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3-*jm*, 6-*j* and isoscalar symbols for the icosahedral group

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Abstract. Using a complex base with a numerical system of labelling we calculate symmetrised coupling symbols (the 3-*jm* symbols) for the icosahedral group. We make full use of Racah's Lemma and explicitly state all the phase standardisations involved. The 3-*jm* symbols are chosen in a manner that leads to them possessing reordering symmetries that are almost as straightforward as in the case of SO(3). We state the basic isoscalars and use the 3-*jm*'s to obtain invariant 6-*j* symbols.

1. Introduction

In this paper we study coupling theory for the icosahedral group (I). This is the symmetry group of the icosahedron and of the dodecahedron. Coupling theory has been developed for this group before (Golding 1973) but we feel that our approach leads to coupling symbols in a form that is substantially easier to use. We repeat the earlier work in an improved notation (due to McLellan 1961) and with explicitly stated phase standardisations for both I and SO(3). Certain unconventional features of Golding's theory (attaching *J* labels to irreducible representations of I for example) are removed. In addition, we calculate the 6-*j* symbols and give the isoscalar factors for the basic irreps. A detailed discussion of the relationship between this paper and Golding (1973) is given in § 5.1.

The motivation for undertaking this work has been the recent work of Khlopin *et al* (1978). They show that Jahn–Teller models with continuous symmetries can be set up for icosahedral symmetry by the judicious selection of coupling strengths. This is an analogous situation to that known to exist for octahedral symmetry (Pooler 1978).

There exist several systems which possess exact or approximate icosahedral symmetry. For example, in crystalline boron carbide ($B_{12}C_3$) the twelve boron atoms form a nearly regular icosahedron. This was discovered by Zdanov and Sevastianov (1941), who used x-ray diffraction techniques, and confirmed by Clark and Hoard (1943). A summary of the properties of boron carbide can be found in Durrant and Durrant (1970).

Also there exist rare-earth double nitrates in which a rare-earth ion is surrounded by twelve oxygen atoms located almost exactly at the vertices of a regular icosahedron. Such an ion can be treated as though it were acted on by a crystal field of icosahedral symmetry instead of the real field of C_{3v} symmetry (see Judd 1955, 1957). The systems in which this would seem to be a good approximation do, however, involve half-integer irreps.

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For other examples of icosahedral symmetry see the references in Khlopin *et al* (1978). A Klug, in a private communication to Cohan (1958), has stated that certain proteins have icosahedral symmetry.

In order to be able to construct a coupling theory for the icosahedral group we need to know some details of the group, and in particular, of its representation theory. The group has five integer irreducible representations (irreps) (an integer irrep is one that is equivalent to a real one). There are several notations in use for the irreps. The notation used here is given in the first column of table 1 together with alternatives (in parentheses). The second column gives the dimensionality [ ] of each irrep and the rest of the table the non-trivial Kronecker products for the group with the symmetric parts of the squares given in square brackets. Repeated irreps occur in Kronecker squares and therefore the group is not simply reducible, although it possesses only real characters.

In the following section we set up a basis of 'kets' that are irreducible under both SO(3) and I. These are expressed in terms of SO(3) ⊃ SO(2) vectors with stated phase standardisations. The basis states are chosen to have simple time reversal properties. A numerical labelling is selected following McLellan (1961) because that leads to ease of application. In § 2.2 we state Racah's Lemma, which will be used to arrive at icosahedral coupling, and define isoscalar factors. There we also give the connection between icosahedral coupling coefficients and the related symmetrised symbols (the 3-*jm* symbols).

In § 3.1 we show how we can define 3-*jm* symbols that have reordering symmetries which are almost as straightforward as those for SO(3) and in § 3.2 we discuss the labelling of repeated irreps. Then in § 3.3 we see how our choice of 3-*jm* properties limits the phase freedom in the definition of the isoscalar factors. Then we state the symmetry of the 3-*jm* symbols under complex conjugation. We then know enough to calculate the 3-*jm* symbols (§ 3.5) which are tabulated in table 3. In § 4 we use the 3-*jm*'s to evaluate 6-*j* symbols and discuss their properties. In the final section (§ 5) we discuss the relation of Golding's (1973) work (§ 5.1), discuss questions of reality (§ 5.2) and summarise the paper (§ 5.3).

2. The group chain SO(3) ⊃ I

2.1. *An* SO(3) ⊃ I *basis*

It is economical to make full use of SO(3) when setting up coupling theory for point groups. Coupling for SO(3) is known and that of I can be found using Racah's Lemma. While doing this it is important to bear in mind the difference between an SO(3) property and a subgroup property. The permutation symmetry of a triple of irreps of the subgroup is an example of the latter type of property. A triple of irreps $(\Gamma_1\Gamma_2\Gamma_3\beta)$ has the defining property that the Kronecker product of any two of the irreps (found from table 1) contains the third irrep of type β. Before using Racah's Lemma it is necessary to specify the phase standardisations to be used in SO(3) and I.

First we choose standard irreps. We do this by specifying bases. This involves two phase choices. We must specify the representation matrices and the connection between conjugate irreps (these are equivalent representations of both groups). For the rotation group we choose the representation matrices of Wigner (1959 ch 15) and the 1-*jm* (or 1-*j* or 2-*jm*) which connects conjugate irreps to be

$$(j)_{mm'} = (-1)^{j-m}\delta(m, -m'). \qquad (2.1.1a)$$

Table 1. The Kronecker products for the icosahedral group. This table also serves to summarise the notations for icosahedral irreps.

Irrep(Γ)	Dimension $[\Gamma]$	Product with T_1	T_2	G	H
$A(\Gamma_1)$	1	T_1	T_2	G	H
$T_1(\Gamma_2$ or $F_1)$	3	$A+[T_1]+H$	$G+H$	T_2+G+H	T_1+T_2+G+H
$T_2(\Gamma_3$ or $F_2)$	3		$A+[T_2]+H$	T_1+G+H	T_1+T_2+G+H
$G(\Gamma_4$ or $U)$	4			$A+[T_1+T_2]+G+H$	T_1+T_2+G+2H
$H(\Gamma_5$ or $V)$	5				$A+[T_1+T_2+G]+G+2H$

For the definition of 1-*jm* symbol see Wigner (1940 p 106) or Butler (1975 p 549). j and m have their usual meanings. Equation (2.1.1*a*) implies that the effect of the time reversal operator θ on SO(3) bases kets is

$$\theta|jm\rangle \equiv |\bar{j}m\rangle = (-1)^{j+m}|j-m\rangle \tag{2.1.1b}$$

where $\bar{j}$ stands for the complex conjugate irrep. McLellan (1961) has chosen bases of SO(3) that are also standardised with respect to I:

$$|Jc\Gamma\gamma\rangle = \sum_m C(Jmc\Gamma\gamma)|Jm\rangle \tag{2.1.2}$$

where the detailed definitions are to follow. c distinguishes between repeated icosahedral group irreps within a given SO(3) one. It is not required for the low J irreps and we drop it. $C(Jm\Gamma\gamma)$ form a unitary matrix. As some are not real the form of equations (2.1.1) is not preserved by this transformation. The basis (2.1.2) could be chosen to be real but we see no advantage in so doing and the use of the complex base leads to a more compact notation (examine table 2, for example). We discuss this point in slightly more detail in § 5.2. Here we choose the basis so that we have the representation matrices given in McLellan (1961 § 3). The effect of time-reversal is specified by requiring

$$C(J-m\Gamma-\gamma) = (-1)^{J+m}\bar{C}(Jm\Gamma\gamma) \tag{2.1.3}$$

which implies, using equation (2.1.1*b*),

$$\theta|\Gamma\gamma\rangle \equiv |\bar{\Gamma}\gamma\rangle = |\Gamma-\gamma\rangle \tag{2.1.4}$$

where we have made a particular choice of numerical label as listed in table 2 (due to McLellan 1961). Note that if we extended our considerations to the double icosahedral group I* then, keeping to McLellan's labelling,

$$\theta|\Gamma\gamma\rangle = \begin{cases} |\Gamma-\gamma\rangle, & \gamma>0 \\ -|\Gamma-\gamma\rangle, & \gamma<0 \end{cases}$$

where equation (2.1.3) is now only for positive γ. Equation (2.1.4) can be expressed in terms of a 1-*jm* symbol:

$$(\bar{\Gamma})_{\gamma'\gamma} = (\Gamma)_{\gamma'\gamma} = \delta(\gamma', -\gamma).$$

The above standardisations specify the required basis up to a phase factor for each irrep.

In order to have the usual relationship between 3-*jm*'s and 1-*jm*'s,

$$[\Gamma]^{1/2}\begin{pmatrix}\Gamma & \Gamma & A\\ \gamma' & \gamma & 0\end{pmatrix}=(\Gamma)_{\gamma'\gamma}$$

and isoscalars involving A positive we need $|A\ 0\rangle=+|0\ 0\rangle$ and because of the requirement (2.1.4) the phases have to be real, but are otherwise arbitrary. To specify I coupling totally we need only consider those bases that involve the following branching laws, expressed in the form $J\to\Sigma\Gamma$:

$0\to A,\qquad 1\to T_1,\qquad 2\to H,\qquad 3\to T_2\oplus G\qquad$ and $\qquad 4\to H\oplus G.$

The bases with these phases chosen are given in table 2; they correspond in phase to those of Golding (1973). We include a note of Golding's notation which is harder to use. They differ in the sign of $|4G\gamma\rangle$ from McLellan's (1961). We note that Cohan (1958) has also produced an SO(3) ⊃ I basis.

Table 2. A complex basis standardised according to the group chain SO(3) ⊃ I.

In Golding's (1973) notation	SO(3) ⊃ I state	Linear combinations of $\|jm\rangle$ states
$\|0\ A\ a\rangle$	$\|0\ A\ 0\rangle$	$\|0\ 0\rangle$
$\|1\ T_1\ \pm1\rangle$	$\|1\ T_1\ \pm1\rangle$	$-\|1\ \pm1\rangle$
$\|1\ T_1\ 0\rangle$	$\|1\ T_1\ 0\rangle$	$\mathrm{i}\|1\ 0\rangle$
$\|2\ V\ \pm2\rangle$	$\|2\ H\ \pm2\rangle$	$-\|2\ \pm2\rangle$
$\|2\ V\ \pm1\rangle$	$\|2\ H\ \pm1\rangle$	$\mathrm{i}\|2\ \pm1\rangle$
$\|2\ V\ 0\rangle$	$\|2\ H\ 0\rangle$	$\|2\ 0\rangle$
$\|3\ T_2\ \mp1\rangle$	$\|3\ T_2\ \pm2\rangle$	$-(2/5)^{1/2}\|3\mp3\rangle-(3/5)^{1/2}\,\mathrm{i}\|3\ \pm2\rangle$
$\|3\ T_2\ 0\rangle$	$\|3\ T_2\ 0\rangle$	$\mathrm{i}\|3\ 0\rangle$
$\|3\ U^{\nu}_{\kappa}\rangle$	$\|3\ G\ \pm2\rangle$	$(3/5)^{1/2}\|3\mp3\rangle-(2/5)^{1/2}\,\mathrm{i}\|3\ \pm2\rangle$
$\|3\ U^{\lambda}_{\mu}\rangle$	$\|3\ G\ \pm1\rangle$	$\|3\ \pm1\rangle$
$\|4\ U^{\nu}_{\kappa}\rangle$	$\|4\ G\ \pm2\rangle$	$\mp(1/15)^{1/2}\|4\mp3\rangle\pm(14/15)^{1/2}\,\mathrm{i}\|4\ \pm2\rangle$
$\|4\ U^{\lambda}_{\mu}\rangle$	$\|4\ G\ \pm1\rangle$	$\pm(8/15)^{1/2}\,\mathrm{i}\|4\mp4\rangle\pm(7/15)^{1/2}\|4\ \pm1\rangle$
$\|4\ V\ \pm2\rangle$	$\|4\ H\ \pm2\rangle$	$(14/15)^{1/2}\,\mathrm{i}\|4\mp3\rangle-(1/15)^{1/2}\|4\ \pm2\rangle$
$\|4\ V\ \pm1\rangle$	$\|4\ H\ \pm1\rangle$	$-(7/15)^{1/2}\|4\mp4\rangle-(8/15)^{1/2}\,\mathrm{i}\|4\ \pm1\rangle$
$\|4\ V\ 0\rangle$	$\|4\ H\ 0\rangle$	$\|4\ 0\rangle$

2.2. *Coupling for* SO(3) ⊃ I *and Racah's Lemma*

We have not yet specified the phase connection that we are going to use for SO(3) coupling. As it is frequently used we decided on the Condon and Shortley (1970) phase convention which means that in terms of the 3-*jm* symbols of Rotenberg *et al* (1959) we have as coupling coefficient for SO(3) in the SO(3) ⊃ SO(2) base

$$\langle J_1m_1;J_2m_2|J_m\rangle=(-1)^{J_2-J_1-m}(2J+1)^{1/2}\begin{pmatrix}J_1 & J_2 & J\\ m_1 & m_2 & -m\end{pmatrix}. \qquad (2.2.1)$$

Changing to the SO(3) ⊃ I base (2.1.2) we obtain coupling coefficients in that base:

$$\langle J_1\Gamma_1\gamma_1;J_2\Gamma_2\gamma_2|J\Gamma\gamma\rangle$$
$$=\sum_{m_1m_2m}\bar{C}(J_1m_1\Gamma_1\gamma_1)\bar{C}(J_2m_2\Gamma_2\gamma_2)C(Jm\Gamma\gamma)\langle J_1m_1;J_2m_2|Jm\rangle \qquad (2.2.2)$$

where we have omitted the multiplicity label c. Then by Racah's Lemma (see Racah (1949) for original SO(3) derivation and Wybourne (1974 § 19.14) for a discussion of the generalisation to other groups) for low J,

$$\langle J_1\Gamma_1\gamma_1; J_2\Gamma_2\gamma_2|J\Gamma\gamma\rangle = \sum_\beta \langle J_1\Gamma_1; J_2\Gamma_2| |J\Gamma\rangle_\beta \langle\Gamma_1\gamma_1; \Gamma_2\gamma_2|\beta\Gamma\gamma\rangle \tag{2.2.3}$$

where $\langle\Gamma_1\gamma_1; \Gamma_2\gamma_2|\beta\Gamma\gamma\rangle$ is an icosahedral coupling coefficient, β is a multiplicity label distinguishing between equivalent Γ's in $\Gamma_1\otimes\Gamma_2$ and the component independent factor $\langle J_1\Gamma_1; J_2\Gamma_2| |J\Gamma\rangle_\beta$ is known as an isoscalar factor. The isoscalars are real as is shown in § 3.4. When there is only one way of constructing a Γ state from J_1 and J_2 states the isoscalar factor reduces to a phase.

The above series of equations specifies the icosahedral coupling coefficients $\langle\Gamma_1\gamma_1; \Gamma_2\gamma_2|\beta\Gamma\gamma\rangle$ up to a phase factor between the isoscalars and the coupling coefficients. This is arbitrary unless we fix a relationship between the coupling coefficients and a symmetric 3-*jm* symbol (see Butler 1975 § 5). If the 3-*jm* symbols have the usual properties (listed in § 3) we have only one phase per triple left which we use to have as many positive isoscalars as possible. We decide on the so-called sensible phase convention:

$$\langle\Gamma_1\gamma_1; \Gamma_2\gamma_2|\beta\Gamma\gamma\rangle = [\Gamma]^{1/2}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma\\ \gamma_1 & \gamma_2 & -\gamma\end{pmatrix}^\beta \tag{2.2.4}$$

where $\beta = 1$ or 2.

Racah's Lemma (2.2.3) could be expressed in terms of 3-*jm* symbols for SO(3) and I. This would lead naturally to another type of isoscalar factor (see Butler 1975 § 13):

$$\begin{pmatrix}J_1 & J_2 & J\\ \Gamma_1 & \Gamma_2 & \Gamma\end{pmatrix}^\beta = \frac{[\Gamma]^{1/2}}{[J]^{1/2}}(-1)^{J+J_1-J_2}\langle J_1\Gamma_1; J_2\Gamma_2| |J\Gamma\rangle_\beta. \tag{2.2.5}$$

The phase factor arises from the use of the 'non-sensible' Condon and Shortley phase. It is easier to expand coupled kets and pick out coupling symbols directly (see example in § 3.5) rather than find SO(3) 3-*jm*'s in the SO(3) $\supset$ I basis with the aid of

$$\begin{pmatrix}J_1 & J_2 & J\\ \Gamma_1\gamma_1 & \Gamma_2\gamma_2 & \Gamma\gamma\end{pmatrix} = \sum_{m_1 m_2 m} \bar{C}(J_1m_1\Gamma_1\gamma_1)\bar{C}(J_2m_2\Gamma_2\gamma_2)\bar{C}(Jm\Gamma\gamma)\begin{pmatrix}J_1 & J_2 & J\\ m_1 & m_2 & m\end{pmatrix}$$

and then find the isoscalars of type (2.2.5). Also working with coupling coefficients means that orthonormality can be checked at a glance. For these two reasons the actual calculation is performed in terms of coupling coefficients and then conversion is made to 3-*jm* symbols. In table 4 we give the values of both types of isoscalars for low J.

3. The isosahedral 3-*jm* symbols

3.1. Reordering symmetries

Before evaluating the icosahedral 3-*jm* symbols we discuss the symmetries that we require them to possess together with the phase freedom that allows these requirements to be met. Firstly, we note that if we reorder the columns of a general 3-*jm* symbol then it is multiplied by a unitary matrix:

$$\begin{pmatrix}\Gamma_{\pi(1)} & \Gamma_{\pi(2)} & \Gamma_{\pi(3)}\\ \gamma_{\pi(1)} & \gamma_{\pi(2)} & \gamma_{\pi(3)}\end{pmatrix} = \sum_{\beta'} m(\pi\Gamma_1\Gamma_2\Gamma_3)_{\beta\beta'}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}^{\beta'},$$

π being a permutation of (123). For a general discussion of reordering symmetries see, for example, Butler (1975 § 6). For a simply reducible group m reduces to a phase which can be chosen to be +1 for even permutations and $(-1)^{\Gamma_1+\Gamma_2+\Gamma_3}$ for odd permutations, where $(-1)^{\Gamma}$ is a number of modulus one defined for each Γ. In the case of the icosahedral group we can choose phases to make the symmetries as simple for all but one triple. A similar situation occurs in octahedral double-group coupling theory (Harnung 1973).

In the approach used in this paper the phase freedom used to obtain maximally symmetric 3-*jm* symbols is that of the isoscalars. Often no such freedom exists. An obvious example is a 3-*jm* symbol involving only one irrep. For such symbols we must, in general, choose $m(\pi)$ according to whether the identity occurs in the symmetric, antisymmetric or mixed symmetry part of $\Gamma\otimes\Gamma\otimes\Gamma$. If a mixed symmetry part exists, then we cannot diagonalise $m(\pi)$ for all π. For a finite group we can ascertain this by ascertaining whether

$$\sum_R \chi^{(\Gamma)}(R)^3 = \sum_R \chi^{(\Gamma)}(R^3) \tag{3.1.1}$$

where $\chi^{(\Gamma)}(R)$ is the character of the element R. For the icosahedral group equation (3.1.1) is true for all irreps which means that there are no mixed-symmetry subspaces. (Such groups are called simple phase groups.) This implies that the rule for the triples $(\Gamma\Gamma\Gamma\beta)$ is the same as for the triples of form $(\Gamma\Gamma\Gamma'\beta)$, namely, that the matrix $m(\pi)$ can be chosen diagonal and that it must be $+\delta_{\beta\beta'}$ for even permutations and $\pm\delta_{\beta\beta'}$ for odd ones according to whether Γ' chosen in the βth manner is in the symmetric or antisymmetric part of $\Gamma\otimes\Gamma$ respectively. If all the irreps involved are different then we can make $m(\pi)_{\beta\beta'}=\delta_{\beta\beta'}$ but we choose to make it $\pm\delta_{\beta\beta'}$ for odd π so that m resembles the familiar simply reducible version as closely as possible.

We can summarise our choices as follows. First, we define

$$(-1)^{\Gamma} = \begin{cases} +1, & \text{if } \Gamma \text{ is in the symmetric part of } \Gamma\otimes\Gamma \\ -1, & \text{if } \Gamma \text{ is in the antisymmetric part of } \Gamma\otimes\Gamma \end{cases}$$

which means that

$$(-1)^{\Gamma} = \begin{cases} +1 & \text{for } \Gamma = A, G \text{ or } H \\ -1 & \text{for } \Gamma = T_1 \text{ or } T_2. \end{cases} \tag{3.1.2}$$

Then according to the discussion in the preceding paragraph $m_{\beta\beta'}=(-1)^{\Gamma_1+\Gamma_2+\Gamma_3}\delta_{\beta\beta'}$ except for the triple (HHG1). This is because G occurs in the symmetric and in the antisymmetric part of $H\otimes H$. We use the multiplicity label 1 for the antisymmetric case (this is because G occurs first in $J=3$ which is an odd irrep of SO(3)—see§ 3.2 for a fuller discussion of our choice of multiplicity labels). Apart from G, irreps either always occur in the symmetric part of squares or always in the antisymmetric. Thus the reordering symmetries of the 3-*jm* symbols are

$$\begin{pmatrix} \Gamma_2 & \Gamma_1 & \Gamma \\ \gamma_2 & \gamma_1 & \gamma \end{pmatrix}^{\beta} = (-1)^{\Gamma_1+\Gamma_2+\Gamma}(-1)^{q(\Gamma_1\Gamma_2\Gamma_3\beta)}\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}^{\beta} \tag{3.1.3}$$

where $(-1)^{q(\Gamma_1\Gamma_2\Gamma_3\beta)}$ equals -1 if $(\Gamma_1\Gamma_2\Gamma_3\beta)$ is any permutation of (HHG1) and +1 otherwise. This equation is a mnemonic of the symmetry.

3.2. *Multiplicity*

In order to calculate the icosahedral coupling symbols we shall couple together two states to form a third which transforms in the standard way under I. That is in the way that all states belonging to that irrep in table 2 do. We treat multiplicity by choosing repeated irreps to transform in different ways under SO(3). First, we choose the vectors to be coupled to have the lowest J values that give a non-vanishing result. Then we take the resultant to have all the available J values. These states must necessarily be orthogonal and they form the repeated irreps. We number these in order of increasing J. For the above cases we choose isoscalar phases to give the symmetry properties mentioned in § 3.1. Once we have covered one order of each triple then all other symbols are fixed. This procedure gives a consistent labelling of repeated irreps. We may not label arbitrarily because of the requirements imposed by the 3-*jm* reordering symmetries. For example, $(HHG1)$ means that we have coupled $2H$ to $2H$ to form $3G$ and $(HGH1)$ that we have coupled $2H$ to $3G$ to form $2H$ whereas $(HHG2)$ refers to $2H$ coupled to $2H$ to give $4G$ and $(HGH2)$ to $2H$ coupled with $3G$ to give $4H$.

3.3. *Isoscalar phases*

By choosing symmetric 3-*jm* symbols (carried out in § 3.2) and by fixing the relation between coupling coefficients and 3-*jm* symbols we have implicitly chosen most of the isoscalar symbol phases. We may still choose one basic isoscalar to be positive for each triple (a basic isoscalar is one used in the calculation of the coupling symbols for I—all others are fixed).

For triples consisting of three equivalent irreps we choose to have the isoscalar positive (that is $\langle J_1\Gamma; J_1\Gamma| |J\Gamma\rangle_\beta \geqslant 0$). If we have only two equivalent irreps then we make $\langle J_1\Gamma; J_1\Gamma| |J\Gamma'\rangle_\beta$ positive. If all irreps are inequivalent then we could choose to have all isoscalars positive corresponding to the fact that we could have $m(\pi)_{\beta\beta'} = \delta_{\beta\beta'}$. Having chosen $m_{\beta\beta'} = (-1)^{\Gamma_1+\Gamma_2+\Gamma}(-1)^{q(\Gamma\Gamma\Gamma\beta)}\delta_{\beta\beta'}$ we can only choose one positive—we choose those with $(\Gamma_1\Gamma_2\Gamma) = (T_2GT_1)$, (T_2HT_1), (GHT_1) and (T_2GH).

The remaining isoscalars are fixed by our choice of reordering symmetries (3.1.3) and of the relation between coupling coefficients and 3-*jm* symbols. These choices lead to the following connections between isoscalars:

$$\langle J_2\Gamma_2; J_1\Gamma_1| |J\Gamma\rangle_\beta = (-1)^{J_1+J_2+J}(-1)^{\Gamma_1+\Gamma_2+\Gamma}(-1)^{q(\Gamma_1\Gamma_2\Gamma\beta)}\langle J_1\Gamma_1; J_2\Gamma_2| |J\Gamma\rangle_\beta \qquad (3.3.1a)$$

and

$$\langle J\Gamma; J_2\Gamma_2| |J_1\Gamma_1\rangle_\beta = (-1)^{J_1+J_2+J}(-1)^{\Gamma_1+\Gamma_2+\Gamma}(-1)^{q(\Gamma_1\Gamma_2\Gamma\beta)}\left(\frac{[J_1][\Gamma]}{[\Gamma_1][J]}\right)^{1/2}\langle J_1\Gamma_1; J_2\Gamma_2| |J\Gamma\rangle_\beta. \qquad (3.3.1b)$$

The latter relation is known as reciprocity for isoscalars (see Wybourne (1974) pp 248–9). One could equally work in terms of symmetrised isoscalars, in which case (3.3.1) becomes

$$\begin{pmatrix} J_1 & J & J_2 \\ \Gamma_1 & \Gamma & \Gamma_2 \end{pmatrix}^\beta = (-1)^{J_1+J_2+J}(-1)^{\Gamma_1+\Gamma_2+\Gamma}(-1)^{q(\Gamma_1\Gamma_2\Gamma\beta)}\begin{pmatrix} J_1 & J_2 & J \\ \Gamma_1 & \Gamma_2 & \Gamma \end{pmatrix}^\beta.$$

3.4. *Conjugation of symbols*

Another 'symmetry' of the 3-*jm* symbols follows from the fact that raising all components of a 3-*jm* symbol is equivalent to complex conjugation

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ -\gamma_1 & -\gamma_2 & -\gamma \end{pmatrix} = \overline{\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix}}, \tag{3.4.1}$$

which implies that

$$\langle \Gamma_1 - \gamma_1; \Gamma_2 - \gamma_2 | \Gamma - \gamma \rangle_\beta = \overline{\langle \Gamma_1 \gamma_1; \Gamma_2 \gamma_2 | \Gamma \gamma \rangle_\beta}.$$

This means that we need only couple to form states with positive components in order to obtain all the symbols. Condition (2.1.3) means that

$$\langle J_1 \Gamma_1 - \gamma_1; J_2 \Gamma_2 - \gamma_2 | J \Gamma - \gamma \rangle_\beta = \overline{\langle J_1 \Gamma_1 \gamma_1; J_2 \Gamma_2 \gamma_2 | J \Gamma \gamma \rangle_\beta}$$

which implies that the isoscalars are real—something we have assumed so far.

3.5. Calculation of the 3-jm symbols

We are now in a position to use Racah's Lemma to find the icosahedral 3-*jm* symbols. The following procedure is followed for one order of each triple and for positive γ. The symmetry relations give all the symbols not evaluated in this process. First we form, using the bases given in table 2,

$$|(J_1 J_2) J \Gamma \gamma\rangle = \sum_{m m_1 m_2} C(Jm\Gamma\gamma) \langle J_1 m_1; J_2 m_2 | Jm \rangle |J_1 m_1\rangle |J_2 m_2\rangle.$$

Then, using the inverse of the transformation given in table 2 we express the coupled states in terms of icosahedral states:

$$|(J_1 J_2) J \Gamma \gamma\rangle = \sum_{\substack{m m_1 m_2 \\ \Gamma_1 \Gamma_2 \gamma_1 \gamma_2}} C(Jm\Gamma\gamma) \langle J_1 m_1; J_2 m_2 | Jm \rangle \times \bar{C}(J_1 m_1 \Gamma_1 \gamma_1) \bar{C}(J_2 m_2 \Gamma_2 \gamma_2) |J_1 \Gamma_1 \gamma_1\rangle |J_2 \Gamma_2 \gamma_2\rangle$$

where $\Gamma_1 \Gamma_2$ range over values such that $\Gamma_1 \subset J_1$, $\Gamma_2 \subset J_2$ and $\Gamma \supset \Gamma_1 \otimes \Gamma_2$. By the above process we have transformed to SO(3) coupling in the SO(3) $\supset$ I base (see 2.1.2). We can break up the product space using Racah's Lemma:

$$|(J_1 J_2) J \Gamma \gamma\rangle = \sum_{\substack{\beta \gamma_1 \gamma_2 \\ \Gamma_1 \Gamma_2}} \langle J_1 \Gamma_1; J_2 \Gamma_2 | \, | J \Gamma \rangle_\beta \langle \Gamma_1 \gamma_1; \Gamma_2 \gamma_2 | \beta \Gamma \gamma \rangle |\Gamma_1 \gamma_1\rangle |\Gamma_2 \gamma_2\rangle.$$

As we have defined the relative phases between the isoscalars and coupling coefficients the decomposition can be performed uniquely using the orthonormality of the coupling coefficients. The isoscalars are also orthonormal in the sense that

$$\sum_{\beta \Gamma_1 \Gamma_2} \langle J_1 \Gamma_1; J_2 \Gamma_2 | \, | J \Gamma \rangle_\beta \langle J_1 \Gamma_1; J_2 \Gamma_2 | \, | J' \Gamma \rangle_{\beta'} = \delta(J, J') \delta(\beta, \beta')$$

and

$$\sum_{J\beta} \langle J_1\Gamma_1; J_2\Gamma_2| \, |J\Gamma\rangle_\beta \langle J_1\Gamma_1'; J_2\Gamma_2'| \, |J\Gamma\rangle_\beta = \delta(\Gamma_1, \Gamma_1')\delta(\Gamma_2, \Gamma_2')$$

which act as a check. Recall that only if J_1 and J_2 are the lowest SO(3) irreps containing Γ_1 and Γ_2 do we define the coupling symbol. Otherwise it is specified. An example should make the above clearer.

From table 2,

$$|(33)1T_10\rangle = \mathrm{i}|(33)10\rangle.$$

Using SO(3) coupling in the SO(3) ⊃ SO(2) base,

$$\begin{aligned}|(33)1T_10\rangle &= \sum_m \mathrm{i}\sqrt{3}\begin{pmatrix} 3 & 3 & 1 \\ m & -m & 0\end{pmatrix}|3m\rangle|3-m\rangle \\ &= (3\mathrm{i}/\sqrt{28})(|33\rangle|3-3\rangle - |3-3\rangle|33\rangle) + (2\mathrm{i}/\sqrt{28})(|3-2\rangle|32\rangle - |32\rangle|3-2\rangle) \\ &\quad + (\mathrm{i}/\sqrt{28})(|31\rangle|3-1\rangle - |3-1\rangle|31\rangle).\end{aligned}$$

Using the inverse of table 2 (recall the unitary nature of the transformation involved),

$$\begin{aligned}|(33)1T_10\rangle = (\tfrac{1}{7})^{1/2}[&(\mathrm{i}/2)|3G-2\rangle|3G2\rangle - (\mathrm{i}/2)|3G2\rangle|3G-2\rangle \\ &+ (\mathrm{i}/2)|3G1\rangle|3G-1\rangle - (\mathrm{i}/2)|3G-1\rangle|3G1\rangle] \\ &- (\tfrac{3}{7})^{1/2}[-(\mathrm{i}/\sqrt{2})|3G2\rangle|3T_2-2\rangle + (\mathrm{i}/\sqrt{2})|3G-2\rangle|3T_22\rangle] \\ &+ (\tfrac{3}{7})^{1/2}[(\mathrm{i}/\sqrt{2})|3T_22\rangle|3G-2\rangle - (\mathrm{i}/\sqrt{2})|3T_2-2\rangle|3G2\rangle]\end{aligned}$$

where we have broken the sum up into the different portions and extracted the isoscalars by making the coupling coefficients orthonormal and using the phase convention for isoscalars. We can see that

$$\langle 3G; 3G| \, |1T_1\rangle = (\tfrac{1}{7})^{1/2},$$
$$\langle 3G; 3T_2| \, |1T_1\rangle = -\langle 3T_2; 3G| \, |1T_1\rangle = (\tfrac{3}{7})^{1/2},$$

and

$$\langle G-2; G2|T_10\rangle = \langle G1; G-1|T_10\rangle = \mathrm{i}/2,$$
$$\langle G2; T_2-2|T_10\rangle = -\mathrm{i}/\sqrt{2},$$

the other symbols being related to these by the symmetry properties. The relation (2.2.4) then gives the 3-*jm* symbols as tabulated in table 3. The basic isoscalars, in both forms, are tabulated in table 4. The 3-*jm* symbols agree with Golding (1973 table 4) after differences of notation and phase standardisation are allowed for with the exception of

$$\begin{pmatrix} T_2 & H & T_1 \\ 0 & 0 & 0\end{pmatrix} = \frac{1}{\sqrt{5}}.$$

He makes this $1/\sqrt{15}$ which does not lead to orthonormality.

Table 3. The icosahedral 3-*jm* symbols. The triples are listed in standard order and the symbols are in standard form. Nonstandard symbols can be obtained by using equation (3.1.3) and/or equation (3.4.1).

$$\begin{pmatrix}\Gamma & \Gamma & A\\ \gamma & \gamma' & 0\end{pmatrix} = \frac{\delta(\gamma,\gamma')}{[\Gamma]^{1/2}}$$

$$\begin{pmatrix}T_1 & T_1 & T_1\\ -1 & 1 & 0\end{pmatrix} = \frac{-i}{\sqrt{6}}$$

H	T_1	T_1	1
0	−1	1	$1/\sqrt{30}$
−2	1	1	$-1/\sqrt{5}$
−1	1	0	$-1/\sqrt{10}$
0	0	0	$-2/\sqrt{15}$

H	H	T_1	1
−2	1	1	$i/\sqrt{15}$
−1	0	1	$i/\sqrt{10}$
−2	2	0	$-i\sqrt{2}/\sqrt{15}$
−1	1	0	$-i/\sqrt{30}$

H	H	H	1
−2	1	1	$-\sqrt{3}/\sqrt{35}$
−2	2	0	$\sqrt{2}/\sqrt{35}$
−1	1	0	$-1/\sqrt{70}$
0	0	0	$-\sqrt{2}/\sqrt{35}$

H	H	H	2
2	2	1	$-\sqrt{7}/5\sqrt{3}$
−2	1	1	$2/5\sqrt{21}$
−2	2	0	$1/5\sqrt{14}$
−1	1	0	$-4/5\sqrt{14}$
0	0	0	$6/5\sqrt{14}$

T_2	H	T_1	1
2	2	1	$-\sqrt{2}/\sqrt{15}$
−2	1	1	$\sqrt{2}/\sqrt{15}$
0	−1	1	$-1/\sqrt{15}$
−2	2	0	$1/\sqrt{15}$
0	0	0	$1/\sqrt{5}$

T_2	H	H	1
0	−2	2	$-i/\sqrt{30}$
0	−1	1	$i\sqrt{2}/\sqrt{15}$
2	2	1	$-i/\sqrt{15}$
−2	2	0	$i/\sqrt{10}$

T_2	T_2	H	1
−2	0	2	$1/\sqrt{10}$
2	2	1	$1/\sqrt{5}$
2	−2	0	$1/\sqrt{30}$
0	0	0	$-\sqrt{2}/\sqrt{15}$

$$\begin{pmatrix}T_2 & T_2 & T_2\\ -2 & 2 & 0\end{pmatrix} = \frac{i}{\sqrt{6}}$$

G	H	T_1	1
2	2	1	$3/2\sqrt{15}$
−2	1	1	$1/\sqrt{15}$
−1	0	1	$-1/\sqrt{10}$
1	−2	1	$1/2\sqrt{15}$
−2	2	0	$1/\sqrt{30}$
−1	1	0	$-2/\sqrt{30}$

G	H	H	1
2	2	1	$i\sqrt{3}/2\sqrt{10}$
1	−2	1	$-i\sqrt{3}/2\sqrt{10}$
−2	2	0	$i/2\sqrt{5}$
−1	1	0	$-i/2\sqrt{5}$

G	H	H	2
1	2	2	$-2i/\sqrt{30}$
2	2	1	$i/2\sqrt{30}$
1	−2	1	$-i/2\sqrt{30}$
−2	1	1	$-2i/\sqrt{30}$
−2	2	0	$-i/2\sqrt{5}$
−1	1	0	$-i/2\sqrt{5}$

G	T_2	T_1	1
2	2	1	$-i/2\sqrt{3}$
1	−2	1	$-i/2\sqrt{3}$
−1	0	1	$i/\sqrt{6}$
−2	2	0	$i/\sqrt{6}$

T_2	G	H	1
2	1	2	$1/\sqrt{15}$
0	−2	2	$1/\sqrt{30}$
2	2	1	$-1/2\sqrt{15}$
−2	1	1	$3/2\sqrt{15}$
0	−1	1	$1/\sqrt{30}$
−2	2	0	$-1/\sqrt{10}$

G	G	T_1	1
−2	1	1	$-i/\sqrt{6}$
−2	2	0	$i/2\sqrt{3}$
−1	1	0	$-i/2\sqrt{3}$

G	G	H	1
2	1	2	$-1/\sqrt{30}$
−1	−1	2	$-2/\sqrt{30}$
2	2	1	$-2/\sqrt{30}$
−2	1	1	$1/\sqrt{30}$
−2	2	0	$1/2\sqrt{5}$
−1	1	0	$-1/2\sqrt{5}$

G	G	T_2	1
2	1	2	$i/\sqrt{6}$
−2	2	0	$i/2\sqrt{3}$
−1	1	0	$i/2\sqrt{3}$

G	G	G	1
2	2	1	$i/2\sqrt{3}$
−2	1	1	$i/2\sqrt{3}$

To use table 3 to find a 3-*jm* symbol put it in the following standard form. First, use the reordering symmetries to make $\Gamma_1 \geqslant \Gamma_2 \geqslant \Gamma$ where $A < T_1 < H < T_2 < G$. Then, put the components in the order $|\gamma_1| \geqslant |\gamma_2| \geqslant |\gamma_3|$ whenever possible (i.e. when repeated irreps occur). Next, use the complex conjugation symmetry to make the first non-zero component reading from right to left positive. The triples occur in the table in 'numerical order'—i.e. HT_1T_1 is before HHT_1 and so on.

Table 4. The isoscalar factors involving the basic irreps. The first column contains the conventional symbol and the second the symmetrised version. Other symbols can be obtained from equation (3.3.1).

J_1	Γ_1	J_2	Γ_2	J	Γ	β	$\langle J_1\Gamma_1; J_2\Gamma_2 \vert\vert J\Gamma\rangle_\beta$	$\begin{pmatrix} J_1 & J_2 & J \\ \Gamma_1 & \Gamma_2 & \Gamma \end{pmatrix}^\beta$
1	T_1	1	T_1	1	T_1	1	1	-1
1	T_1	1	T_1	2	H	1	1	1
2	H	2	H	1	T_1	1	1	-1
3	G	3	G	1	T_1	1	$1/\sqrt{7}$	$-1/\sqrt{7}$
3	T_2	3	G	1	T_1	1	$\sqrt{3}/\sqrt{7}$	$-\sqrt{3}/\sqrt{7}$
3	G	2	H	1	T_1	1	$2/\sqrt{7}$	$2/\sqrt{7}$
3	T_2	2	H	1	T_1	1	$\sqrt{3}/\sqrt{7}$	$\sqrt{3}/\sqrt{7}$
3	G	3	G	3	T_2	1	$\sqrt{2}/\sqrt{3}$	$-\sqrt{2}/\sqrt{7}$
3	T_2	3	T_2	3	T_2	1	$1/\sqrt{3}$	$-1/\sqrt{7}$
3	G	3	G	2	H	1	$\sqrt{3}/\sqrt{7}$	$\sqrt{3}/\sqrt{7}$
3	T_2	3	G	2	H	1	$1/\sqrt{7}$	$1/\sqrt{7}$
3	T_2	3	T_2	2	H	1	$\sqrt{2}/\sqrt{7}$	$\sqrt{2}/\sqrt{7}$
2	H	2	H	2	H	1	1	1
2	H	2	H	4	H	2	1	$\sqrt{5}/3$
3	G	3	G	3	G	1	0	0
3	G	3	G	4	G	1	$2\sqrt{2}/\sqrt{11}$	$4\sqrt{2}/3\sqrt{11}$
2	H	2	H	3	T_2	1	1	$-\sqrt{3}/\sqrt{7}$
2	H	2	H	3	G	1	1	$-2/\sqrt{7}$
2	H	2	H	4	G	2	1	$2/3$

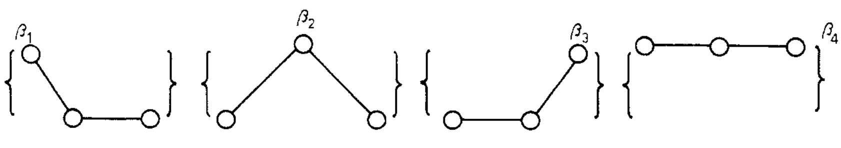
4. Icosahedral 6-*j* symbols

4.1. The definition

For any compact or finite group we can define an invariant 6-*j* symbol by considering the coupling of three kets (see Butler 1975 § 9). The definition reduces to

$$\begin{matrix}\beta_1 & \beta_2 & \beta_3 & \beta_4\end{matrix}$$
$$\begin{Bmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \Gamma_4 & \Gamma_5 & \Gamma_6 \end{Bmatrix}$$
$$= \sum_\gamma \begin{pmatrix} \Gamma_1 & \Gamma_5 & \Gamma_6 \\ \gamma_1 & -\gamma_5 & \gamma_6 \end{pmatrix}^{\beta_1} \begin{pmatrix} \Gamma_4 & \Gamma_2 & \Gamma_6 \\ \gamma_4 & \gamma_2 & -\gamma_6 \end{pmatrix}^{\beta_2}$$
$$\times \begin{pmatrix} \Gamma_4 & \Gamma_5 & \Gamma_3 \\ -\gamma_4 & \gamma_5 & \gamma_3 \end{pmatrix}^{\beta_3} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ -\gamma_1 & -\gamma_2 & -\gamma_3 \end{pmatrix}^{\beta_4}. \tag{4.1.1}$$

As can be seen from equation (4.1.1) the 6-*j* symbol vanishes unless certain irreps form triples. By placing the multiplicity labels above the symbol we enable an extension of a method of Judd's (1963 p 57) for recalling which irreps must form triples to be used. The irreps sitting on the circles are the required ones:



4.2. Properties of the 6-j symbols

The 6-j symbols are real because I has only real characters (see Butler 1975 equation (9.11)). They form the elements of an orthogonal matrix:

$$\sum_{\beta_1\beta_2\Gamma}[\Gamma_3][\Gamma]\overset{\beta_1\quad\beta_2\quad\beta_3\ \ \beta_4}{\begin{Bmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \Gamma_4 & \Gamma_5 & \Gamma\end{Bmatrix}}\overset{\beta_1\quad\beta_2\quad\beta_3'\ \ \beta_4'}{\begin{Bmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3'\\ \Gamma_4 & \Gamma_5 & \Gamma\end{Bmatrix}}=\delta(\Gamma_3,\Gamma_3')\delta(\beta_3,\beta_3')\delta(\beta_4,\beta_4')$$

(see Butler 1975 equation (9.7)). If one of the irreps in the 6-j is the identity we find (Butler 1975 equation (9.18)):

$$\overset{1\quad\ 1\quad\ \beta_3\ \ \beta_4}{\begin{Bmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \Gamma_2 & \Gamma_1 & A\end{Bmatrix}}=\frac{(-1)^{\Gamma_1+\Gamma_2+\Gamma_3}(-1)^{q(\Gamma_1\Gamma_2\Gamma_3\beta_3)}\delta(\beta_3,\beta_4)}{([\Gamma_1][\Gamma_2])^{1/2}}.$$

A symmetry of the symbols involves the partial exchanging of the rows (see Butler 1975 equation (9.8)):

$$\overset{\beta_1\quad\beta_2\quad\beta_3\ \ \beta_4}{\begin{Bmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \Gamma_4 & \Gamma_5 & \Gamma_6\end{Bmatrix}}=\overset{\beta_4\quad\beta_3\quad\beta_2\ \ \beta_1}{\begin{Bmatrix}\Gamma_1 & \Gamma_5 & \Gamma_6\\ \Gamma_4 & \Gamma_2 & \Gamma_3\end{Bmatrix}}.$$

Note that the multiplicity indices move so as to keep themselves attached to the same triple. The symbols are also invariant under even permutations of the columns and under odd permutations they are multiplied by $(-1)^n$, where n is the number of times the triple ($HHG1$) occurs (see Butler 1975 equation (9.9)). This means that some symbols containing an odd number of ($HHG1$) triples *must* vanish. For example,

$$\overset{1\quad\ 2\quad\ 2\ \ 2}{\begin{Bmatrix}G & H & H\\ H & H & H\end{Bmatrix}}=-\overset{1\quad\ 2\quad\ 2\ \ 2}{\begin{Bmatrix}G & H & H\\ H & H & H\end{Bmatrix}}=0.$$

We are left with 216 non-trivial symbols to calculate.

4.3. The calculation of the 6-j symbols

To calculate the 6-j symbols we use the recoupling relation (Butler 1975 equation (9.12)):

$$\sum_{\beta_4}\overset{\beta_1\quad\beta_2\quad\beta_3\ \ \beta_4}{\begin{Bmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \Gamma_4 & \Gamma_5 & \Gamma_6\end{Bmatrix}}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}^{\beta_4}$$

$$=\sum_{\gamma_4\gamma_5\gamma_6}\begin{pmatrix}\Gamma_1 & \Gamma_5 & \Gamma_6\\ \gamma_1 & -\gamma_5 & \gamma_6\end{pmatrix}^{\beta_1}\begin{pmatrix}\Gamma_4 & \Gamma_2 & \Gamma_6\\ \gamma_4 & \gamma_2 & -\gamma_6\end{pmatrix}^{\beta_2}\begin{pmatrix}\Gamma_4 & \Gamma_5 & \Gamma_3\\ -\gamma_4 & \gamma_5 & \gamma_3\end{pmatrix}^{\beta_3}.$$

We choose the 3-jm on the left so as to minimise the number of terms to be summed (usually by setting as many of γ_1, γ_2 and γ_3 equal to zero as is possible). If β_4 can take on two values then we first attempt to use the symmetry properties to obtain a new β_4 that cannot. If this fails we select γ_1, γ_2 and γ_3 so that the $\beta_4=1$ version of the 6-j vanishes, calculate the $\beta_4=2$ version and then use the result to find the other one.

Table 5. Invariant 6-*j* symbols for the icosahedral group. These are in the standard order and form mentioned in the text. Other symbols are related to them by symmetry. We have marked the multiplicity labels of those symbols that change sign under odd column permutations with an asterisk. A blank in the multiplicity column represents 1 1 1 1.

T_1	T_2	G	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	β_1	β_2	β_3	β_4	6-*j* symbol
6	0	0	T_1	T_1	T_1	T_1	T_1	T_1					$1/6$
5	0	0	H	T_1	T_1	T_1	T_1	T_1					$1/6$
4	0	0	H	T_1	T_1	H	T_1	T_1					$1/30$
			H	H	T_1	T_1	T_1	T_1					$-1/2\sqrt{5}$
3	1	2	G	G	T_1	T_1	T_1	T_2					$-1/6\sqrt{2}$
3	1	1	G	T_2	T_1	T_1	T_1	H					$-1/3\sqrt{2}$
3	1	0	T_2	H	T_1	T_1	T_1	H					$1/3\sqrt{5}$
			T_2	H	T_1	T_1	H	T_1					$1/5$
3	0	3	G	G	T_1	T_1	T_1	G					$-1/3\sqrt{2}$
3	0	2	G	G	T_1	T_1	T_1	H					$1/6\sqrt{2}$
3	0	1	G	H	T_1	T_1	T_1	H					$-1/3\sqrt{5}$
			G	H	T_1	T_1	H	T_1					$1/5$
3	0	0	H	H	T_1	T_1	T_1	H					$1/6\sqrt{5}$
			H	H	T_1	H	T_1	T_1					$-1/10$
			H	H	H	T_1	T_1	T_1	1	1	1	1	$7/10\sqrt{21}$
									1	1	1	2	0
2	2	2	G	T_2	T_1	G	T_2	T_1					$1/4$
2	2	1	G	T_2	T_1	H	T_2	T_1					0
			G	T_2	T_1	H	T_1	T_2					$-1/6$
2	2	0	T_2	T_2	H	T_1	T_1	H					$2/15$
			T_2	H	T_1	T_2	H	T_1					$1/5$
2	1	3	G	G	T_1	G	T_2	T_1					$1/6$
2	1	2	G	G	T_1	H	T_1	T_2					$-1/2\sqrt{6}$
			G	G	T_1	T_2	H	T_1					$-1/6$
			G	T_2	T_1	G	H	T_1					$-1/12$
			G	G	H	T_1	T_1	T_2					$-1/2\sqrt{6}$
2	1	1	G	T_2	T_1	H	T_1	H					$-1/\sqrt{60}$
			G	T_2	H	T_1	T_1	H					$1/5\sqrt{6}$
			G	T_2	T_1	H	H	T_1					$2/3\sqrt{10}$
			G	H	T_1	T_2	H	T_1					$-2/15$
			G	T_2	T_1	T_1	H	H	1	1	1	1*	$1/2\sqrt{15}$
									2	1	1	1	$1/2\sqrt{15}$
2	1	0	T_2	H	H	T_1	H	T_1					$-2/5\sqrt{6}$
			T_2	H	T_1	H	H	T_1					$1/15$
			T_2	H	T_1	H	T_1	H	1	1	1	1	$1/5\sqrt{21}$
									1	2	1	1	$-2/\sqrt{105}$
2	0	4	G	G	T_1	G	G	T_1					$-1/12$
2	0	3	G	G	T_1	G	H	T_1					$1/6$
			G	G	T_1	H	T_1	G					0
2	0	2	G	G	H	T_1	T_1	H					$-3/10\sqrt{6}$
			G	G	T_1	H	T_1	H	1	1	1	1*	$1/4\sqrt{15}$
									1	2	1	1	$3/4\sqrt{15}$
			G	G	T_1	H	H	T_1					$1/3\sqrt{10}$
			G	H	T_1	G	H	T_1					$7/60$
2	0	1	G	H	T_1	H	T_1	H	1	1	1	1	$-1/5\sqrt{21}$
									1	2	1	1	$-3/2\sqrt{105}$
			G	H	T_1	H	H	T_1					$1/15$
			G	H	H	T_1	H	T_1	1	1	1	1*	$-2/5\sqrt{6}$
									1	1	1	2	0
2	0	0	H	H	T_1	H	H	T_1					$1/6$

Table 5—continued.

T_1	T_2	G	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	β_1	β_2	β_3	β_4	6-*j* symbol
			H	H	H	H	T_1	T_1	1	1	1	1	$7/10\sqrt{21}$
									1	1	1	2	0
1	3	2	G	G	T_2	T_2	T_2	T_1					$-1/6\sqrt{2}$
1	3	1	G	T_2	H	T_2	T_1	T_2					$1/3\sqrt{2}$
			G	T_2	T_1	H	T_2	T_1					0
1	3	0	T_2	T_2	H	T_2	T_1	H					$1/5$
			T_2	T_2	T_2	H	H	T_1					$-1/3\sqrt{5}$
1	2	3	G	G	T_2	G	T_1	T_2					$1/6$
1	2	2	G	G	T_2	T_2	H	T_1					$-1/2\sqrt{6}$
			G	T_2	H	G	T_2	T_1					$-1/12$
			G	G	T_2	H	T_1	T_2					$1/6$
			G	G	H	T_2	T_2	T_1					$1/2\sqrt{6}$
1	2	1	G	T_2	T_1	T_2	H	H	1	1	1	1*	$-1/2\sqrt{15}$
									2	1	1	1	$-1/2\sqrt{15}$
			G	T_2	H	H	T_2	T_1					$2/3\sqrt{10}$
			G	T_2	H	H	T_1	T_2					$1/2\sqrt{15}$
			G	T_2	H	T_2	T_1	H					$-1/5\sqrt{6}$
			G	T_2	H	T_1	T_2	H					$-2/15$
1	2	0	T_2	T_2	H	H	H	T_1	1	1	1	1	$4/5\sqrt{21}$
									1	1	2	1	$-1/\sqrt{105}$
			T_2	T_2	H	H	T_1	H					$2/5\sqrt{6}$
			T_2	H	H	T_2	H	T_1					$1/15$
1	1	4	G	G	G	G	T_2	T_1					$1/6$
			G	G	T_2	G	G	T_1					$1/4$
1	1	3	G	G	G	T_2	H	T_1					$-1/6$
			G	G	T_2	G	T_1	H					$1/6$
			G	G	T_1	G	H	T_2					0
			G	G	T_1	G	T_2	H					$-1/6$
			G	G	T_1	T_2	H	G					$-1/6$
1	1	2	G	T_2	H	G	T_1	H					$1/5$
			G	G	T_2	H	T_1	H	1	1	1	1*	$1/2\sqrt{10}$
									1	2	1	1	$1/6\sqrt{10}$
			G	G	T_2	H	H	T_1					$1/2\sqrt{10}$
			G	G	T_1	T_2	H	H	1	1	1	1*	$-1/2\sqrt{10}$
									2	1	1	1	$-1/6\sqrt{10}$
			G	G	H	T_2	T_1	H					$-2/15$
			G	G	H	T_2	H	T_1					$1/6\sqrt{10}$
			G	T_2	H	G	H	T_1	1	1	1	1*	$1/4\sqrt{10}$
									1	1	2	1	$-7/12\sqrt{10}$
			G	G	T_1	H	H	T_2					$-1/2\sqrt{10}$
			G	G	H	H	T_1	T_2					$1/6\sqrt{10}$
1	1	1	G	T_2	H	H	H	T_1	1	1	1	1	$-2/5\sqrt{14}$
									1	1	2	1	$-2/3\sqrt{70}$
			G	T_2	H	H	T_1	H					$1/10$
			G	T_2	H	T_1	H	H	1	1	1	1*	$-1/10$
									2	1	1	1	$1/6$
			G	H	H	T_2	H	T_1	1	1	1	1*	$1/10$
									1	1	1	2	$1/6$
			G	T_2	T_1	H	H	H	1	1	1	1*	$-1/2\sqrt{10}$
									2	1	1	1	$1/6\sqrt{10}$
1	1	0	T_2	H	H	T_1	H	H					0
			T_2	H	H	H	H	T_1	1	1	1	1	$-2/5\sqrt{14}$
									1	1	2	1	$-2/3\sqrt{70}$

Table 5—continued.

T_1	T_2	G	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	β_1	β_2	β_3	β_4	6-j symbol
1	0	5	G	G	G	G	G	T_1					1/12
1	0	4	G	G	G	G	H	T_1					−1/6
			G	G	H	G	G	T_1					1/12
1	0	3	G	G	G	H	H	T_1	1	1	2	1	$-1/3\sqrt{10}$
			G	G	H	G	T_1	H					1/30
			G	G	H	H	T_1	G					$-1/3\sqrt{10}$
			G	G	H	G	H	T_1	1	1	1	1*	$1/2\sqrt{10}$
									1	1	2	1	$1/6\sqrt{10}$
1	0	2	G	G	H	H	H	T_1	1	1	1	1	$-3/5\sqrt{14}$
									1	1	2	1	$1/6\sqrt{70}$
			G	G	H	H	T_1	H	1	1	1	1*	−3/20
									1	2	1	1	1/12
			G	H	H	G	H	T_1	1	1	1	2*	−1/8
									1	1	2	2	−1/24
									1	1	1	1	1/40
			G	G	T_1	H	H	H	1	1	1	1	$1/4\sqrt{10}$
									1	2	1	1*	$-1/4\sqrt{10}$
									2	2	1	1	$5/12\sqrt{10}$
1	0	1	G	H	H	H	H	T_1	1	1	1	1*	$-2/5\sqrt{14}$
									1	1	2	2	$7/6\sqrt{70}$
									1	1	1	2	0
									1	1	2	1*	$1/2\sqrt{70}$
			G	H	H	T_1	H	H	1	1	1	1	0
									2	1	1	2	2/15
1	0	0	H	H	H	H	H	T_1	1	1	1	1	−1/10
									1	1	1	2	0
									1	1	2	2	2/15
0	6	0	T_2	T_2	T_2	T_2	T_2	T_2					1/6
0	5	0	T_2	T_2	T_2	T_2	T_2	H					1/6
0	4	0	T_2	T_2	H	T_2	T_2	H					1/30
			T_2	T_2	T_2	T_2	H	H					$1/2\sqrt{5}$
0	3	3	G	G	T_2	T_2	T_2	G					$-1/3\sqrt{2}$
0	3	2	G	G	T_2	T_2	T_2	H					$1/6\sqrt{2}$
0	3	1	G	T_2	H	T_2	T_2	H					1/5
			G	T_2	H	T_2	H	T_2					$1/3\sqrt{5}$
0	3	0	T_2	T_2	T_2	H	H	H					$-1/6\sqrt{5}$
			T_2	T_2	H	T_2	H	H					−1/10
			T_2	T_2	H	H	H	T_2	1	1	1	1	$-1/5\sqrt{21}$
									1	1	2	1	$-3/2\sqrt{105}$
0	2	4	G	G	T_2	G	G	T_2					−1/12
0	2	3	G	G	T_2	G	H	T_2					−1/10
			G	G	H	T_2	T_2	G					0
0	2	2	G	G	T_2	T_2	H	H	1	1	1	1*	$1/4\sqrt{15}$
									2	1	1	1	$3/4\sqrt{15}$
			G	G	T_2	H	H	T_2					$-1/3\sqrt{10}$
			G	T_2	H	G	T_2	H					7/60
			G	G	H	T_2	T_2	H					$3/10\sqrt{6}$
0	2	1	G	T_2	H	H	H	T_2	1	1	1	1	$7/10\sqrt{21}$
									1	1	2	1	0
			G	T_2	H	H	T_2	H					1/15
			G	T_2	H	T_2	H	H	1	1	1	1*	$2/5\sqrt{6}$
									2	1	1	1	0
0	2	0	T_2	H	H	T_2	H	H					1/6

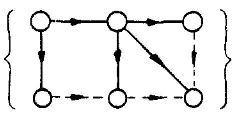
Table 5—continued.

T_1	T_2	G	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	β_1	β_2	β_3	β_4	6-*j* symbol
			T_2	T_2	H	H	H	H	1	1	1	1	$-1/5\sqrt{21}$
									1	1	2	1	$-3/2\sqrt{105}$
0	1	5	G	G	G	G	G	T_2					$1/12$
0	1	4	G	G	G	G	T_2	H					$1/6$
			G	G	T_2	G	G	H					$1/12$
0	1	3	G	G	G	T_2	H	H	2	1	1	1	$-1/3\sqrt{10}$
			G	G	H	G	T_2	H					$1/30$
			G	G	T_2	G	H	H	1	1	1	1*	$1/2\sqrt{10}$
									2	1	1	1	$-1/6\sqrt{10}$
			G	G	H	T_2	H	G					$1/3\sqrt{10}$
0	1	2	G	G	T_2	H	H	H	1	1	1	1	$-1/4\sqrt{10}$
									1	2	1	1*	$-1/4\sqrt{10}$
									2	2	1	1	$-5/12\sqrt{10}$
			G	G	H	H	H	T_2	1	1	1	1	$-1/10\sqrt{14}$
									1	1	2	1	$-2/3\sqrt{70}$
			G	G	H	T_2	H	H	1	1	1	1*	$-3/20$
									2	1	1	1	$1/12$
			G	T_2	H	G	H	H	1	1	2	1*	$-1/8$
									2	1	2	1	$-1/24$
									1	1	1	1	$1/40$
0	1	1	G	T_2	H	H	H	H	1	1	1	1	$1/10\sqrt{14}$
									1	1	2	1	$-1/\sqrt{70}$
									2	1	1	1	$1/2\sqrt{14}$
									2	1	2	1	$-1/3\sqrt{70}$
			G	H	H	T_2	H	H	1	1	1	1	0
									2	1	1	2	$2/15$
0	1	0	T_2	H	H	H	H	H	1	1	1	1	$4/35$
									1	1	2	1	$-1/7\sqrt{5}$
									1	2	2	1	$-17/210$
0	0	6	G	G	G	G	G	G					$1/6$
0	0	5	G	G	G	G	G	H					$-1/12$
0	0	4	G	G	G	G	H	H	2	1	1	1	$1/3\sqrt{10}$
			G	G	H	G	G	H					$7/60$
0	0	3	G	G	G	H	H	H	2	2	2	1	$-1/6\sqrt{10}$
									1	1	2	1	$1/2\sqrt{10}$
			G	G	H	G	H	H	1	1	1	1	$-1/10$
									2	1	2	1	$1/6$
			G	G	H	H	H	G	1	1	1	1	$-2/5\sqrt{14}$
									1	1	2	1	$-2/3\sqrt{70}$
0	0	2	G	H	H	G	H	H	2	2	2	2	$-1/120$
									2	1	1	2	$-3/40$
									1	1	1	1	$1/8$
			G	G	H	H	H	H	1	1	1	1	$-3/20\sqrt{14}$
									1	2	1	1*	$-1/4\sqrt{14}$
									2	2	1	1	$-1/4\sqrt{14}$
									1	1	2	1	$-1/4\sqrt{70}$
									2	2	2	1	$-5/12\sqrt{70}$
									1	2	2	1*	$3/4\sqrt{70}$
0	0	1	G	H	H	H	H	H	1	2	2	1	$3/35$
									1	1	2	1	$3/28\sqrt{5}$
									2	1	2	2	$5/28\sqrt{5}$
									2	2	2	2	$1/105$
									1	1	2	2*	$1/4\sqrt{5}$

Table 5—continued.

T_1	T_2	G	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	β_1	β_2	β_3	β_4	6-*j* symbol
									1	1	1	1	4/35
									2	1	1	2	2/35
0	0	0	H	H	H	H	H	H	1	1	1	2	0
									1	1	2	2	2/35
									1	2	2	2	$-1/7\sqrt{5}$
									2	2	2	2	$-1/210$
									1	1	1	1	$-3/70$

We tabulate the 6-*j* symbols in table 5. The symbols are listed in descending order of $N(T_1)N(T_2)N(G)$ where $N(\Gamma)$ is the number of Γ's occurring in the symbol. All the 6-*j* symbols are either in the table or related to one that is by symmetry (we omit those that vanish by symmetry). The representative is selected in a manner that is an extension of the ordering used in Rotenberg *et al* (1959) for SO(3) 6-*j* symbols. This is summarised in



where irreps linked by solid arrows (say $\Gamma_1 \rightarrow \Gamma_2$) are chosen so that $\Gamma_1 \geq \Gamma_2$ using the same ordering of irreps as above ($A < T_1 < H < T_2 < G$). In the case of dotted arrows we order the irreps if possible (this occurs when there is an equality elsewhere in the symbol). Occasionally this ordering distinguishes between symbols that are equal by symmetry—we only include one.

5. Discussion

5.1. Comparison with the work of Golding

In this paper we have set up coupling theory for the icosahedral group. In doing this we have followed the general guidelines of Butler (1975). Before that general framework had been set up, Golding (1973) calculated what amount to 3-*jm* symbols for the group. The present paper keeps to the same basis states as used in Golding (1973) but we have improved the notation and the definition of multiplicity labels, redefined phases and have improved the treatment of the symmetry of the 3-*jm* symbols resulting from time reversal. The reasons for these changes are that Golding's approach leads to symbols that are somewhat hard to use.

One difficulty is that Golding attaches a J label to each irrep of I. This is an improper procedure because I is a group in its own right and not just a subgroup of SO(3). The low J's that symbols come from can be used to label repeated irreps but the multiplicity label is a property of triples and not of individual irreps. This is particularly important when we calculate 6-*j* symbols as then each irrep occurs in two different triples. We define multiplicity labels properly but using the same general idea as Golding, in § 3.2. In addition to this use of J labels as multiplicity labels, Golding also uses $(-1)^{J_1+J_2+J_3}$

disguised as $(-1)^{\Gamma_1+\Gamma_2+\Gamma_3}$ as the reordering phase. This is subject to the same criticisms as in the multiplicity case.

The second criticism that one can make is that the symmetry of symbols under negation of all components (time reversal) is unnecessarily complicated by the introduction of the phase of this symmetry in SO(3) which has nothing to do with it (property C p 665 of Golding 1973). The use of non-numerical labels for irrep components further complicates the issue. We adopt instead the labelling used by McLellan (1961) whereupon $a' \to -a$. Golding has

$$V\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ a & b & c\end{pmatrix} = (-1)^{\Gamma_1+\Gamma_2+\Gamma_3} V\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ -(a) & -(b) & -(c)\end{pmatrix}$$

$$= \pm(-1)^{\Gamma_1+\Gamma_2+\Gamma_3} V\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ a' & -(b) & -(c)\end{pmatrix} \text{ etc.}$$

This involves four moves to obtain the results summarised in equation (3.4.1). For example,

$$V\begin{pmatrix}4U & U & U\\ \mu & \kappa & \kappa\end{pmatrix} = V\begin{pmatrix}4U & U & U\\ -(\mu) & -(\kappa) & -(\kappa)\end{pmatrix} = -V\begin{pmatrix}4U & U & U\\ \lambda & \nu & \nu\end{pmatrix}$$

which we know because it is an imaginary quantity.

Additionally, the sign of the isoscalars is not stated. It is hoped that by stating all our assumptions of this type we have made it easy to check and use the results of our calculations.

5.2. *Reality*

As the icosahedral group has only integer irreps we could choose a base leading to real 3-*jm* symbols. Such a base is shown in table 6. The real base is more complicated than

Table 6. A real base for the icosahedral group. The polynomials in the third column are proportional to the states when the latter are made up from the lowest possible J states.

Real state	Relation to the complex base	Transformation properties
$\|A\ l\rangle$	$= \|A\ 0\rangle$	~ 1
$\|T_1\ x\rangle$	$= -\mathrm{i}(\|T_1\ 1\rangle - \|T_1\ -1\rangle)/\sqrt{2}$	$\sim x$
$\|T_1\ y\rangle$	$= (\|T_1\ 1\rangle + \|T_1\ -1\rangle)/\sqrt{2}$	$\sim y$
$\|T_1\ z\rangle$	$= -\|T_1\ 0\rangle$	$\sim z$
$\|T_2\ x\rangle$	$= \mathrm{i}(\|T_2\ 2\rangle - \|T_2 -2\rangle)/\sqrt{2}$	$\sim 3xy^2 - x^3 + 6xyz$
$\|T_2\ y\rangle$	$= (\|T_2\ 2\rangle + \|T_2 -2\rangle)/\sqrt{2}$	$\sim y^3 - 3x^2y + 3z(y^2 - x^2)$
$\|T_2\ z\rangle$	$= -\|T_2\ 0\rangle$	$\sim 3zx^2 + 3zy^2 - 2z^3$
$\|G\ \alpha\rangle$	$= (\|G\ 2\rangle + \|G\ -2\rangle)/\sqrt{2}$	$\sim (3x^2y - y^2) + 2(zy^2 - zx^2)$
$\|G\ \beta\rangle$	$= \mathrm{i}(\|G\ 2\rangle - \|G\ -2\rangle)/\sqrt{2}$	$\sim x^3 - 3xy^2 - 4xyz$
$\|G\ \gamma\rangle$	$= (\|G\ 1\rangle + \|G\ -1\rangle)/\sqrt{2}$	$\sim (x^2 + y^2 - 4z^2)y$
$\|G\ \delta\rangle$	$= \mathrm{i}(\|G\ 1\rangle - \|G\ -1\rangle)/\sqrt{2}$	$\sim (x^2 + y^2 - 4z^2)x$
$\|H\ \theta\rangle$	$= -\|H\ 0\rangle$	$\sim 2z^2 - x^2 - y^2$
$\|H\ \epsilon\rangle$	$= (\|H\ 2\rangle + \|H\ -2\rangle)/\sqrt{2}$	$\sim \sqrt{3}(x^2 - y^2)$
$\|H\ x\rangle$	$= -(\|H\ 1\rangle + \|H\ -1\rangle)/\sqrt{2}$	$\sim 2\sqrt{3}yz$
$\|H\ y\rangle$	$= -\mathrm{i}(\|H\ 1\rangle - \|H\ -1\rangle)/\sqrt{2}$	$\sim 2\sqrt{3}xz$
$\|H\ z\rangle$	$= -\mathrm{i}(\|H\ 2\rangle - \|H\ -2\rangle)/\sqrt{2}$	$\sim 2\sqrt{3}xy$

the one in table 2 from the SO(3) ⊃ I point of view and leads to symbols which have some of the symmetries 'hidden'. For example consider

$$\begin{pmatrix} H & H & H \\ \epsilon & \epsilon & x \end{pmatrix}^2 = -\begin{pmatrix} H & H & H \\ y & z & \epsilon \end{pmatrix}^2 = -\begin{pmatrix} H & H & H \\ z & z & x \end{pmatrix}^2 = \frac{\sqrt{7}}{5\sqrt{6}}.$$

The information contained in these three symbols is contained in our single $\begin{pmatrix} H & H & H \\ -2 & -1 & -2 \end{pmatrix}^2$. Another advantage of the complex base is that the numerical labels carry information. Often we can easily spot 3-*jm* symbols that vanish—sometimes the SO(3) rules ($\gamma_1 + \gamma_2 + \gamma_3 = 0$) are kept in the subgroup and always two components add to form a unique third. A comparison of table 2 with table 6 should demonstrate the compactness of the notation that we can use with a complex base. The fact that the 3-*jm*'s are complex seems a small price to pay for the ease of application and we have therefore chosen to tabulate the complex 3-*jm*'s. If the symbols are required in the real basis then they can be found by using (Butler 1975 equation (11.6)):

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ x_1 & x_2 & x_3 \end{pmatrix}^\beta = \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}^\beta \langle \Gamma_1\gamma_1|\Gamma_1 x_1\rangle\langle \Gamma_2\gamma_2|\Gamma_2 x_2\rangle\langle \Gamma_3\gamma_3|\Gamma_3 x_3\rangle.$$

Work is currently in progress on real I* coupling at the Inorganic Chemistry Department at the University of Copenhagen (T Damhus, private communication).

5.3. Concluding remarks

We have set up coupling theory for I using a complex basis with a numerical labelling system. This base is expressed in terms of SO(3) ⊃ SO(2) vectors $|jm\rangle$ with an explicit phase standardisation. With the aid of Racah's Lemma we obtained coupling coefficients for I that have a phase standardisation selected with the definition of symmetrised 3-*jm* symbols in mind. We tabulated the isoscalar factors for the basic irreps so as to facilitate checking and the changing of the phase convention.

Having followed this procedure we were left with a theory of icosahedral coupling that contains no information originating in another group in contradistinction to Golding (1973). The symmetries of the 3-*jm* and the multiplicity labels are easy to use and are defined entirely in terms of subgroup properties. Finally, we discussed the relationship to our work of that of Golding and explained why we did not use a real basis. It is hoped that this paper will enable icosahedral group calculations to be performed with relatively little effort.

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