoms occur in the calculation of $6j$ symbols. During the $6j$ calculation a set of basis triads emerges (essentially one per irrep). All other triads are fixed relative to this basis set by choosing the phases (and magnitudes in the case of multiplicity) of a set of basis $6j$ symbols. Once all phases are chosen, all other $6j$ follow recursively. The $3jm$ factors are calculated after the $6j$ of the group and the $6j$ of the subgroup. Again, once all phase and multiplicity choices are made, all other $3jm$ follow recursively. (Note that not one of our transformation coefficient calculations (see I) uses $3jm$ factors which contain coupling phase information.) A branching choice occurs for each non-primitive ket, and this is well understood, but in some cases an extra phase choice must be made, one we are calling the continuous orientation choice. The occurrence of a complex primitive irrep in the group or subgroup seems to be a necessary condition for the appearance of such a choice. It is not a sufficient condition however. SO_2 has a complex primitive but there is no orientation choice for $SO_3 \supset SO_2$. (It is clear from equation (58) of Butler (1976) that all $3jm$ choices for $SO_3 \supset SO_2$ are ket choices.)

Bickerstaff and Wybourne (1981) have argued that when one makes a continuous orientation choice one is fixing a relationship between basis triads (they call them 'product antecedents') of the group and subgroup. Because of this restriction a transformation between sets of $3jm$ factors with different orientation choices requires non-unity primitive transformation coefficients.

A continuous orientation choice occurs in the point group embeddings $D_n \supset C_n$, $D_{odd} \supset C_2$, $T \supset C_3$ and $C_{mn} \supset C_n$ (see table 1). However, the most striking example of this sort of choice occurs in the continuous group branching $SU_3 \supset SO_3$ (Bickerstaff *et al* 1982). If the phase of the $3jm$ factor

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}^{SU_3}_{SO_3} \tag{2.1}$$

is changed to

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}' = e^{i\theta}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \tag{2.2}$$

then from

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}' = \langle 11|11\rangle'\langle 11|11\rangle'\langle 11|11\rangle'\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}. \tag{2.3}$$

Table 1. Occurrence of orientation phase choices in subgroup chains of SO_3.

No orientation choice, no complex values necessary	$SO_3 \supset SO_2$, $SO_3 \supset D_\infty$, $SO_3 \supset K$, $SO_3 \supset O$, $D_\infty \supset C_\infty$, $D_\infty \supset D_n$, $D_{mn} \supset D_n$, $O \supset D_4$, $O \supset T$.
No orientation choice, complex values necessary	$K \supset D_3$.
Continuous orientation choice, no complex values necessary	$T \supset C_3$, $D_n \supset C_n$, $D_{odd} \supset C_2$, $C_{mn} \supset C_n$.
Double root orientation choice, complex values necessary	$K \supset T$, $K \supset D_5$, $O \supset D_3$, $T \supset D_2$.

(Butler 1975, equation (11.6)) one obtains (since $1^*(SU_3) = 1^2(SU_3)$)

$$\langle 11|11\rangle' = e^{-i\theta/3} = \langle 1^2 1|1^2 1\rangle^* \tag{2.4}$$

entirely analogous to the $D_3 \supset C_3$ example discussed in I. This can be explained by the basis triad concept. In choosing the phase of the $3jm$ factor we are relating the basis triad (111) of SU_3 to the basis triad (111) of SO_3 via the kets $|1(SU_3)1(SO_3)\rangle$. It is important to realise that we do not have a branching freedom for this $3jm$ because the ket $|1(SU_3)1(SO_3)\rangle$ is primitive. Orientation-type choices also occurred in the $SU_6 \supset SU_2 \times SU_3$ and $SU_3 \supset U_1 \times SU_2$ branchings considered in Bickerstaff *et al* (1982).

The 'double root' choices are not so straightforward. In these cases there is no Schur's lemma freedom left in the Racah–Wigner algebra but also no equations which fix the $3jm$ completely. Instead a double root occurs for one primitive $3jm$, both solutions leading to a consistent set of $3jm$ factors. In I we showed that the two roots in the $T \supset D_2$ calculation correspond to two orientations of a tetrahedron, $\pi/2$ apart. In that case the two tetrahedra had the same three-fold axes, though the character of a three-fold rotation about xyz was different for the two tetrahedra, equivalent to switching C_3 and C_3^{-1} in the character table. This may be determined by the methods discussed in § 5 of the present paper. In figure 2 of I we see that in one case xyz is through a vertex and in the other case through a face of the tetrahedron. This correspondence of operations is not a general property of double root choices. For example, the two roots for $O \supset D_3$ correspond to the two orientations shown in figure 1. In this case the two cubes have different four-fold axes, and therefore different irrep matrices, but the character table is the same. For maximal embeddings of rotation point groups a double root occurs only for $T \supset D_2$, $O \supset D_3$, $K \supset D_5$ and $K \supset T$. We know of no continuous group examples.

How the double root choice is related to labelling choices in the character tables of group and subgroup is unknown. Observe that while there are two distinct orientations of an icosahedron about a D_3 triangle (similar to $O \supset D_3$), and further that while certain $K \supset D_3$ $3jm$ are complex and appear at first sight to be a double root occurrence, no such choice exists as only one value satisfies the equations.

We have previously reported (Gruber and Millman 1980, pp 99–104) that the complex numbers in the $T \supset D_2$ calculation cannot be removed by changing the $3jm$ complex conjugation symmetries. (Damhus (1981) showed that it is possible to obtain real coefficients for the $T \supset C_3$ and the (non-maximal) $T \supset C_2$ embedding.) The $3jm$ for $O \supset D_3$, $K \supset D_5$ and $K \supset T$ also contain essentially complex double roots. The $K \supset D_3$ embedding is the only point group case where complex $3jm$ are necessary, but no double root, and hence no orientation choice, occurs (see table 1).

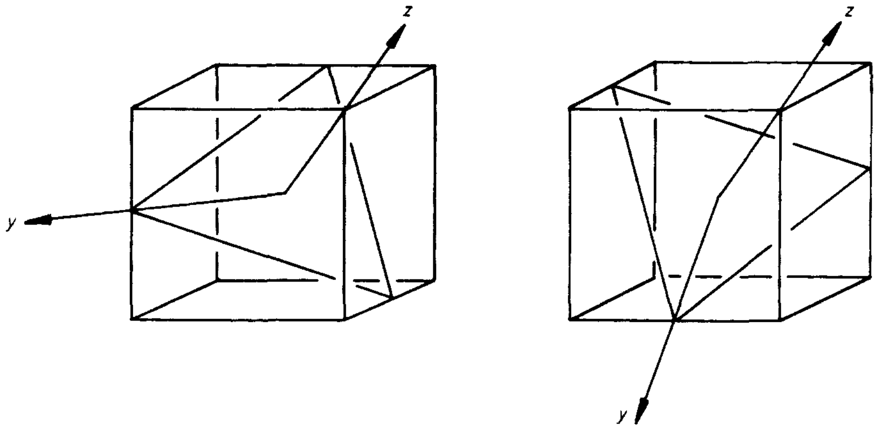

Figure 1. Orientations of $O \supset D_3$. The two orientations of the cube about a D_3 triangle are related by a $\pi/3$ rotation about the z axis. Though the cube has been drawn as fixed in the diagram it is the D_3 triangle which should be considered to be fixed since the $D_3 \supset C_3$ orientation choice fixes the two-fold axes of D_3 and the $O \supset D_3$ choice fixes the orientation of the other axes of O relative to these.

3. Transformation of odd-parity kets to the *JM* basis

In I we showed how to transform from pure rotation point group bases of SO_3 to the standard angular momentum basis $SO_3 \supset SO_2$ (the *JM* basis). Butler (1981) contains a complete set of such tables. The transformations between bases of O_3 may be easily determined from these pure rotation coefficients.

Of the thirty two point groups eleven are pure rotation groups. The rest are either direct products of a rotation group and the two element inversion group C_i (e.g. O_h, D_{4h}) or contain reflections but are isomorphic to a pure rotation group (e.g. $T_d \sim O$, $C_{4v} \sim D_4$). We denote the rotation–inversion groups G_i ($=C_i \times G$). Note that $O_3 = C_i \times SO_3$. The jm symbols for $G_i \supset H_i$ may be obtained directly from the tables for $G \supset H$.

For the rotation–reflection groups the j and jm symbols are just those of the pure rotation groups to which they are isomorphic. The only non-trivial cases are for a rotation–inversion group G_i containing a rotation–reflection group $\tilde{G}$, isomorphic to G. The branching rules are

$$\lambda^+(G_i) \to \lambda(\tilde{G}) \qquad (3.1)$$
$$\lambda^-(G_i) \to \tilde{\lambda}(\tilde{G})$$

where

$$\tilde{\lambda} = \lambda \times \varepsilon \qquad (3.2)$$

and ε is determined by

$$0^-(G_i) \to \varepsilon(\tilde{G}) \qquad (3.3)$$

The non-zero $3jm$ factors containing only even-parity irreps are unity and the rest are calculated by the methods of § 4 of Butler and Ford (1979) and are tabulated by Butler (1981).

To calculate transformation coefficients between an arbitrary point group basis of O_3 and the *JM* basis we note that the even-parity coefficients are the same as for the corresponding pure rotation chain. The pseudoscalar transformation coefficient $\langle 0^-(O_3)0(SO_2)|0^-(O_3)0^-(G_i)\varepsilon(\tilde{G})e(H)\rangle$ is real or imaginary, with a free sign, depending on the $2jm$ factor$(0^-0^-\varepsilon e)^T$, since

$$\langle 0^-0|0^-0^-\varepsilon e\rangle^* = \begin{pmatrix} 0^- \\ 0 \end{pmatrix}^* \langle 0^-0|0^-0^-\varepsilon e\rangle \begin{pmatrix} 0^- \\ 0^- \\ \varepsilon \\ e \end{pmatrix} \tag{3.4}$$

and $\binom{0^-}{0} = +1$.

(Butler (1981) overlooked this point and implies that the pseudoscalar coefficients are real. This was pointed out to us by Piepho (1981). In the $3jm$ tables of Butler (1981) the pseudoscalar $2jm$ have often been chosen -1 (e.g. $\binom{\tilde{0}}{0} = -1$ for all $D_n \supset C_n$), in order to have as many real $3jm$ factors as possible, see table 1.)

The odd-parity transformation coefficients are calculated by coupling the pseudoscalar kets to the even-parity kets, using $3jm$ factors (or coupling coefficients) to give:

$$\langle J^-M|J^-\lambda^-\tilde{\lambda}\tilde{l}\rangle = \langle J^+M|J^+\lambda^+\lambda l\rangle\langle 0^-0|0^-0^-\varepsilon e\rangle(-1)^{2J}|J|^{1/2} \begin{pmatrix} J^{-*} & J^+ & 0^- \\ \lambda^{-*} & \lambda^+ & 0^- \\ \tilde{\lambda}^* & \lambda & \varepsilon \\ \tilde{l}^* & l & e \end{pmatrix}^* \begin{pmatrix} J^- \\ \lambda^- \\ \tilde{\lambda} \\ \tilde{l} \end{pmatrix}. \tag{3.5}$$

Changing the sign of the pseudoscalar transformation coefficient has the effect of inversion, since it changes the sign of all odd-parity transformation coefficients. It is another choice of relative orientation of the group schemes, in addition to the choice of even-parity primitive transformation coefficient (I equation (3.2)). This extra choice is necessary because the irrep $\frac{1}{2}^+$ (O_3) is not faithful and therefore does not contain all the irreps of O_3 in its Kronecker powers. Instead, the irrep $\frac{1}{2}^- = \frac{1}{2}^+ \times 0^-$ is faithful. However, it is more convenient to attach the 0^- kets to the even-parity transformation coefficients than to build up the entire set from the $\frac{1}{2}^-$ transformation coefficients.

4. Cartesian basis functions

Transformations to the *JM* basis of O_3 are useful in constructing combinations of point group kets which transform as functions of x, y and z. For example, the electric dipole operator transforms as $1^-(O_3)$ and so the standard choice of spherical harmonics, namely,

$$|1^-(O_3)0(SO_2)\rangle = z \qquad |1^-(O_3)\pm 1(SO_2)\rangle = \mp\sqrt{\tfrac{1}{2}}\,(x \pm \mathrm{i}y) \tag{4.1}$$

can be used to construct combinations of point group kets which transform as various polarisations of the electric dipole operator. Cartesian expressions derived from our transformation coefficient tables have proved useful to the work of Churcher and Stedman (1981a, b) on Raman selection rules and Stedman and Minard (1981) on lattice strain, and are central to several discussions in Piepho and Schatz (1982).

5. Orientations of rotation–reflection groups

We can determine the orientation of axes and mirror planes of any selected point group-chain by transforming to the *JM* basis. The effect of rotations on *JM* kets is given by the rotation matrices (Messiah 1961, appendix C). If I is inversion, σ_h a reflection in the xy plane and σ_v a reflection in the xz plane, then we have

$$\begin{aligned} I|J^{\pm}M\rangle &= \pm|J^{\pm}M\rangle \\ \sigma_h|J^{\pm}M\rangle &= \pm(-1)^{M}|J^{\pm}M\rangle \\ \sigma_v|J^{\pm}M\rangle &= \pm(-1)^{J-M}|J^{\pm}-M\rangle. \end{aligned} \tag{5.1}$$

Reflections in other planes may be generated by rotating, reflecting and rotating back. Note that a reflection is the same as a rotation by π about an axis perpendicular to the mirror plane, followed by an inversion. For even-parity kets the inversion has no effect.

One must be careful about which groups are being considered when drawing diagrams. For example, our $3jm$ tables make an orientation choice for $D_3 \supset C_3$ so that the y axis is a two-fold axis (see I, equation (4.11)). The D_3 operations will then transform the triangle in figure 2 into itself. If we consider instead $C_{3v} \supset C_3$ the xz plane is a mirror plane and so C_{3v} transforms a different triangle into itself (figure 3). Altmann and Herzig (1981, figures 1(*b*) and 2 and equation (6.1)) make similar observations. Note that we do not need to consider odd-parity kets to determine the orientation of mirror planes.

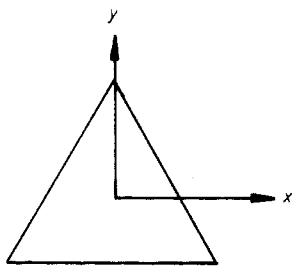

Figure 2. Orientation of D_3. Here the y axis is a two-fold axis.

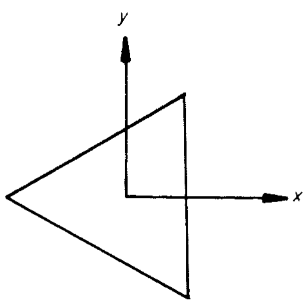

Figure 3. Orientation of C_{3v}. Here the xz plane is a mirror plane.

6. Characters of representations

The character of irreps under the symmetry operations may be determined by transforming to the *JM* basis and using the rotation matrices and the reflection operators discussed in the previous section. Alternatively, we can by-pass the *JM* basis by generating a set of rotated transformation coefficients. We have shown that choosing a particular relationship between the primitive transformation coefficients corresponds to a rotation of the axes (I equation (3.3)). If the group schemes and phase choices are identical then the transformation coefficients are precisely the matrix elements of the operation and hence the characters (traces) may be determined directly. This is analogous to the usual construction of $SO_3 \supset SO_2$ rotation matrices (Messiah 1961, equation (C70)).

Consider the $D_3 \supset C_3$ example of I. We can choose

$$\langle \tfrac{1}{2}(D_3)\, \tfrac{1}{2}(C_3) | \tfrac{1}{2}(D_3)\, \tfrac{1}{2}(C_3)\rangle' = e^{i\alpha/2} = \langle \tfrac{1}{2} - \tfrac{1}{2} | \tfrac{1}{2} - \tfrac{1}{2}\rangle' \tag{6.1}$$

corresponding to a rotation of the primed kets by an angle α about z (this is misprinted in I as $\alpha/2$ at the bottom of p 2893). We then find that

$$\langle \tfrac{3}{2}\,\tfrac{3}{2} | \tfrac{3}{2}\,\tfrac{3}{2}\rangle' = \tfrac{1}{2}(e^{-3i\alpha/2} + e^{3i\alpha/2}) \tag{6.2}$$

(from I equation (4.13), with the same orientation choice for both kets). For $\alpha = 2\pi/3$ we have the matrix element, and hence the character, -1, consistent with the D_3 character table of I. Note that a rotation which is not a multiple of $2\pi/3$ is not allowed and the coefficient will become unnormalised if such a rotation is attempted.

7. Coincidence of groups

With the above tools for finding axes and mirror planes, we return to a study of the orientation questions. In this section we show that coincidence of the axes and mirror planes of the group is not sufficient to guarantee that the primitive transformation coefficients between two sets of $3jm$ factors (with different orientation choices or symmetrised with respect to different subgroup schemes) can be chosen unity. This is immediately apparent in the $D_3 \supset C_3$ example discussed above. A $\pi/3$ rotation about the z axis brings the two-fold axes into coincidence but, as we showed in I, a change in orientation phase equivalent to a rotation which is a multiple of $2\pi/3$ (i.e. a symmetry operation of D_3) is necessary if one wants to have unity primitive transformation coefficients.

The situation is even more complex if we wish to consider transformations between the bases of a group, symmetrised with respect to different subgroups. In general such transformations require non-unity primitive transformation coefficients because in general a rotation is needed to bring the axes into coincidence. Obviously the transformation from, for example, $O \supset D_3 \supset C_3$ to $O \supset D_4 \supset C_4$ requires a rather complicated rotation because in the first case the z axis is through a corner and in the second case a face of the cube. Even when the z axes are the same, such as for $D_4 \supset C_4$ and $D_4 \supset D_2 \supset C_2$, a rotation is needed unless the orientation phases are chosen appropriately.

For rotation–reflection groups the situation is complicated by the existence of a sign choice for the pseudoscalar transformation coefficients. This sign choice is another choice of relative orientation of the two schemes, in addition to the choice of even-parity primitive transformation coefficients (see § 3), and has the effect of inversion.

Consider the following example. The phase choices of Butler (1981) are such that we can transform between the schemes $D_4 \supset C_4$ and $D_4 \supset D_2 \supset C_2$ with unity primitive transformation coefficients and therefore, by isomorphism, between $D_{2d} \supset S_4$ and $D_{2d} \supset C_{2v} \supset C_2$. However, since the transformation coefficient

$$\langle 2(D_{2d})2(S_4)|2(D_{2d})0(C_{2v})0(C_2)\rangle = -1 \qquad (7.1)$$

care must be taken if the chains $D_{4h} \supset D_{2d} \supset S_4$ and $D_{4h} \supset D_{2d} \supset C_{2v} \supset C_2$ are considered. The transformation between these schemes contains the even-parity coefficient (identical to (7.1))

$$\langle 2^+(D_{4h})2(D_{2d})2(S_4)|2^+(D_{4h})2(D_{2d})0(C_{2v})0(C_2)\rangle = -1 \qquad (7.2)$$

and the pseudoscalar

$$\langle 0^-22|0^-200\rangle = \pm 1. \qquad (7.3)$$

The pseudoscalar coefficient is real because of the $2jm$ choices. If it is chosen to be $+1$ then application of the Racah factorisation lemma gives an apparent contradiction because if we attempt to factorise out the $D_{4h} \supset D_{2d}$ transformation factors we obtain two different signs for $\langle 2(D_{2d})2(S_4)|2(D_{2d})0(C_{2v})0(C_2)\rangle$, one for each of equations (7.2) and (7.3). This shows that the two D_{2d} groups are not identical, even though both have axes and mirror planes in the same places.

If we desire factorisation we have several options. The $3jm$ choices can be changed to reverse the sign in equation (7.2). Another option is to rotate by $\pi/2$ about z, which is accomplished by a suitable choice of the primitive coefficients (i.e. those transforming as $\frac{1}{2}^+$ (D_{4h})). This rotation has no effect on the pseudoscalar (equation (7.3)), but changes equation (7.2) to

$$\langle 2^+22|2^+200\rangle = +1. \qquad (7.4)$$

Finally, we can obtain factorisation by changing the sign of the pseudoscalar transformation coefficient. This changes the sign of all odd-parity transformation coefficients and is equivalent to an inversion. Note that all of these changes result in D_{2d} groups with axes and mirror planes in the same place.

8. Conclusions

The building up method brings to the fore the question of the number and meaning of the free phases in the Racah–Wigner algebra. All continuous phase freedoms are easily understood in terms of Schur's lemmas. All $6j$ choices relate triads to basis triads and most $3jm$ choices relate kets to the primitive ket, and neither type has an effect on orientation. Sometimes a continuous phase freedom in the $3jm$ arises, which links basis triads in group and subgroup, and this affects the orientation. Double root orientation choices are not a result of Schur's lemmas.

In our first paper we pointed out the existence of orientation phases and gave some examples. Here we have extended the work to all point groups and some continuous groups, and pointed out that we cannot predict the existence of orientation choices for other groups without detailed study of the $3jm$ factors. We have also observed that identical orientation of the symmetry axes and mirror planes of the group schemes does not guarantee that the groups are identical. Identical groups are required for applications of Schur's lemma, such as the Wigner–Eckart theorem or the Racah factorisation lemma.

It may appear that our rather lengthy discussion of axes and bases has removed the main advantage of the building up method—that one only needs character theory results in order to calculate $3jm$ and $6j$. This is not the case. The calculations are still done using only the equations which arise from the Racah–Wigner algebra and this discussion demonstrates that while the orientation structure of point group chains is subtle we can always deduce the information that is necessary for a particular application directly from the tables of $3jm$ factors.

However, many applications require no basis information. For example the multi-quark hadron dissociation calculations of Bickerstaff and Wybourne (1981) require only a consistent set of $3jm$ and $6j$. Other calculations may require information such as the transformation properties of various orientations of an electric or magnetic field, that is, only bases for $1^{\pm}(O_3)$. We have shown how these properties may be deduced.

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