

## Spin-orbit coupling coefficients for icosahedral molecules

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**Summary.** A self-consistent set of real spin-orbit coupling coefficients for the icosahedral double group is derived. Construction of the basis, resolution of multiplicities by spherical operator techniques, and typical applications to Zeeman and crystal-field problems for transition-metal atoms and lanthanides in icosahedral environments are described.

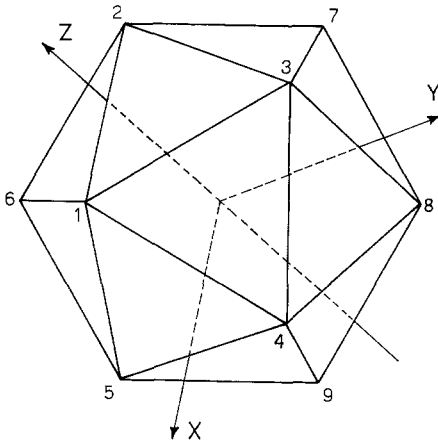
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### 1 Introduction

The successful synthesis of cage molecules with rigorous icosahedral symmetry [1] continues to raise interest in the icosahedral point group  $I_h$ . In a previous publication we have presented tables of coupling coefficients for the single-valued irreducible representations of the rotational subgroup  $I$  [2]. These tables were based on the symmetry functions of Boyle and Parker [3]. The purpose of the present paper is to extend this analysis to the icosahedral double group  $I^*$ , by providing a suitable complex symmetry basis and corresponding spin-orbit coupling coefficients. In this way a complete set of practical group-theoretical tables for the study of icosahedral and dodecahedral molecules is made available.

### 2 The real orbital basis of Boyle and Parker

In their paper on a vibrating icosahedral cage Boyle and Parker [3] have presented a real symmetry basis for the orbital representations of the icosahedral rotational group  $I$ . The Cartesian  $xyz$ -frame was made to coincide with a set of mutually orthogonal two-fold axes [4], as shown in Fig. 1. At first sight this scheme is somewhat unusual in that a symmetry element of low rotational order is elected for quantization of the symmetry functions. However, it should be noted that the coordinate frame as a whole is compatible with the standard frame for the tetrahedral subgroup  $T \subset I$ . This provides a connection between icosahedral symmetry functions and the elaborate symmetry bases which are



**Fig. 1.** Projection of the icosahedron on a plane perpendicular to a three-fold axis illustrating the coordinate convention of Boyle and Parker [3]. Note that the edge intersected by the  $y$ -axis is parallel to the  $z$ -axis. A different choice is possible where this edge is parallel to the  $x$ -axis [4]

available for cubic groups (see e.g. [5]). In this way Boyle and Parker obtained a convenient realization for all single-valued irreducible representations of  $I$ . Their component labelling is shown in Table 1. The corresponding defining transformation matrices may be found in the appendix of the original paper [3]. The  $xyz$ -labels in the table follow the usual conventions for the cubic groups. This is not the case though for the  $\epsilon\theta$ -labels of  $H$  which do not correspond to standard components  $z^2$  and  $x^2 - y^2$  transforming as  $(2z^2 - x^2 - y^2)$  and  $\sqrt{3}(x^2 - y^2)$  resp., but to linear combinations thereof as specified in Eq. (1).

$$\begin{aligned} |H\theta\rangle &= \sqrt{3/8}|Hz^2\rangle + \sqrt{5/8}|Hx^2 - y^2\rangle \\ |H\epsilon\rangle &= -\sqrt{5/8}|Hz^2\rangle + \sqrt{3/8}|Hx^2 - y^2\rangle \end{aligned} \quad (1)$$

The real basis of Boyle and Parker is *almost* adapted to the group-subgroup hierarchy  $I \supset T \supset D_2$ . The exceptions are the  $\theta$  and  $\epsilon$  components of  $H$  which form a reducible basis for the two-non-degenerate complex-conjugate representations of  $T$ . Apparently this exception was introduced to avoid the use of complex functions. However, there is also a more fundamental and interesting group-theoretical reason. When constructing a symmetry basis for a group it is often desirable to define symmetry functions in such a way that real coupling coefficients result. As shown by Damhus, a necessary and sufficient condition for the existence of real coupling coefficients is that the group contain a fixed inner

**Table 1.** Component labelling in the real orbital basis of Boyle and Parker [3]

Representation	Components
$A$	$ Aa\rangle$
$T_1$	$ T_1x\rangle,  T_1y\rangle,  T_1z\rangle$
$T_2$	$ T_2x\rangle,  T_2y\rangle,  T_2z\rangle$
$G$	$ Ga\rangle,  Gx\rangle,  Gy\rangle,  Gz\rangle$
$H$	$ H\theta\rangle,  H\epsilon\rangle,  Hx\rangle,  Hy\rangle,  Hz\rangle$

automorphism carrying all standard representations into their complex conjugates [6]. This means that there should be some symmetry element, the *conjugating* element  $R_0 \in G$ , such that the automorphism  $R \rightarrow R_0^{-1}RR_0$  with  $R \in G$  takes the representational matrices  $\mathbb{D}^f(R)$  into their complex conjugates, i.e.:

$$\mathbb{D}^f(R_0^{-1}RR_0) = \overline{\mathbb{D}^f(R)} \quad (2)$$

As Bickerstaff and Damhus have demonstrated, this condition is incompatible with a tetrahedral symmetry adaptation of an icosahedral basis [7]. Hence by avoiding a complete  $I \supset T$  symmetrization Boyle and Parker have ensured the reality of the Clebsch–Gordan coupling coefficients.

Complete tables of these coefficients for the real basis set have been published previously [2]. These tables have proven to be a valuable tool for the study of the intricate icosahedral Jahn–Teller equations of type  $G \times (g + h)$  and  $H \times (g + 2h)$  [8, 9].

Evidently alternative reference frames with a pentagonal or trigonal axis of quantization [5, 10] continue to be of interest, especially for problems which contain a pentagonal or trigonal perturbation. A case in point is the study of lanthanide double nitrates, such as  $\text{Eu}_2\text{Mg}_3(\text{NO}_3)_{12} \cdot 24\text{H}_2\text{O}$  [11] where the lanthanide ion is surrounded by twelve oxygens forming a trigonally distorted icosahedron. Such a problem clearly requires a reference frame with a trigonal principal axis. For general purposes though, the frame adopted by Boyle and Parker is useful, because it has three equivalent coordinate axes. This leads to a greater simplicity of the coupling algebra. We will continue to use this coordinate frame in the subsequent treatment of the icosahedral double group  $I^*$ .

### 3 Complex orbital and spin basis

The icosahedral double group contains – in addition to the five orbital representations – four irreducible spin representations. These may conveniently be denoted by the Griffith labels  $E', E'', U', W'$  [12]. In this section we will discuss the construction of a suitable symmetry basis which allows a simple description of spin-orbit couplings. As in the case of the single group such a construction cannot be based on a tetrahedral symmetry adaptation since the  $I^* \supset T^*$  hierarchy gives rise to a complex coupling algebra [7].

For this reason we have applied a classical rotation-group approach. In such an approach the standard definitions of the spherical  $J$  representations of  $SU(2)$  are extrapolated to the irreducible representations of a finite subgroup. For the  $I^*$  group under study this approach turns out to be very successful, since no less than six  $J$  levels transform irreducibly under the elements of  $I^*$ . These are the integral  $J$  values 0, 1, 2 corresponding respectively to  $A, T_1, H$  orbital representations, and the half-integral  $J$  values 1/2, 3/2, 5/2 corresponding respectively to  $E', U', W'$  spin representations [12]. Hence symmetry bases for these representations can be defined directly by means of the standard representational matrices for the corresponding  $J$  levels [13, 14]. Relevant matrices for the icosahedral generators are listed in appendix A [15]. We recall that the classical standardization of these matrices includes a fixed inner automorphism of the type discussed in Eq. (2), the conjugating element  $R_0$  being a two-fold rotation about the  $y$ -axis. In our convention this element is labeled  $C_2^{3,8}$ . It connects  $|JM\rangle$  and  $|J-M\rangle$  kets in the following way:

$$C_2^{3,8}|JM\rangle = (-1)^{J-M}|J-M\rangle \quad (3)$$

The  $|JM\rangle$  basis thus satisfies the reality condition for the coupling coefficients. As a further result of the rotation group approach the non-trivial orbital representations  $T_1$  and  $H$  adopt a complex format. Table 2 specifies the conversion formulae which relate this complex orbital basis to the real basis of Boyle and Parker. The expressions used are in line with the usual conventions for real and complex forms of the spherical harmonics [13]. The table also shows the component labelling of the double-valued spin representations. In practice the representation matrices for the  $U'$  and  $W'$  representations were obtained by forming third and fifth symmetrized Kronecker powers of the standard  $\mathbb{D}^{E'}(R)$

**Table 2.** Complex orbital and spin basis for  $I^*$

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Single-valued orbital representations<sup>a</sup>

$A$   $|Aa\rangle$

$T_1$   $|T_11\rangle = (-|T_1x\rangle - i|T_1y\rangle)/\sqrt{2}$   
 $|T_1-1\rangle = (|T_1x\rangle - i|T_1y\rangle)/\sqrt{2}$   
 $|T_10\rangle = |T_1z\rangle$

$T_2$   $|T_21\rangle = (-|T_2x\rangle - i|T_2y\rangle)/\sqrt{2}$   
 $|T_2-1\rangle = (|T_2x\rangle - i|T_2y\rangle)/\sqrt{2}$   
 $|T_20\rangle = |T_2z\rangle$

$G$   $|Gi\rangle = i|Ga\rangle$   
 $|G1\rangle = (-|Gx\rangle - i|Gy\rangle)/\sqrt{2}$   
 $|G-1\rangle = (|Gx\rangle - i|Gy\rangle)/\sqrt{2}$   
 $|G0\rangle = |Gz\rangle$

$H$   $|H2\rangle = (\sqrt{5}|H\theta\rangle + \sqrt{3}|H\epsilon\rangle + i\sqrt{8}|Hz\rangle)/4$   
 $|H-2\rangle = (\sqrt{5}|H\theta\rangle + \sqrt{3}|H\epsilon\rangle - i\sqrt{8}|Hz\rangle)/4$   
 $|H1\rangle = (-i|Hx\rangle - |Hy\rangle)/\sqrt{2}$   
 $|H-1\rangle = (-i|Hx\rangle + |Hy\rangle)/\sqrt{2}$   
 $|H0\rangle = (\sqrt{3}|H\theta\rangle - \sqrt{5}|H\epsilon\rangle)/2\sqrt{2}$

Double-valued spin representations<sup>b</sup>

$E'$   $|E'\alpha\rangle, |E'\beta\rangle$

$E''$   $|E''\alpha\rangle, |E''\beta\rangle$

$U'$   $|U'\frac{3}{2}\rangle, |U'\frac{1}{2}\rangle, |U' - \frac{1}{2}\rangle, |U' - \frac{3}{2}\rangle$

$W'$   $|W'\frac{5}{2}\rangle, |W'\frac{3}{2}\rangle, |W'\frac{1}{2}\rangle, |W' - \frac{1}{2}\rangle, |W' - \frac{3}{2}\rangle, |W' - \frac{5}{2}\rangle$

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<sup>a</sup> The complex forms of  $T_1$  and  $H$  are analogous to the standard spherical harmonics  $Y_{lm}$  with  $l=1$  and  $l=2$  respectively [13]. The  $T_2$  representation is the irrational conjugate of  $T_1$

<sup>b</sup>  $U'$  and  $W'$  are constructed from symmetrized powers of the  $(\alpha\beta)$  spinor [16]. The  $E''$  representation is the irrational conjugate of  $E'$

matrices [16]. In this way six icosahedral representations have been defined using  $SU(2)$  representation theory. Three representations remain: the orbital representations  $T_2$  and  $G$  which form a basis for the  $J = 3$  level, and the spin representation  $E''$  which occurs in the decomposition of the  $J = 7/2$  level.

The  $T_2$  and  $E''$  species can easily be dealt with as they are *irrational conjugates* of  $T_1$  and  $E'$  respectively. This means that their representational matrices can be obtained from the  $\mathbb{D}^{T_1}(R)$  and  $\mathbb{D}^{E'}(R)$  matrices by simply changing the sign of  $\sqrt{5}$  on every occurrence [2]. The resulting matrices are listed in appendix A. It can immediately be verified that they obey the fixed inner automorphism of the  $C_2^{3,8}$  element. In Table 2 the complex  $T_2$  basis is related to the real basis of Boyle and Parker. On the other hand, the construction of a symmetry basis for the four-fold degenerate  $G$  representation is less straightforward, since this representation is self-conjugate. A useful strategy is to transform the three  $x, y, z$  components of  $G$  into a complex form using the standard basis relationships. The inner automorphism then requires that the remaining  $|Ga\rangle$  component should be multiplied by  $i$ . The phase-adapted component  $i|Ga\rangle$  will be denoted as  $|Gi\rangle$  (cf. Table 2). The generator matrices for this new basis are given in Appendix A, and the transformation formulae are displayed in Table 2.

This completes the construction of a complex orbital and spin basis for  $I^*$  which mimics the classical Wigner–Racah approach to the rotational group.

#### 4 The calculation of coupling coefficients

The coupling of icosahedral representations can most conveniently be described by Clebsch–Gordan coefficients of the type  $\langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle$ . These coefficients indicate how  $\Gamma_i$  and  $\Gamma_j$  representations combine to yield a resultant  $\Gamma$ .

$$|\Gamma \gamma\rangle = \sum_{\gamma_i \gamma_j} |\Gamma_i \gamma_i\rangle |\Gamma_j \gamma_j\rangle \langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle \quad (4)$$

The coefficients in this equation are – except for an overall phase – defined by the symmetry properties of the three representations involved. In the present section we show how these coefficients can be calculated, and discuss the specific characteristics of the coupling in the complex spin-orbit basis described in the previous section.

##### 4.1 The $A$ matrix method

The calculation of the  $\langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle$  coefficients was based on the  $A$  matrix method [2, 17, 18]. For a point group  $G$ , of order  $|G|$ , the elements of this matrix are given by:

$$A_{gg'} = \frac{1}{|G|} \sum_{R \in G} D_{\gamma_i \gamma_i}^{R_i}(R) D_{\gamma_j \gamma_j}^{R_j}(R) \overline{D_{\gamma \gamma'}^R(R)} \quad (5)$$

Here  $g$  and  $g'$  are compound indices denoting the respective triads  $\gamma_i \gamma_j \gamma$  and  $\gamma_i' \gamma_j' \gamma'$ . The coupling coefficients are obtained by normalizing a given column of  $A$ .

$$\langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle_{g_0} = |\Gamma|^{1/2} A_{gg_0} / (A_{g_0 g_0})^{1/2} \quad (6)$$

In Eq. (6)  $|\Gamma|$  is the dimension of  $\Gamma$  and  $g_0$  is any allowed triad of  $\gamma$ 's. Solutions

corresponding to different choices of  $g_0$  will differ by at most an overall phase factor. No attempt has been made to fix such external phase factors. If the  $\Gamma_i \times \Gamma_j$  product contains  $\Gamma$  more than once, different sets of coupling coefficients may be obtained by varying  $g_0$ . From these sets a complete separation of the product multiplicity may always be obtained [17]. Equations (5) and (6) also hold for the coupling of double-valued representations, provided the summation in Eq. (5) is extended over the double group  $G^*$ , of order  $2|G|$ . It can easily be shown that only an even number of double-valued representations can give rise to allowed coupling triads.

As in Ref. [2], a computer program was used to generate columns of the  $A$  matrix and to tabulate numerical coefficients. These were converted to algebraic expressions and typeset using computer editing to minimize human error. Selected tables of coefficients are presented in Appendix B, while a print-out of the complete Clebsch–Gordan series of orbit-orbit and spin-orbit couplings is made available as supplementary material. As expected, all coefficients are real. The form of the tables is the same as in our previous publication of coefficients for the icosahedral Boyle–Parker basis [2] and follows Griffith’s presentation of the cubic coupling coefficients [12, 19].

#### 4.2 The permutational symmetry of the coupling coefficients

As indicated by Griffith [20], it is usual for a Clebsch–Gordan formalism to define the phases of the coefficients in such a way that permutation of  $\Gamma_i \gamma_i$  and  $\Gamma_j \gamma_j$  does not change the coefficients when  $\Gamma_i \neq \Gamma_j$ , i.e.:

$$\langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle = \langle \Gamma_j \gamma_j \Gamma_i \gamma_i | \Gamma \gamma \rangle \quad (i \neq j) \quad (7)$$

Permutations involving the product representation  $\Gamma$  are not allowed, because of the complex conjugation of  $\mathbb{D}^\Gamma$  in Eq. (5). Nonetheless, for a basis which incorporates a fixed inner automorphism, an interesting relationship between  $\Gamma_i \times \Gamma_j = \Gamma$  and  $\Gamma_i \times \Gamma = \Gamma_j$  products can be established. To derive this relationship, the automorphism operation  $R_0$  is used to define new basis sets, denoted by a star.

$$|\Gamma \gamma^* \rangle \equiv R_0 |\Gamma \gamma \rangle \quad (8)$$

As an example the starred components of a Wigner–Racah basis may be obtained from Eq. (3) as:

$$|JM^* \rangle = (-1)^{J-M} |J-M \rangle \quad (9)$$

The corresponding bra’s are easily formed by inverting Eq. (8):

$$\langle \Gamma \gamma^* | = \langle \Gamma \gamma | R_0^{-1} \quad (10)$$

Combining these definitions with the matrix relation in Eq. (2) yields:

$$\begin{aligned} \overline{D}_{\gamma\gamma'}^{\Gamma}(R) &= \overline{\langle \Gamma \gamma | R | \Gamma \gamma' \rangle} \\ &= \langle \Gamma \gamma | R_0^{-1} R R_0 | \Gamma \gamma' \rangle \\ &= \langle \Gamma \gamma^* | R | \Gamma \gamma'^* \rangle \\ &= D_{\gamma^* \gamma'^*}^{\Gamma}(R) \end{aligned} \quad (11)$$

From this equation it is clear that the starred basis transforms as the complex

conjugate of the original basis. This result may now be substituted in Eq. (5) to relate the  $A$  matrices for  $\Gamma_i \times \Gamma_j = \Gamma$  and  $\Gamma_i \times \Gamma = \Gamma_j$  products.

$$A_{gg'}^{\Gamma_i \times \Gamma_j = \Gamma} = A_{g^*g'^*}^{\Gamma_i \times \Gamma = \Gamma_j} \quad (12)$$

with

$$g^* = (\gamma_i \quad \gamma^* \quad \gamma_j^*), \quad g'^* = (\gamma'_i \quad \gamma'^* \quad \gamma'_j^*)$$

Since the coupling coefficients are proportional to these matrix elements, one finally obtains from Eqs. (6) and (12):

$$|\Gamma|^{-1/2} \langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle_{g_0} = |\Gamma_j|^{-1/2} \langle \Gamma_i \gamma_i \Gamma \gamma^* | \Gamma_j \gamma_j^* \rangle_{g_0^*} \quad (13)$$

The starred components in the right-hand side of this equation can be replaced by components of the original basis, using the explicit forms of the inner automorphism relation, as specified in Appendix A.

### 4.3 Spherical symmetry properties of the coupling coefficients

The tables reveal an important consequence of the rotation group approach adopted in Sect. 3. Indeed, all representations of  $I^*$  that can be defined as irreducible images of spherical representations must couple in exactly the same way as the corresponding  $J$  levels. Coupling coefficients involving these representations will thus coincide – except for the external phase – with the well known Wigner coefficients which describe the coupling at the level of the spherical group [21].

A case in point is the  $T_1 \times T_1 = A + T_1 + H$  product which matches precisely the vector addition of two  $L = 1$  momenta:  $P \times P = S + P + D$ . This equivalence of icosahedral and spherical coupling coefficients also implies that standard operator techniques of angular momentum theory can be transferred to icosahedral basis sets. As an example the  $|H1\rangle$  component of the  $T_1 \times T_1 = H$  product may be obtained from the  $|H2\rangle$  component by lowering the pseudo- $M_L$  values of the  $T_1$  kets with a shift operator.

$$\begin{aligned} |H1\rangle &= \frac{1}{2} \mathcal{L}^- |H2\rangle = \frac{1}{2} (\mathcal{L}^- |T_1 1\rangle) |T_1 1\rangle + \frac{1}{2} |T_1 1\rangle (\mathcal{L}^- |T_1 1\rangle) \\ &= \frac{1}{\sqrt{2}} |T_1 0\rangle |T_1 1\rangle + \frac{1}{\sqrt{2}} |T_1 1\rangle |T_1 0\rangle \end{aligned} \quad (14)$$

The same linear combination indeed emerges from the corresponding  $T_1 \times T_1 = H$  coupling table.

A further interesting application of these operator techniques involves the assignment of pseudo- $J$  values to icosahedral spin-orbit levels. To this end the  $\mathcal{J}^2$  operator is expressed as  $\mathcal{L}^2 + \mathcal{S}^2 + \mathcal{L}^+ \mathcal{S}^- + \mathcal{L}^- \mathcal{S}^+ + 2\mathcal{L}_z \mathcal{S}_z$ . Clearly this operator will be defined if the coupled spin and orbit representations are irreducible images of spherical representations. It is not required that the resultant representation itself is also an irreducible image. As an example consider the  $T_1 \times W' = E''$  coupling table, given in the appendix. In this case the orbit and spin parts correspond respectively to  $L = 1$  and  $S = 5/2$  representations. This correspondence allows us to operate with  $\mathcal{L}$  and  $\mathcal{S}$  operators in the respective subspaces. Using the expressions for the  $E''$  kets from the appropriate coupling table, one obtains:

$$\mathcal{J}^2 |(T_1 \times W') E'' \alpha\rangle = 63/4 |(T_1 \times W') E'' \alpha\rangle \quad (15)$$

and similarly for  $|E''\beta\rangle$ . The pseudo- $J$  value associated with the  $E''$  spin-orbit level is thus seen to be  $7/2$ . In this way a correspondence can be established between the  $T_1 \times W' = E''$  coupling and the coupling in a  ${}^6P_{7/2}$  level. At this point a note of warning is in order. A correspondence such as the one just mentioned indicates only that a formal equivalence relation exists between both types of coupling. It does not imply a spherical parentage relation such as occurs in the theory of transition-metal ions.

#### 4.4 The separation of product multiplicities

Assignments of pseudo- $J$  values prove to be particularly useful for separation of the many product multiplicities that occur in the icosahedral double group. For the spin-orbit coupling tables no less than eight multiplicities must be addressed:

$$\begin{aligned}
 T_1 \times W' &= 2W' \\
 T_2 \times W' &= 2W' \\
 G \times U' &= 2W' \\
 G \times W' &= 2U' \\
 G \times W' &= 2W' \\
 H \times U' &= 2W' \\
 H \times W' &= 2U' \\
 H \times W' &= 3W'
 \end{aligned} \tag{16}$$

The cases involving  $T_1$  and  $H$  representations have straightforward solutions since spin and orbit representations have definite  $S$  and  $L$  assignments. Pseudo- $J$  values may thus be used to distinguish equisymmetric icosahedral product representations.

$$\begin{aligned}
 T_1 \times W' &= W'(J = 5/2) + W'(J = 7/2) \\
 H \times U' &= W'(J = 5/2) + W'(J = 7/2) \\
 H \times W' &= U'(J = 3/2) + U'(J = 9/2) \\
 H \times W' &= W'(J = 5/2) + W'(J = 7/2) + W'(J = 9/2)
 \end{aligned} \tag{17}$$

In Eq. (17) the half-integer values in brackets denote the pseudo- $J$  values associated with particular coupling results. These values are also specified in the coupling tables of the appendix. The actual calculation of these solutions proceeds via a Schmidt orthogonalisation of two columns of the  $A$  matrix, such that one resulting column has zero entries for the coupling of the highest pseudo- $M_J$  orbit and spin components. This column thus will describe the spin-orbit level of lower pseudo- $J$  value while its orthogonal counterpart will correspond to the level of higher resultant  $J$ .

The remaining four cases involving the  $T_2$  and  $G$  representations cannot be dealt with in this way since the orbit representations do not match a complete  $L$  manifold. In order to solve these problems we must first turn the spin-orbit products into spin-spin products by using the permutation rule of Eq. (13). The latter products are easily separable using pseudo- $L$  values.



$$\begin{aligned}
 W' \times W' &= T_2(L=3) + T_2(L=5) \\
 W' \times W' &= G(L=3) + G(L=4) \\
 W' \times U' &= G(L=3) + G(L=4)
 \end{aligned} \tag{18}$$

Coefficients obtained by this procedure may then be transformed back into a spin-orbit form, yielding the results in the tables. It is noteworthy that for the three cases involving  $G$  Schmidt orthogonalisation is unnecessary since the relevant  $A$  matrices already contain orthogonal columns which precisely correspond to the separation proposed in Eq. (18).

## 5 Examples of use of the tables

### 5.1 Icosahedral symmetry adaptation of a $L = 3$ manifold

As mentioned before, the  $|LM\rangle$  kets with  $L = 3$  span the reducible representation  $T_2 + G$ . The symmetry adaptation of this basis can be realised in three steps. In the first the  $|LM\rangle$  kets are decomposed into  $L_1$  and  $L_2$  states with known icosahedral symmetry:

$$|LM\rangle = \sum_{M_1 + M_2 = M} |L_1 M_1\rangle |L_2 M_2\rangle \langle L_1 M_1 L_2 M_2 | LM\rangle \tag{19}$$

The coefficients  $\langle L_1 M_1 L_2 M_2 | LM\rangle$  in Eq. (19) are the Wigner coefficients for the addition of two angular momenta [21]. With  $L = 3$ ,  $L_1 = 1$ ,  $L_2 = 2$  Eq. (19) yields:

$$\begin{aligned}
 |F \pm 3\rangle &= |P \pm 1\rangle |D \pm 2\rangle \\
 |F \pm 2\rangle &= (\sqrt{2}|P \pm 1\rangle |D \pm 1\rangle + |P0\rangle |D \pm 2\rangle) / \sqrt{3} \\
 |F \pm 1\rangle &= (\sqrt{6}|P \pm 1\rangle |D0\rangle + 2\sqrt{2}|P0\rangle |D \pm 1\rangle + |P \mp 1\rangle |D \pm 2\rangle) / \sqrt{15} \\
 |F0\rangle &= (|P + 1\rangle |D - 1\rangle + \sqrt{3}|P0\rangle |D0\rangle + |P - 1\rangle |D + 1\rangle) / \sqrt{5}
 \end{aligned} \tag{20}$$

In the second step the icosahedral symmetry adaptation of the  $L_1$  and  $L_2$  states is introduced, i.e.:

$$\begin{aligned}
 |L_1 M_1\rangle &= \sum_{\Gamma_1 \in L_1} \sum_{\gamma_1 \in \Gamma_1} |\Gamma_1 \gamma_1\rangle \langle \Gamma_1 \gamma_1 | L_1 M_1\rangle \\
 |L_2 M_2\rangle &= \sum_{\Gamma_2 \in L_2} \sum_{\gamma_2 \in \Gamma_2} |\Gamma_2 \gamma_2\rangle \langle \Gamma_2 \gamma_2 | L_2 M_2\rangle
 \end{aligned} \tag{21}$$

For the case under consideration, Eq. (21) adopts a particularly simple form since both  $P$  and  $D$  states transform irreducibly in  $I$  (as  $T_1$  and  $H$ , respectively) and

$$\begin{aligned}
 \langle \Gamma_1 \gamma_1 | P M_1\rangle &= \delta_{\Gamma_1 T_1} \delta_{\gamma_1 M_1} \\
 \langle \Gamma_2 \gamma_2 | D M_2\rangle &= \delta_{\Gamma_2 H} \delta_{\gamma_2 M_2}
 \end{aligned} \tag{22}$$

Hence in Eq. (20)  $P$  and  $D$  can be replaced by  $T_1$  and  $H$ , respectively.

Finally in the third step the  $|\Gamma_1 \gamma_1\rangle |\Gamma_2 \gamma_2\rangle$  ket products are recoupled to  $|\Gamma \gamma\rangle$  states with irreducible symmetry characteristics.

$$|\Gamma_1 \gamma_1\rangle |\Gamma_2 \gamma_2\rangle = \sum_{\Gamma \in \Gamma_1 \times \Gamma_2} \sum_{\gamma \in \Gamma} |\Gamma \gamma\rangle \langle \Gamma_1 \gamma_1 \Gamma_2 \gamma_2 | \Gamma \gamma\rangle \tag{23}$$

The coupling coefficients in this expression are contained in a single row of the  $\Gamma_1 \times \Gamma_2$  coupling tables. As an example, the recoupling of the  $|T_1 + 1\rangle|H + 2\rangle$  product reads:

$$|T_1 + 1\rangle|H + 2\rangle = (-3|T_2 + 1\rangle - \sqrt{5}|T_2 - 1\rangle - \sqrt{3}|G + 1\rangle + \sqrt{15}|G - 1\rangle)/4\sqrt{2} \quad (24)$$

Substitution of the recoupling expressions in Eq. (20) then yields the icosahedral symmetries of the  $F$  levels:

$$\begin{aligned} |F \pm 3\rangle &= (-3|T_2 \pm 1\rangle - \sqrt{5}|T_2 \mp 1\rangle - \sqrt{3}|G \pm 1\rangle + \sqrt{15}|G \mp 1\rangle)/4\sqrt{2} \\ |F \pm 2\rangle &= (\sqrt{3}|T_2 0\rangle \pm 2|Gi\rangle + |G0\rangle)/2\sqrt{2} \\ |F \pm 1\rangle &= (-\sqrt{3}|T_2 \pm 1\rangle + \sqrt{15}|T_2 \mp 1\rangle + 3|G \pm 1\rangle + \sqrt{5}|G \mp 1\rangle)/4\sqrt{2} \\ |F0\rangle &= (|T_2 0\rangle - \sqrt{3}|G0\rangle)/2 \end{aligned} \quad (25)$$

In principle the method can be extended to manifolds of arbitrary high  $L$  or  $J$  value. It avoids complicating multiplicity issues since the product form of the resultant states (see Eq. (23)) provides a complete labelling system. Equation (25) has obvious applications to the finite group symmetry adaptation of the levels of a rare earth atom, enclosed by a  $C_{60}$  cage. Such endohedral  $M@C_n$  clusters are currently at the focus of intense research activity [22]. Further applications might involve the analysis of half-integral  $J$  eigen levels of rotational tensor Hamiltonians for icosahedral molecules [23].

### 5.2 Zeeman splitting of $U'$ states

The perturbation Hamiltonian for a system in a magnetic field is:

$$\mathcal{H} = -\mu \cdot \mathbf{H} \quad (26)$$

where  $\mathbf{H}$  is the magnetic field vector and  $\mu$  is the magnetic dipole operator. The corresponding Zeeman effect for an icosahedral  $U'$  state is described to first order by a  $4 \times 4$  perturbation matrix with elements:

$$\langle U'i | \mathcal{H} | U'j \rangle = \langle U'i | -\mu | U'j \rangle \cdot \mathbf{H} \quad (27)$$

Since the magnetic dipole operator transforms as  $T_1$  each matrix element in Eq. (27) can be factorized into a  $U'T_1U'$  coupling coefficient and a parameter  $K$ .

$$\begin{aligned} \langle U'i | -\mu_z | U'j \rangle &= K \langle U'i | T_1 0 U'j \rangle \\ \langle U'i | -\mu_x | U'j \rangle &= K (-\langle U'i | T_1 + 1 U'j \rangle + \langle U'i | T_1 - 1 U'j \rangle) \sqrt{2} \\ \langle U'i | -\mu_y | U'j \rangle &= iK (\langle U'i | T_1 + 1 U'j \rangle + \langle U'i | T_1 - 1 U'j \rangle) \sqrt{2} \end{aligned} \quad (28)$$

Here we have made use of the relationship between real and complex  $T_1$  components as given in Table 2. In order to convert these expressions into a spin Hamiltonian formalism the parameter  $K$  must be replaced by a more convenient  $g$  factor. This factor will be defined in such a way that the energy of the  $|U' + 3/2\rangle$  component in a magnetic field along the  $z$  direction equals  $3/2g\beta H_z$  ( $\beta$  is the Bohr magneton). Hence one has by definition:

$$\langle U' + 3/2 | -\mu_z | U' + 3/2 \rangle \equiv 3/2g\beta \quad (29)$$

Combining Eqs. (28) and (29) yields:

$$K = \frac{\sqrt{15}}{2} g\beta \quad (30)$$

The Hamiltonian can then be rewritten as follows:

$$\mathcal{H} = g\beta\mathcal{S} \cdot \mathbf{H} \quad (31)$$

Here  $\mathcal{S}$  is an effective spin operator. Its matrix form can be derived from Eqs. (28) and (30).

$$\begin{aligned} \langle U'i|\mathcal{S}_z|U'j\rangle &= \frac{\sqrt{15}}{2} \langle U'i|T_1 0U'j\rangle \\ \langle U'i|\mathcal{S}_x|U'j\rangle &= \frac{\sqrt{15}}{2\sqrt{2}} (-\langle U'i|T_1 + 1U'j\rangle + \langle U'i|T_1 - 1U'j\rangle) \\ \langle U'i|\mathcal{S}_y|U'j\rangle &= \frac{i\sqrt{15}}{2\sqrt{2}} (\langle U'i|T_1 + 1U'j\rangle + \langle U'i|T_1 - 1U'j\rangle) \end{aligned} \quad (32)$$

Note that the coupling coefficients involved are all real. Hence bra's and kets in these coefficients can be interchanged to attain the familiar  $\langle T_1 0U'j|U'i\rangle$  and  $\langle T_1 \pm 1U'j|U'i\rangle$  format of the  $T_1 \times U' = U'$  coupling table. In this way the matrix elements of the spin operators are readily obtained. They are listed in Table 3. It is easily verified that the matrices in the table obey the commutation relations of angular momentum theory, i.e.:

$$[\mathcal{S}_x, \mathcal{S}_y] = i\mathcal{S}_z \quad (\text{and cyclic permutations}) \quad (33)$$

Once again this illustrates the residual spherical symmetry of the icosahedral coupling coefficients. As a result the Zeeman splitting of an icosahedral  $U'$  level will be isotropic with eigenvalues  $\pm 3/2g\beta H$ ,  $\pm 1/2g\beta H$ . This splitting pattern is formally equivalent to the splitting of a quartet spin level. It is different though

**Table 3.** Matrix form of the spin Hamiltonian for icosahedral  $U'$  states<sup>a</sup>

$$\begin{aligned} \mathcal{S}_z &= \begin{bmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{bmatrix} \\ \mathcal{S}_x &= \begin{bmatrix} 0 & \sqrt{\frac{3}{2}} & 0 & 0 \\ \sqrt{\frac{3}{2}} & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{\frac{3}{2}} \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 \end{bmatrix} \\ \mathcal{S}_y &= \begin{bmatrix} 0 & -\sqrt{\frac{3}{2}} & 0 & 0 \\ \sqrt{\frac{3}{2}} & 0 & -1 & 0 \\ 0 & 1 & 0 & -\sqrt{\frac{3}{2}} \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 \end{bmatrix} \end{aligned}$$

<sup>a</sup> The component ordering is:  $|U' + 3/2\rangle$ ,  $|U' + 1/2\rangle$ ,  $|U' - 1/2\rangle$ ,  $|U' - 3/2\rangle$ .

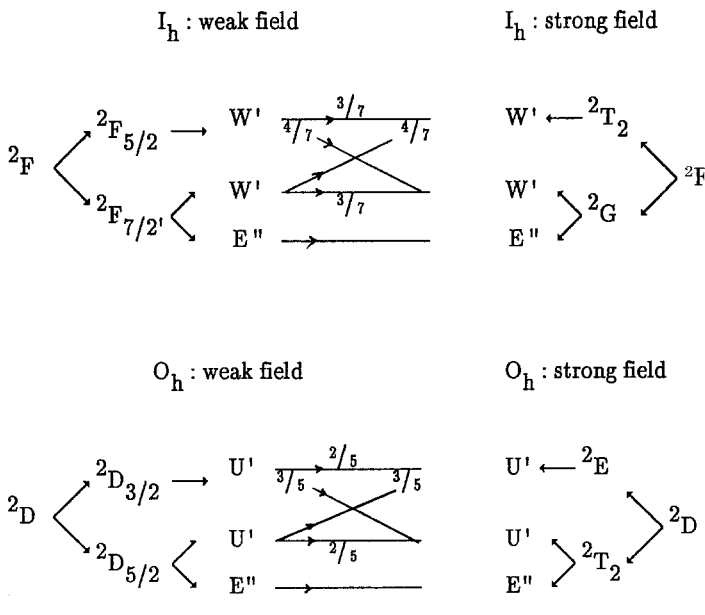
from the Zeeman effect in an *octahedral*  $U'$  state, which is in principle anisotropic [24].

The isotropy of the Zeeman effect for all icosahedral and some octahedral  $U'$  states has an interesting group-theoretical background. It points to the presence of a  $SO(3)$  invariance group in the  $SO(5)$  symmetry of the fourfold degenerate  $U'$  state [25].

### 5.3 Crystal field splitting of ${}^2F$ terms

As a final example we examine the crystal field splitting of  ${}^2F$  terms in an icosahedral environment. This application should be useful to describe the spectral features of a lanthanide inside a  $C_{60}$  cage. The branching rules governing this splitting are schematically represented in Table 4. Two coupling limits must be considered. In the weak-field limit spin-orbit coupling prevails. It resolves the free ion multiplet into  ${}^2F_{7/2}$  and  ${}^2F_{5/2}$  levels. A small crystal field perturbation of icosahedral symmetry will lead to further branching into  $W'(7/2)$ ,  $E''(7/2)$  and  $W'(5/2)$  crystal field components. By contrast, in the strong-field coupling limit the primary branching process is the  ${}^2F \rightarrow {}^2T_2 + {}^2G$  crystal field splitting. The spin-orbit components of these states are  $W'(T_2)$ ,  $W'({}^2G)$  and  $E''({}^2G)$ . Clearly since only one  $E''$  level is present the  $E''(7/2)$  and  $E''({}^2G)$  states must coincide. On the other hand, it can be expected that the composition of the two  $W'$  states will vary as a function of the coupling conditions. The  $W'$  eigenfunctions of the strong field limit can be determined from the  $T_2 \times E' = W'$  and  $G \times E' = W'$

**Table 4.** Comparison of branching schemes for  ${}^2F$  terms in icosahedral fields and  ${}^2D$  terms in cubic fields. Relative weights of the  $W'$  and  $U'$  branches are indicated



coupling tables. For example, the  $|W' + 5/2\rangle$  components read:

$$\begin{aligned} |W'(^2T_2) + 5/2\rangle &= (\sqrt{2}|T_2 0\rangle|E'\alpha\rangle + 3|T_2 + 1\rangle|E'\beta\rangle + \sqrt{5}|T_2 - 1\rangle|E'\beta\rangle)/4 \\ |W'(^2G) + 5/2\rangle &= (2\sqrt{2}|Gi\rangle|E'\alpha\rangle + \sqrt{2}|G0\rangle|E'\alpha\rangle + 3|G + 1\rangle|E'\beta\rangle \\ &\quad - 3\sqrt{5}|G - 1\rangle|E'\beta\rangle)/8 \end{aligned} \quad (34)$$

In the weak-field limit the starting eigenfunctions are the  $|JM\rangle$  kets of the free ion. These may be determined using the familiar techniques of atomic spectroscopy [21]. As an example, the  $|5/2\ 5/2\rangle$  ket is given by:

$$|5/2\ 5/2\rangle = (|F + 2\rangle|1/2\ 1/2\rangle - \sqrt{6}|F + 3\rangle|1/2 - 1/2\rangle)\sqrt{7} \quad (35)$$

Icosahedral symmetry adaptation of these functions can be achieved by following the general procedure outlined in the first example of this section. In the case of the  $J = 5/2$  term this symmetry adaptation is particularly straightforward since this manifold forms an irreducible basis for the  $W'(5/2)$  representation. Furthermore, the  $S = 1/2$  spin part matches the  $E'$  representation, while the icosahedral symmetry of the  $L = 3$  orbit part is specified in Eq. (25). Combining Eqs (25) and (35) one thus obtains for the  $|W'(5/2) + 5/2\rangle$  component

$$\begin{aligned} |W'(5/2) + 5/2\rangle &= (2\sqrt{3}|T_2 0\rangle|E'\alpha\rangle + 4|Gi\rangle|E'\alpha\rangle + 2|G0\rangle|E'\alpha\rangle \\ &\quad + 3\sqrt{6}|T_2 + 1\rangle|E'\beta\rangle + \sqrt{30}|T_2 - 1\rangle|E'\beta\rangle \\ &\quad + 3\sqrt{2}|G + 1\rangle|E'\beta\rangle - 3\sqrt{10}|G - 1\rangle|E'\beta\rangle)/4\sqrt{14} \end{aligned} \quad (36)$$

The overlap integrals between this function and the equisymmetric strong field components of Eq. (34) are as follows:

$$\begin{aligned} \langle W'(^2T_2) + 5/2 | W'(5/2) + 5/2 \rangle &= \sqrt{3/7} \\ \langle W'(^2G) + 5/2 | W'(5/2) + 5/2 \rangle &= \sqrt{4/7} \end{aligned} \quad (37)$$

Alternatively one may write:

$$(3 \times 1/2)^{5/2} = \sqrt{3/7}(T_2 \times E)^{W'} + \sqrt{4/7}(G \times E)^{W'} \quad (38)$$

This equation illustrates the mixing of the  $W'$  levels as a function of the coupling scheme. It shows that the distribution of the weak-field level  $W'(5/2)$  over  $W'(^2T_2)$  and  $W'(^2G)$  strong-field levels follows a ratio of 3:4. This is precisely the ratio of the orbital degeneracies of the parent  $^2T_2$  and  $^2G$  states. From normalization conditions it further follows that the other weak field level  $W'(7/2)$  will have the inverse branching ratio of 4:3.

Interestingly, an analogous pattern can be shown to hold for the  $^2D$  terms in cubic symmetries (cf. Table 4).

## 6 Discussion

In the spherical symmetry group  $\langle J_1 M_1 J_2 M_2 | JM \rangle$  coupling coefficients are related to the so-called  $3j$ -symbols which have a well defined permutational symmetry. The use of these compact symbols was advocated primarily because it reduces the length of tables of coupling coefficients. Furthermore the permutational symmetry of the symbols proved to be a very important tool for working out general expressions of complicated coupling processes. With the implementation of Clebsch-Gordan algorithms the need for compressed symbols has disappeared. However, the algebraic versatility of Wigner's  $3j$ -symbols continues to be of considerable importance.

For the finite point groups the situation is somewhat different. Here too compact so-called  $3T$  symbols have been introduced to incorporate the permutational symmetry of the  $\langle T_1\gamma_1 T_2\gamma_2 | T\gamma \rangle$  coefficients. However, this necessitated the use of delicate phase factors which have an *ad hoc* character. The product multiplicity problems in these groups add to the confusion. Hence, since there is no real algebraic advantage of adopting these coefficients for the finite point groups, we have chosen to present our results in the direct coupling format, introduced by Griffith [12]. A glance at such tables immediately exposes the structure of a product representation. Read horizontally the tables reveal how a particular ket product is distributed over the coupled states.

On the methodological level coupling coefficients for cubic and icosahedral groups are usually calculated via a subduction method [26]. In order to solve multiplicity problems this procedure may require the use of secondary basis sets (see e.g. [10]). In contrast the  $A$  matrix method which we have used in the present paper is entirely based on the symmetry properties of the finite point group. The programming of the basic expression in Eq. (5) makes use of a cyclic coset expansion of  $I$  in its tetrahedral subgroup, as described previously [2]. This greatly facilitates the implementation of the method.

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#### *Supplementary material*

A print-out of the complete Clebsch–Gordan series of orbit-orbit and spin-orbit couplings (88 tables) is made available.

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## Appendix A

The complex orbital and spin basis for the icosahedral group is defined by a set of representational matrices for relevant generators. A row vector notation is adopted, i.e.:

$$R(\cdots |T\gamma\rangle \cdots) = (\cdots |T\gamma\rangle \cdots) \mathbb{D}^T(R)$$

The standard order of the components is  $(1, -1, 0)$  for  $T_1$  and  $T_2$ ,  $(i, 1, -1, 0)$  for  $G$ ,  $(2, -2, 1, -1, 0)$  for  $H$ ,  $(\alpha, \beta)$  for  $E'$  and  $E''$ ,  $(3/2, 1/2, -1/2, -3/2)$  for  $U'$ , and  $(5/3, 3/2, 1/2, -1/2, -3/2, -5/2)$  for  $W'$ . The relevant symmetry elements are defined in the figure. The poles of all these elements fall in the positive hemisphere. The representational matrices for the fundamental spinor representation  $E'$  follow the conventions given by Altmann [15]. The golden number  $(\sqrt{5} + 1)/2$  is denoted by  $\phi$ . Its irrational conjugate  $(-\sqrt{5} + 1)/2$  is equal to  $-\phi^{-1}$ .

	$C_2^{3,8}$		$C_3^{1,4,3}$
$T_1, T_2$	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$1/2$	$\begin{bmatrix} -i & i & -\sqrt{2} \\ -i & i & \sqrt{2} \\ -i\sqrt{2} & -i\sqrt{2} & 0 \end{bmatrix}$
$G$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$	$1/2$	$\begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & -i & i & -\sqrt{2} \\ 0 & -i & i & \sqrt{2} \\ 0 & -i\sqrt{2} & -\sqrt{2} & 0 \end{bmatrix}$
$H$	$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$	$1/4$	$\begin{bmatrix} -1 & -1 & 2i & -2i & \sqrt{6} \\ -1 & -1 & -2i & 2i & \sqrt{6} \\ -2 & 2 & 2i & 2i & 0 \\ -2 & 2 & -2i & -2i & 0 \\ -\sqrt{6} & -\sqrt{6} & 0 & 0 & -2 \end{bmatrix}$
$E', E''$	$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$	$1/2$	$\begin{bmatrix} 1-i & -1-i \\ 1-i & 1+i \end{bmatrix}$
$U'$	$\begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$	$1/4$	$\begin{bmatrix} -1-i & -\sqrt{3}(1-i) & \sqrt{3}(1+i) & 1-i \\ -\sqrt{3}(1+i) & -1+i & -1-i & -\sqrt{3}(1-i) \\ -\sqrt{3}(1+i) & 1-i & -1-i & \sqrt{3}(1-i) \\ -1-i & \sqrt{3}(1-i) & \sqrt{3}(1+i) & -1+i \end{bmatrix}$

$$W' \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad 1/8 \begin{bmatrix} -1+i & \sqrt{5}(1+i) & \sqrt{10}(1-i) & -\sqrt{10}(1+i) & -\sqrt{5}(1-i) & 1+i \\ -\sqrt{5}(1-i) & 3+3i & \sqrt{2}(1-i) & \sqrt{2}(1+i) & 3-3i & -\sqrt{5}(1+i) \\ -\sqrt{10}(1-i) & \sqrt{2}(1+i) & -2+2i & 2+2i & -\sqrt{2}(1-i) & \sqrt{10}(1+i) \\ -\sqrt{10}(1-i) & -\sqrt{2}(1+i) & -2+2i & -2-2i & -\sqrt{2}(1-i) & -\sqrt{10}(1+i) \\ -\sqrt{5}(1-i) & -3-3i & \sqrt{2}(1-i) & -\sqrt{2}(1+i) & 3-3i & \sqrt{5}(1+i) \\ -1+i & -\sqrt{5}(1+i) & \sqrt{10}(1-i) & \sqrt{10}(1+i) & -\sqrt{5}(1-i) & -1-i \end{bmatrix}$$

$C_5^{1,12}$

$$T_1 \quad 1/4 \begin{bmatrix} \phi-2i\phi & -\phi^{-2} & \sqrt{2}(\phi^{-1}+i) \\ -\phi^{-2} & \phi+2i\phi & \sqrt{2}(\phi^{-1}-i) \\ -\sqrt{2}(\phi^{-1}+i) & \sqrt{2}(\phi^{-1}-i) & 2\phi \end{bmatrix}$$

$$T_2 \quad 1/4 \begin{bmatrix} -\phi^{-1}+2i\phi^{-1} & -\phi^2 & \sqrt{2}(\phi-i) \\ -\phi^2 & -\phi^{-1}-2i\phi^{-1} & -\sqrt{2}(\phi+i) \\ \sqrt{2}(\phi-i) & -\sqrt{2}(\phi+i) & -2\phi^{-1} \end{bmatrix}$$

$$G \quad 1/4\sqrt{2} \begin{bmatrix} -1 & -\sqrt{5}(1+i) & -\sqrt{5}(1-i) & -i\sqrt{10} \\ -\sqrt{5}(1+i) & -\sqrt{2}(2+i) & \sqrt{2} & 1+3i \\ -\sqrt{5}(1-i) & \sqrt{2} & -\sqrt{2}(2-i) & -1+3i \\ -i\sqrt{10} & 1+3i & -1+3i & \sqrt{2} \end{bmatrix}$$

$$H \quad 1/16 \begin{bmatrix} -3\phi^{-2}-4i\phi^2 & \phi^{-4} & -2\phi^3+2i\phi^{-2} & 2\phi^{-3}+2i\phi^{-2} & -\sqrt{6}\phi^{-1}(1-2i) \\ \phi^{-4} & -3\phi^2+4i\phi^2 & -2\phi^{-3}+2i\phi^{-2} & 2\phi^3+2i\phi^{-2} & -\sqrt{6}\phi^{-1}(1+2i) \\ -2\phi^3+2i\phi^{-2} & -2\phi^{-3}+2i\phi^{-2} & 4-8i & -4 & -2\sqrt{6}(1+i\phi) \\ 2\phi^{-3}+2i\phi^{-2} & 2\phi^3+2i\phi^{-2} & -4 & 4+8i & 2\sqrt{6}(1-i\phi) \\ -\sqrt{6}\phi^{-1}(1-2i) & -\sqrt{6}\phi^{-1}(1+2i) & -2\sqrt{6}(1+i\phi) & 2\sqrt{6}(1-i\phi) & 2\phi^3-2\phi^{-2} \end{bmatrix}$$

$$E' \quad 1/2 \begin{bmatrix} \phi-i & -i\phi^{-1} \\ -i\phi^{-1} & \phi+i \end{bmatrix}$$

$$E'' \quad 1/2 \begin{bmatrix} -\phi^{-1}-i & i\phi \\ i\phi & -\phi^{-1}+i \end{bmatrix}$$

$$U' \quad 1/8 \begin{bmatrix} -\phi^{-1}-i\phi^4 & -\sqrt{3}(2+i) & -\sqrt{3}(\phi^{-1}-i\phi^{-2}) & i\phi^{-3} \\ -\sqrt{3}(2+i) & 3+\phi+i(3-\phi^{-4}) & -i(4+\phi^{-3}) & -\sqrt{3}(\phi^{-1}+i\phi^{-2}) \\ -\sqrt{3}(\phi^{-1}-i\phi^{-2}) & -i(4+\phi^{-3}) & 3+\phi+i(3-\phi^{-4}) & \sqrt{3}(2-i) \\ i\phi^{-3} & -\sqrt{3}(\phi^{-1}+i\phi^{-2}) & \sqrt{3}(2-i) & -\phi^{-1}+i\phi^4 \end{bmatrix}$$



$$\begin{array}{ccccccc}
 -7-10\phi^{-1}(1+5\phi) & -\sqrt{5}\phi(4-3i) & \sqrt{10}\phi^{-3}+i\phi^2 & \sqrt{10}\phi^{-2}(2+i) & \sqrt{5}(\phi^{-3}-i\phi^{-4}) & -i\phi^{-5} \\
 -\sqrt{5}\phi(4-3i) & -5+6\phi^{-1}(3+7\phi) & -2\sqrt{2}(5\phi-2)-i\sqrt{2}(5\phi-2) & -\sqrt{2}(2\phi+3)+i\sqrt{2}(3\phi-1) & \sqrt{5}(\phi^{-3}+i\phi^{-4}) & \sqrt{5}(\phi^{-3}+i\phi^{-4}) \\
 \sqrt{10}(\phi^{-3}+i\phi^2) & -2\sqrt{2}(5\phi-2)-i\sqrt{2}(5\phi-2) & 2\phi^3-2i\phi^2 & -2i(\phi+8) & -\sqrt{10}\phi^{-2}(2-i) & -\sqrt{10}\phi^{-2}(2-i) \\
 \sqrt{10}\phi^{-2}(2+i) & -\sqrt{2}(2\phi+3)+i\sqrt{2}(3\phi-1) & -2i(\phi+8) & 2\phi^3+2i\phi^2 & 2\sqrt{2}(5\phi-2)-i\sqrt{2}(5\phi-2) & \sqrt{10}(\phi^{-3}-i\phi^2) \\
 \sqrt{5}(\phi^{-3}-i\phi^{-4}) & i(7\phi-8) & -\sqrt{2}(2\phi+3)-i\sqrt{2}(3\phi-1) & 2\sqrt{2}(5\phi-2)-i\sqrt{2}(5\phi-2) & 6\phi^{-1}-5+i(3+7\phi) & \sqrt{5}\phi(4+3i) \\
 -i\phi & \sqrt{5}(\phi^{-3}+i\phi^{-4}) & -\sqrt{10}\phi^{-2}(2-i) & \sqrt{10}(\phi^{-3}-i\phi^2) & \sqrt{5}\phi(4+3i) & -7-10\phi+i(5\phi+1)
 \end{array}$$

W<sup>1</sup> 1/32

**Appendix B**

Tables of Clebsch–Gordan coupling coefficients for typical orbit  $\times$  orbit and spin  $\times$  orbit products in the icosahedral double group. The orbit  $\times$  orbit products  $T_1 \times T_1$  (Table B1) and  $T_1 \times H$  (Table B2) are needed for working the examples described in the main text. Tables B3 to B6 give all products of an orbit representation and the spin 1/2 representation  $E'$ , and Tables B7 to B10 list the equivalent products for the spin 3/2 representation  $U'$ . Table B11 and B12 illustrate the resolution of multiplicities in the partial products  $T_2 \times W' = 2W' + \dots$  and  $H \times W' = 3W' + \dots$ .

**Table B1.**  $T_1 \times T_1 = A + T_1 + H$

$T_1$ $T_1$	$A$	$T_1$			$H$				
		0	1	-1	2	-2	1	-1	0
0 0	$\frac{1}{\sqrt{3}}$	.	.	.	.	.	.	.	$\frac{\sqrt{2}}{\sqrt{3}}$
0 1	.	.	$\frac{1}{\sqrt{2}}$	.	.	.	$\frac{1}{\sqrt{2}}$	.	.
0 -1	.	.	.	$-\frac{1}{\sqrt{2}}$	.	.	.	$\frac{1}{\sqrt{2}}$	.
1 0	.	.	$-\frac{1}{\sqrt{2}}$	.	.	.	$\frac{1}{\sqrt{2}}$	.	.
1 1	.	.	.	.	1	.	.	.	.
1 -1	$-\frac{1}{\sqrt{3}}$	$-\frac{1}{\sqrt{2}}$	.	.	.	.	.	.	$\frac{1}{\sqrt{6}}$
-1 0	.	.	.	$\frac{1}{\sqrt{2}}$	.	.	.	$\frac{1}{\sqrt{2}}$	.
-1 1	$-\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{2}}$	.	.	.	.	.	.	$\frac{1}{\sqrt{6}}$
-1 -1	.	.	.	.	.	1	.	.	.

**Table B3.**  $T_1 \times E' = E'(J = \frac{1}{2}) + U'(J = \frac{3}{2})$

$T_1$ $E'$	$E'$		$U'$			
	$\alpha$	$\beta$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$
0 $\alpha$	$\frac{1}{\sqrt{3}}$	.	.	$\frac{\sqrt{2}}{\sqrt{3}}$	.	.
0 $\beta$	.	$-\frac{1}{\sqrt{3}}$	.	.	$\frac{\sqrt{2}}{\sqrt{3}}$	.
1 $\alpha$	.	.	1	.	.	.
1 $\beta$	$-\frac{\sqrt{2}}{\sqrt{3}}$	.	.	$\frac{1}{\sqrt{3}}$	.	.
-1 $\alpha$	.	$\frac{\sqrt{2}}{\sqrt{3}}$	.	.	$\frac{1}{\sqrt{3}}$	.
-1 $\beta$	.	.	.	.	.	1

Table B2.  $T_1 \times H = T_1 + T_2 + G + H$ 

$T_1$	$H$	$T_1$		$T_2$			$G$				$H$					
		0	1	-1	0	1	-1	$i$	0	1	-1	2	-2	1	-1	0
0	2	.	.	.	$\frac{1}{2\sqrt{2}}$	.	.	$\frac{1}{\sqrt{6}}$	.	.	.	$\frac{\sqrt{2}}{\sqrt{3}}$	.	.	.	.
0	-2	.	.	.	$\frac{1}{2\sqrt{2}}$	.	.	$-\frac{1}{\sqrt{6}}$	.	.	.	.	$-\frac{\sqrt{2}}{\sqrt{3}}$	.	.	.
0	1	.	$\frac{\sqrt{3}}{\sqrt{10}}$	.	.	$\frac{1}{2}$	.	.	$\frac{\sqrt{3}}{2\sqrt{5}}$	.	$\frac{1}{\sqrt{6}}$	.	.	$\frac{1}{\sqrt{6}}$	.	.
0	-1	.	$\frac{\sqrt{3}}{\sqrt{10}}$	.	.	$-\frac{1}{2}$	.	.	$-\frac{1}{2\sqrt{5}}$	.	.	.	.	$-\frac{1}{\sqrt{6}}$	.	.
0	0	$\frac{\sqrt{2}}{\sqrt{5}}$	.	.	$\frac{\sqrt{3}}{2\sqrt{5}}$	.	.	.	$-\frac{3}{2\sqrt{5}}$	.	.	.	.	.	.	.
1	2	.	.	.	.	$-\frac{3}{4\sqrt{2}}$	.	.	$-\frac{\sqrt{3}}{4\sqrt{2}}$	.	$\frac{\sqrt{15}}{4\sqrt{2}}$	.	.	.	.	.
1	-2	.	$-\frac{\sqrt{3}}{\sqrt{5}}$	.	.	$\frac{1}{4\sqrt{2}}$	.	.	$\frac{1}{4\sqrt{6}}$	.	$\frac{\sqrt{3}}{4\sqrt{10}}$	.	.	$-\frac{1}{\sqrt{3}}$	.	.
1	1	.	.	.	$\frac{1}{2}$	.	.	$\frac{1}{\sqrt{3}}$	$\frac{1}{2\sqrt{5}}$	.	.	$-\frac{1}{\sqrt{3}}$	.	.	.	.
1	-1	$-\frac{\sqrt{3}}{\sqrt{10}}$	.	.	$\frac{1}{2\sqrt{5}}$	.	.	.	$-\frac{\sqrt{3}}{2\sqrt{5}}$	.	.	.	.	.	.	$-\frac{1}{\sqrt{2}}$
1	0	.	$-\frac{1}{\sqrt{10}}$	.	.	$-\frac{\sqrt{3}}{4\sqrt{5}}$	.	.	$\frac{3}{4\sqrt{5}}$	.	$\frac{1}{4}$	.	.	$-\frac{1}{\sqrt{2}}$	.	.
-1	2	.	$-\frac{\sqrt{3}}{\sqrt{5}}$	.	.	$-\frac{1}{4\sqrt{10}}$	.	.	$\frac{\sqrt{3}}{4\sqrt{10}}$	.	$\frac{1}{4\sqrt{6}}$	.	.	$\frac{1}{\sqrt{3}}$	.	.
-1	-2	.	$-\frac{\sqrt{3}}{\sqrt{5}}$	.	.	$-\frac{3}{4\sqrt{2}}$	.	.	$-\frac{\sqrt{3}}{4\sqrt{2}}$	.	$-\frac{\sqrt{15}}{4\sqrt{2}}$	.	.	.	.	$\frac{1}{\sqrt{2}}$
-1	1	$-\frac{\sqrt{3}}{\sqrt{10}}$	.	.	$\frac{1}{2\sqrt{5}}$	.	.	.	$-\frac{\sqrt{3}}{2\sqrt{5}}$	.	.	.	.	.	.	.
-1	-1	.	.	.	$\frac{1}{2}$	.	.	$-\frac{1}{\sqrt{3}}$	$\frac{1}{2\sqrt{5}}$	.	.	.	.	$\frac{1}{\sqrt{3}}$	.	.
-1	0	.	$-\frac{1}{\sqrt{10}}$	.	.	$\frac{\sqrt{3}}{4}$	.	.	$-\frac{\sqrt{3}}{4\sqrt{5}}$	.	$\frac{1}{4}$	.	.	.	$\frac{1}{\sqrt{2}}$	.

Table B4.  $T_2 \times E' = W'$ 

$T_2$	$E'$	$W'$					
		$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
0	$\alpha$	$\frac{1}{2\sqrt{2}}$	.	$\frac{1}{2}$	.	$\frac{\sqrt{5}}{2\sqrt{2}}$	.
0	$\beta$	.	$-\frac{\sqrt{5}}{2\sqrt{2}}$	.	$-\frac{1}{2}$	.	$-\frac{1}{2\sqrt{2}}$
1	$\alpha$	.	$-\frac{1}{4}$	.	$\frac{\sqrt{5}}{2\sqrt{2}}$	.	$-\frac{\sqrt{5}}{4}$
1	$\beta$	$\frac{3}{4}$	.	$\frac{1}{2\sqrt{2}}$	.	$-\frac{\sqrt{5}}{4}$	.
-1	$\alpha$	.	$\frac{\sqrt{5}}{4}$	.	$-\frac{1}{2\sqrt{2}}$	.	$-\frac{3}{4}$
-1	$\beta$	$\frac{\sqrt{5}}{4}$	.	$-\frac{\sqrt{5}}{2\sqrt{2}}$	.	$\frac{1}{4}$	.

Table B5.  $G \times E' = E'' + W'$ 

$G$	$E'$	$E''$		$W'$					
		$\alpha$	$\beta$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
$i$	$\alpha$	$\frac{1}{2}$	.	$\frac{1}{2\sqrt{2}}$	.	.	.	$-\frac{\sqrt{5}}{2\sqrt{2}}$	.
$i$	$\beta$	.	$\frac{1}{2}$	.	$-\frac{\sqrt{5}}{2\sqrt{2}}$	.	.	.	$\frac{1}{2\sqrt{2}}$
0	$\alpha$	$\frac{1}{2}$	.	$\frac{1}{4\sqrt{2}}$	.	$-\frac{3}{4}$	.	$\frac{\sqrt{5}}{4\sqrt{2}}$	.
0	$\beta$	.	$-\frac{1}{2}$	.	$-\frac{\sqrt{5}}{4\sqrt{2}}$	.	$\frac{3}{4}$	.	$-\frac{1}{4\sqrt{2}}$
1	$\alpha$	.	.	.	$\frac{3}{8}$	.	$\frac{\sqrt{5}}{4\sqrt{2}}$	.	$\frac{3\sqrt{5}}{8}$
1	$\beta$	$-\frac{1}{\sqrt{2}}$	.	$\frac{3}{8}$	.	$-\frac{3}{4\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8}$	.
-1	$\alpha$	.	$\frac{1}{\sqrt{2}}$	.	$\frac{\sqrt{5}}{8}$	.	$\frac{3}{4\sqrt{2}}$	.	$-\frac{3}{8}$
-1	$\beta$	.	.	$-\frac{3\sqrt{5}}{8}$	.	$-\frac{\sqrt{5}}{4\sqrt{2}}$	.	$-\frac{3}{8}$	.



Table B8.  $T_2 \times U' = E'' + U' + W'$

$T_2$	$U'$	$E''$	$U'$		$W'$	
		$\alpha$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$
0	$\frac{3}{2}$	$\beta$	$\frac{3}{2}$	$-\frac{3}{2}$	$\frac{3}{2}$	$-\frac{3}{2}$
0	$\frac{1}{2}$	$\frac{\sqrt{5}}{2\sqrt{6}}$	$\frac{1}{2\sqrt{15}}$	$\frac{1}{2}$	$\frac{\sqrt{3}}{2\sqrt{5}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$
0	$-\frac{1}{2}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{\sqrt{2}}{2\sqrt{5}}$	$-\frac{1}{2}$	$-\frac{1}{\sqrt{10}}$	$\frac{1}{4}$
0	$-\frac{3}{2}$	$\frac{\sqrt{5}}{2\sqrt{6}}$	$\frac{1}{2}$	$\frac{\sqrt{2}}{2\sqrt{5}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{\sqrt{5}}{4}$
1	$\frac{3}{2}$	$-\frac{\sqrt{5}}{4\sqrt{3}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{3\sqrt{3}}{8}$	$-\frac{\sqrt{15}}{8\sqrt{2}}$
1	$\frac{1}{2}$	$\frac{\sqrt{5}}{4}$	$\frac{1}{2\sqrt{10}}$	$-\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{7}{8\sqrt{10}}$	$-\frac{5}{8\sqrt{2}}$
1	$-\frac{1}{2}$	$\frac{1}{4}$	$-\frac{\sqrt{3}}{2\sqrt{10}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{8\sqrt{5}}$	$-\frac{7}{8\sqrt{2}}$
1	$-\frac{3}{2}$	$\frac{\sqrt{3}}{4}$	$\frac{\sqrt{2}}{2\sqrt{2}}$	$\frac{1}{2\sqrt{10}}$	$-\frac{3\sqrt{3}}{8\sqrt{5}}$	$\frac{\sqrt{15}}{8\sqrt{2}}$
-1	$\frac{3}{2}$	$\frac{\sqrt{3}}{4}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{10}}$	$\frac{\sqrt{15}}{8\sqrt{2}}$	$-\frac{3\sqrt{3}}{8\sqrt{2}}$
-1	$\frac{1}{2}$	$\frac{1}{4}$	$-\frac{1}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{10}}$	$-\frac{7}{8\sqrt{2}}$	$\frac{1}{8\sqrt{5}}$
-1	$-\frac{1}{2}$	$\frac{\sqrt{5}}{4}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2\sqrt{2}}$	$-\frac{1}{8}$	$\frac{7}{8\sqrt{10}}$
-1	$-\frac{3}{2}$	$-\frac{\sqrt{5}}{4\sqrt{3}}$	$\frac{\sqrt{5}}{2\sqrt{6}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{\sqrt{15}}{8\sqrt{2}}$	$-\frac{\sqrt{3}}{8\sqrt{2}}$



Table B10:  $H \times U' = E'(J = \frac{1}{2}) + E''(J = \frac{1}{2}) + U'(J = \frac{3}{2}) + W'(J = \frac{5}{2}) + W''(J = \frac{7}{2})$

H	U'	E'		E''		U'		W'(J = 5/2)					W''(J = 7/2)					
		$\alpha$	$\beta$	$\alpha$	$\beta$	3/2	1/2	-1/2	-3/2	-5/2	5/2	3/2	1/2	-1/2	-3/2	-5/2		
2	3/2	.	.	.	$\frac{\sqrt{15}}{8}$	.	.	.	.	.	.	$\frac{\sqrt{7}}{16\sqrt{2}}$	.	.	.	$-\frac{3\sqrt{35}}{16\sqrt{2}}$		
2	1/2	.	.	$\frac{3}{8}$	.	.	.	.	.	.	.	$-\frac{\sqrt{21}}{16}$	.	.	$-\frac{\sqrt{105}}{16\sqrt{2}}$	.	$\frac{\sqrt{21}}{16\sqrt{2}}$	
2	-1/2	.	.	.	$\frac{1}{8}$	.	$\frac{2}{\sqrt{7}}$	.	.	.	.	$-\frac{\sqrt{15}}{16\sqrt{2}}$	.	.	.	.	.	
2	3/2	$\frac{\sqrt{2}}{\sqrt{5}}$	.	$-\frac{\sqrt{3}}{8\sqrt{5}}$	.	$\frac{\sqrt{2}}{\sqrt{5}}$	$\frac{4}{\sqrt{35}}$	.	.	.	.	$-\frac{\sqrt{7}}{16\sqrt{10}}$	.	$\frac{\sqrt{5}}{16\sqrt{7}}$	.	$-\frac{\sqrt{7}}{16\sqrt{2}}$	.	$\frac{\sqrt{7}}{16\sqrt{10}}$
-2	3/2	.	$-\frac{\sqrt{2}}{\sqrt{5}}$	$-\frac{1}{8}$	$\frac{\sqrt{5}}{8\sqrt{5}}$	.	.	.	.	.	.	$-\frac{\sqrt{21}}{16\sqrt{2}}$	.	$-\frac{\sqrt{5}}{16\sqrt{7}}$	.	$-\frac{\sqrt{15}}{16\sqrt{14}}$	.	$-\frac{\sqrt{7}}{16\sqrt{10}}$
-2	1/2	.	.	.	$-\frac{3}{8}$	.	.	.	.	.	.	$-\frac{\sqrt{21}}{16}$	.	.	.	$\frac{\sqrt{15}}{16\sqrt{14}}$	.	$-\frac{\sqrt{3}}{16\sqrt{14}}$
-2	-3/2	.	.	$-\frac{\sqrt{15}}{8}$	.	.	.	.	.	.	.	$\frac{\sqrt{105}}{16\sqrt{2}}$	.	.	$-\frac{\sqrt{7}}{16\sqrt{2}}$	.	.	.
1	3/2	.	.	$\frac{\sqrt{3}}{4}$	.	.	$-\frac{\sqrt{3}}{\sqrt{7}}$	.	.	.	.	.	$-\frac{\sqrt{7}}{8}$	.	$-\frac{\sqrt{35}}{8\sqrt{2}}$	.	.	.
1	1/2	.	.	.	$\frac{1}{4}$	.	.	.	.	.	.	$-\frac{\sqrt{15}}{8\sqrt{14}}$	.	.	.	$\frac{\sqrt{21}}{8}$	.	$\frac{\sqrt{21}}{8\sqrt{2}}$



Table B10 (continued)

H	U'	E'		E''		U'		W'(J = 5/2)					W'(J = 7/2)									
		$\alpha$	$\beta$	$\alpha$	$\beta$	3/2	1/2	-1/2	-3/2	-5/2	5/2	3/2	1/2	-1/2	-3/2	-5/2	5/2	3/2	1/2	-1/2	-3/2	-5/2
1	-1/2	$-\frac{\sqrt{3}}{\sqrt{10}}$	.	$-\frac{3}{4\sqrt{5}}$	.	.	.	.	.	.	$-\frac{\sqrt{21}}{8\sqrt{10}}$	.	.	$-\frac{\sqrt{21}}{8\sqrt{2}}$	.	$-\frac{\sqrt{21}}{8\sqrt{10}}$	.	$\frac{\sqrt{15}}{8\sqrt{7}}$	.	$-\frac{\sqrt{21}}{8\sqrt{2}}$	.	$-\frac{\sqrt{21}}{8\sqrt{10}}$
1	3/2	.	$\frac{1}{\sqrt{10}}$	.	$\frac{\sqrt{3}}{4\sqrt{5}}$	.	$\frac{\sqrt{2}}{\sqrt{5}}$	.	.	.	.	$\frac{\sqrt{7}}{8\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	.	$-\frac{\sqrt{7}}{8\sqrt{10}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	.	$-\frac{\sqrt{7}}{8\sqrt{2}}$	.	$-\frac{\sqrt{7}}{8\sqrt{10}}$
-1	1/2	$-\frac{1}{\sqrt{10}}$	.	$-\frac{\sqrt{3}}{4\sqrt{5}}$	.	$\frac{\sqrt{2}}{\sqrt{5}}$	.	.	.	.	$-\frac{\sqrt{7}}{8\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	.	$-\frac{\sqrt{7}}{8\sqrt{10}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	.	$-\frac{\sqrt{7}}{8\sqrt{2}}$	.	$-\frac{\sqrt{7}}{8\sqrt{10}}$	
-1	1/2	.	$\frac{\sqrt{3}}{\sqrt{10}}$	.	$\frac{3}{4\sqrt{5}}$	.	.	.	.	.	$-\frac{\sqrt{21}}{8\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	.	$-\frac{\sqrt{21}}{8\sqrt{10}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	.	$-\frac{\sqrt{21}}{8\sqrt{2}}$	.	$-\frac{\sqrt{21}}{8\sqrt{10}}$	
-1	-1/2	.	.	$-\frac{1}{4}$	.	.	.	$-\frac{\sqrt{2}}{\sqrt{5}}$	.	$-\frac{1}{\sqrt{35}}$	.	.	$-\frac{1}{\sqrt{35}}$	.	$-\frac{\sqrt{21}}{8\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	.	$-\frac{\sqrt{21}}{8\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	
-1	-3/2	.	.	$-\frac{\sqrt{3}}{4}$	.	.	.	.	.	$-\frac{1}{\sqrt{35}}$	.	.	$-\frac{1}{\sqrt{35}}$	.	$-\frac{\sqrt{21}}{8\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	.	$-\frac{\sqrt{21}}{8\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8\sqrt{7}}$	
0	3/2	.	.	.	$\frac{1}{4\sqrt{2}}$	.	.	.	.	$-\frac{3\sqrt{2}}{\sqrt{35}}$	.	.	$-\frac{3\sqrt{2}}{\sqrt{35}}$	.	$-\frac{\sqrt{35}}{16\sqrt{7}}$	.	$-\frac{\sqrt{35}}{16\sqrt{7}}$	.	$-\frac{\sqrt{35}}{16\sqrt{7}}$	.	$-\frac{\sqrt{35}}{16\sqrt{7}}$	
0	1/2	$\frac{1}{\sqrt{5}}$	.	$-\frac{3\sqrt{3}}{4\sqrt{10}}$	.	$-\frac{1}{\sqrt{5}}$	.	.	.	$-\frac{\sqrt{3}}{\sqrt{35}}$	.	.	$-\frac{\sqrt{3}}{\sqrt{35}}$	.	$-\frac{3\sqrt{7}}{16}$	.	$-\frac{3\sqrt{7}}{16}$	.	$-\frac{3\sqrt{7}}{16}$	.	$-\frac{3\sqrt{7}}{16}$	
0	-1/2	.	$-\frac{1}{\sqrt{5}}$	.	$\frac{3\sqrt{3}}{4\sqrt{10}}$	.	$-\frac{1}{\sqrt{5}}$	.	.	$-\frac{\sqrt{3}}{\sqrt{35}}$	.	.	$-\frac{\sqrt{3}}{\sqrt{35}}$	.	$-\frac{3\sqrt{7}}{16}$	.	$-\frac{3\sqrt{7}}{16}$	.	$-\frac{3\sqrt{7}}{16}$	.	$-\frac{3\sqrt{7}}{16}$	
0	-3/2	.	.	$-\frac{1}{4\sqrt{2}}$	.	.	.	$\frac{1}{\sqrt{5}}$	.	$\frac{3\sqrt{2}}{\sqrt{35}}$	.	.	$\frac{3\sqrt{2}}{\sqrt{35}}$	.	$-\frac{\sqrt{21}}{16}$	.	$-\frac{\sqrt{21}}{16}$	.	$-\frac{\sqrt{21}}{16}$	.	$-\frac{\sqrt{21}}{16}$	

Table B11.  $T_2 \times W' = 2W'$

$T_2$	$W'$	$W'$						$W'$					
		$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
0	$\frac{5}{2}$	$\frac{\sqrt{5}}{6\sqrt{2}}$	.	$\frac{\sqrt{5}}{4}$	.	.	.	$-\frac{1}{24\sqrt{2}}$	.	$\frac{1}{8}$	.	$-\frac{3\sqrt{5}}{8\sqrt{2}}$	.
0	$\frac{3}{2}$	.	$-\frac{7}{6\sqrt{10}}$	.	$\frac{1}{4}$	.	.	.	$\frac{5}{24\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8}$	.	$\frac{3\sqrt{5}}{8\sqrt{2}}$
0	$\frac{1}{2}$	$\frac{\sqrt{5}}{4}$	.	$-\frac{\sqrt{2}}{3\sqrt{5}}$	.	$-\frac{1}{4}$	.	$\frac{1}{8}$	.	$-\frac{5}{12\sqrt{2}}$	.	$\frac{\sqrt{5}}{8}$	.
0	$-\frac{1}{2}$	.	$\frac{1}{4}$	.	$\frac{\sqrt{2}}{3\sqrt{5}}$	.	$-\frac{\sqrt{5}}{4}$	.	$-\frac{\sqrt{5}}{8}$	.	$\frac{5}{12\sqrt{2}}$	.	$-\frac{1}{8}$
0	$-\frac{3}{2}$	.	.	$-\frac{1}{4}$	.	$\frac{7}{6\sqrt{10}}$	.	$-\frac{3\sqrt{5}}{8\sqrt{2}}$	.	$\frac{\sqrt{5}}{8}$	.	$-\frac{5}{24\sqrt{2}}$	.
0	$-\frac{5}{2}$	.	.	.	$-\frac{\sqrt{5}}{4}$	.	$-\frac{\sqrt{5}}{6\sqrt{2}}$	.	$\frac{3\sqrt{5}}{8\sqrt{2}}$	.	$-\frac{1}{8}$	.	$\frac{1}{24\sqrt{2}}$
1	$\frac{5}{2}$	.	$\frac{\sqrt{5}}{4}$	.	$-\frac{5}{12\sqrt{2}}$	.	.	.	$-\frac{1}{16}$	.	$\frac{5\sqrt{5}}{24\sqrt{2}}$	.	$\frac{3\sqrt{5}}{16}$
1	$\frac{3}{2}$	$\frac{1}{4}$	.	$-\frac{1}{4\sqrt{2}}$	.	$-\frac{\sqrt{5}}{6}$	.	$\frac{\sqrt{5}}{16}$	.	$\frac{\sqrt{5}}{8\sqrt{2}}$	.	$-\frac{25}{48}$	.
1	$\frac{1}{2}$	.	$-\frac{1}{4\sqrt{10}}$	.	$-\frac{1}{2}$	.	$-\frac{5}{12\sqrt{2}}$	.	$-\frac{5}{8\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8}$	.	$\frac{5\sqrt{5}}{24\sqrt{2}}$
1	$-\frac{1}{2}$	$\frac{\sqrt{5}}{4\sqrt{2}}$	.	$-\frac{1}{2\sqrt{5}}$	.	$-\frac{1}{4\sqrt{2}}$	.	$\frac{1}{8\sqrt{2}}$	.	$\frac{5}{8}$	.	$\frac{\sqrt{5}}{8\sqrt{2}}$	.
1	$-\frac{3}{2}$	.	$\frac{1}{2}$	.	$-\frac{1}{4\sqrt{10}}$	.	$\frac{\sqrt{5}}{4}$	.	$-\frac{\sqrt{5}}{16}$	.	$-\frac{5}{8\sqrt{2}}$	.	$-\frac{1}{16}$
1	$-\frac{5}{2}$	.	.	$\frac{\sqrt{5}}{4\sqrt{2}}$	.	$\frac{1}{4}$	.	$\frac{9}{16}$	.	$\frac{1}{8\sqrt{2}}$	.	$\frac{\sqrt{5}}{16}$	.
-1	$\frac{5}{2}$	.	$-\frac{1}{4}$	.	$-\frac{\sqrt{5}}{4\sqrt{2}}$	.	.	.	$-\frac{\sqrt{5}}{16}$	.	$-\frac{1}{8\sqrt{2}}$	.	$-\frac{9}{16}$
-1	$\frac{3}{2}$	$-\frac{\sqrt{5}}{4}$	.	$\frac{1}{4\sqrt{10}}$	.	$-\frac{1}{2}$	.	$\frac{1}{16}$	.	$\frac{5}{8\sqrt{2}}$	.	$\frac{\sqrt{5}}{16}$	.
-1	$\frac{1}{2}$	.	$\frac{1}{4\sqrt{2}}$	.	$\frac{1}{2\sqrt{5}}$	.	$-\frac{\sqrt{5}}{4\sqrt{2}}$	.	$-\frac{\sqrt{5}}{8\sqrt{2}}$	.	$-\frac{5}{8}$	.	$-\frac{1}{8\sqrt{2}}$
-1	$-\frac{1}{2}$	$\frac{5}{12\sqrt{2}}$	.	$\frac{1}{2}$	.	$\frac{1}{4\sqrt{10}}$	.	$-\frac{5\sqrt{5}}{24\sqrt{2}}$	.	$\frac{\sqrt{5}}{8}$	.	$\frac{5}{8\sqrt{2}}$	.
-1	$-\frac{3}{2}$	.	$\frac{\sqrt{5}}{6}$	.	$\frac{1}{4\sqrt{2}}$	.	$-\frac{1}{4}$	.	$\frac{25}{48}$	.	$-\frac{\sqrt{5}}{8\sqrt{2}}$	.	$-\frac{\sqrt{5}}{16}$
-1	$-\frac{5}{2}$	.	.	$\frac{5}{12\sqrt{2}}$	.	$-\frac{\sqrt{5}}{4}$	.	$-\frac{3\sqrt{5}}{16}$	.	$-\frac{5\sqrt{5}}{24\sqrt{2}}$	.	$\frac{1}{16}$	.



Table B12 (continued)

$H$	$W'$	$W'(J = \frac{5}{2})$	$W'(J = \frac{7}{2})$	$W'(J = \frac{9}{2})$
$-1$	$\frac{5}{2}$	$-\frac{\sqrt{2}}{\sqrt{7}}$	$-\frac{\sqrt{35}}{16}$	$-\frac{\sqrt{2}}{16}$
$-1$	$\frac{3}{2}$	$-\frac{\sqrt{6}}{\sqrt{35}}$	$-\frac{11\sqrt{7}}{48\sqrt{10}}$	$-\frac{11\sqrt{7}}{48\sqrt{2}}$
$-1$	$\frac{1}{2}$	$0$	$-\frac{7\sqrt{7}}{48}$	$-\frac{11}{24\sqrt{2}}$
$-1$	$-\frac{1}{2}$	$\frac{\sqrt{6}}{\sqrt{35}}$	$\frac{\sqrt{7}}{16}$	$\frac{1}{8}$
$-1$	$-\frac{3}{2}$	$0$	$\frac{\sqrt{35}}{48\sqrt{2}}$	$\frac{\sqrt{5}}{48}$
$-1$	$-\frac{5}{2}$	$0$	$\frac{5\sqrt{7}}{16\sqrt{2}}$	$-\frac{5}{16}$
$0$	$\frac{5}{2}$	$-\frac{\sqrt{5}}{\sqrt{14}}$	$-\frac{\sqrt{5}}{16\sqrt{21}}$	$-\frac{\sqrt{5}}{16\sqrt{6}}$
$0$	$\frac{3}{2}$	$\frac{1}{\sqrt{70}}$	$\frac{\sqrt{15}}{16\sqrt{7}}$	$-\frac{\sqrt{15}}{16\sqrt{2}}$
$0$	$\frac{1}{2}$	$\frac{2\sqrt{2}}{\sqrt{35}}$	$-\frac{\sqrt{5}}{8\sqrt{21}}$	$\frac{\sqrt{5}}{8\sqrt{6}}$
$0$	$-\frac{1}{2}$	$\frac{2\sqrt{2}}{\sqrt{35}}$	$-\frac{\sqrt{5}}{8\sqrt{21}}$	$\frac{\sqrt{5}}{8\sqrt{6}}$
$0$	$-\frac{3}{2}$	$\frac{1}{\sqrt{70}}$	$-\frac{\sqrt{21}}{8\sqrt{2}}$	$-\frac{\sqrt{15}}{16\sqrt{2}}$
$0$	$-\frac{5}{2}$	$0$	$-\frac{\sqrt{5}}{8\sqrt{6}}$	$-\frac{17}{16\sqrt{15}}$