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Phase-fixed double-group 3-Γ symbols. VI. Real 3-Γ symbols and coupling coefficients for the group hierarchy $I^* \supset C_5^*$

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It is demonstrated that for the group-subgroup hierarchy $I^* \supset C_5^*$, one may choose standard irreducible matrix representations and corresponding all-real sets of 3-Γ symbols which obey a formalism just as elegant as the classical one for the 3-j symbols of the rotation double group. The 3-Γ symbols are phase-fixed by the specification of basis functions (or, equivalently, subduction coefficients) generating them and based on functions first given by McLellan.

Other icosahedral double-group hierarchies are also briefly discussed.

Key words: Icosahedral double group — real phase-fixed three-gamma symbols and coupling coefficients — standard irreducible matrix representations — complex conjugation of matrix representations by inner automorphism.

1. Introduction

The present paper, by discussing the icosahedral double group, completes a series of papers of which the two first ones dealt with 3-Γ symbols and coupling coefficients in general [1] and with such quantities for double groups in particular [2], while the following papers [3–5] discussed 3-Γ symbols for the dihedral, tetrahedral, and octahedral double groups, respectively. For terminology and notation not explained here we refer to [1] and [2].

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At the present time, so many applications or potential applications of the icosahedral group I and its double group I^* are known [6; 7; 8, Refs. given on p. 1059; 9, Introduction; 10] that it is clearly of interest to investigate the possibilities of establishing smoothly working Wigner–Racah algebras for these groups. Besides, the icosahedral groups present some intriguing problems with respect to subgroup adaption (like did the octahedral double group [5]) and the unique feature of a triple multiplicity (the triple WVW, see below).

Although the icosahedral groups have been known to mathematicians for more than a century (e.g., Hamilton 1856, cited in [11], p. 67; Klein's 1884 lectures [12]; the character table of I^*, Frobenius 1899 [13]; see also the bibliography [14]), the *detailed* representation theory has been worked out only in the last decades, chiefly by physicists and chemists. Several authors [8, 15–19] have dealt with *icosahedral invariants*, i.e. bases in various specified spaces for the totally symmetric irrep of I. However, the task of furnishing physically suitable concrete realizations of *all* the irreps of I (and I^*) was undertaken first by Cohan [20] and, independently, by McLellan [6] and was later attacked from a different point of view by Boyle and Ożgo [21]. The spherical harmonic approach to icosahedral reps is presented in modern mathematical terms in a paper by Huber [22], while Schmelzer [23] and Ceulemans [24] treat cyclically and otherwise equivalent bases generating icosahedral irreps. Finally, some recent publications give sets of symmetry coefficients for I^* [25, 26] or just I [9, 27]; these will be commented upon below in this paper.

Table 1 gives our present notation for the irreps of I^* along with some relevant rep-theoretical information.

Table 1. The icosahedral double group[a] I^*

Irreps[d]	*Dimension*	*Frobenius–Schur classification*[b]	*vector/spin classification*[c]
$A = 1_{I^*}(\Gamma_1)$	1	first kind	vector
$\mathrm{T}_1(\mathrm{F}_1, \Gamma_2)$	3		
$\mathrm{T}_2(\mathrm{F}_2, \Gamma_3)$	3		
$\mathrm{U}(\mathrm{G}, \Gamma_4)$	4		
$\mathrm{V}(\mathrm{H}, \Gamma_5)$	5		
$\mathrm{E}_1(\mathrm{E}', \mathrm{E}_{1/2}, \Gamma_6)$	2	second kind	spin
$\mathrm{E}_2(\mathrm{E}'', \mathrm{E}_{7/2}, \Gamma_7)$	2		
$\mathrm{X}(\mathrm{U}', \mathrm{G}_{3/2}, \Gamma_8)$	4		
$\mathrm{W}(\mathrm{W}', \mathrm{I}_{5/2}, \Gamma_9)$	6		

[a] Alternative notations for the icosahedral group include P, Y, and K, of which the latter is also sometimes used for the rotation group, R_3. See the discussion by Boyle [45].
[b] See ([1], Sect. 5.2).
[c] See ([2], Sect. 2.1).
[d] Alternative notations in parentheses collected from other works [6, 9, 21, 25, 27, 28, 29, 36, 44, 45]; still another system is found in the quasi-numerical labels used by Butler [26]. See also the discussion by Boyle [45].

Table 2. Icosahedral irrep triples. The table displays those irrep triples $\Gamma_1\Gamma_2\Gamma_3$ for which $\Gamma_1 \otimes \Gamma_2 \otimes \Gamma_3$ contains A at least once. (Only one of the permuted forms of each unordered triple is given.) The number of occurrences of A in $\Gamma_1 \otimes \Gamma_2 \otimes \Gamma_3$ is given, using – whenever relevant – the labels "s" and "a" to indicate the symmetry/antisymmetry of the fix-vectors (cf. [1], Sect. 3.2). Thus, for example, for WVW we have dim $\mathscr{F}_s(\mathrm{WVW}) = 1$ and dim $\mathscr{F}_a(\mathrm{WVW}) = 2$. Note that either two or none of the irreps in a triple figuring here are of the second kind ([2], Sect. 2.1)

A A A	s	$\mathrm{T_1 A T_1}$	s	$\mathrm{U T_2 T_1}$	1
$\mathrm{T_1 T_1 T_1}$	a	$\mathrm{T_1 V T_1}$	s	$\mathrm{V T_2 T_1}$	1
$\mathrm{T_2 T_2 T_2}$	a	$\mathrm{T_2 A T_2}$	s	$\mathrm{V U T_1}$	1
U U U	s	$\mathrm{T_2 V T_2}$	s	$\mathrm{V U T_2}$	1
V V V	$2s$	U A U	s		
		$\mathrm{U T_1 U}$	a	$\mathrm{E_2 E_1 U}$	1
		$\mathrm{U T_2 U}$	a	$\mathrm{X E_1 T_1}$	1
		U V U	s	$\mathrm{X E_1 V}$	1
		V A V	s	$\mathrm{X E_2 T_2}$	1
		$\mathrm{V T_1 V}$	a	$\mathrm{X E_2 V}$	1
		$\mathrm{V T_2 V}$	a	$\mathrm{W E_1 T_2}$	1
		V U V	$s+a$	$\mathrm{W E_1 U}$	1
				$\mathrm{W E_1 V}$	1
		$\mathrm{E_1 A E_1}$	a	$\mathrm{W E_2 T_1}$	1
		$\mathrm{E_1 T_1 E_1}$	s	$\mathrm{W E_2 U}$	1
		$\mathrm{E_2 A E_2}$	a	$\mathrm{W E_2 V}$	1
		$\mathrm{E_2 T_2 E_2}$	s	$\mathrm{W X T_1}$	1
		X A X	a	$\mathrm{W X T_2}$	1
		$\mathrm{X T_1 X}$	s	W X U	2
		$\mathrm{X T_2 X}$	s	W X V	2
		X U X	s		
		X V X	a		
		W A W	a		
		$\mathrm{W T_1 W}$	$2s$		
		$\mathrm{W T_2 W}$	$2s$		
		W U W	$s+a$		
		W V W	$s+2a$		

2. The icosahedral irrep triples; primary and supplementary j-values

Table 2 gives a listing of those irrep triples $\Gamma_1\Gamma_2\Gamma_3$ of I^* for which $\Gamma_1 \otimes \Gamma_2 \otimes \Gamma_3$ contains the totally symmetric irrep $\mathrm{A} = 1_{I^*}$ at least once, i.e. for which dim $\mathscr{F}(\Gamma_1\Gamma_2\Gamma_3) > 0$ (cf. [1], Sect. 3.1). The table is derivable by standard arguments ([1], Sect. A.1) from the character table and may be assimilated from existing tables (see [28], App. 2 or, for the triples $\Gamma\Gamma\Gamma$, [29]).

In Table 3a we have reproduced some relevant subduction relations for $R_3^* \to I^*$. The procedure described in ([2], Sect. 4) leads us to assign to the icosahedral irreps certain irreps of R_3^* (i.e., j-values) in the way shown in Table 3b.

The permutational symmetry of the triple UUU and the multiplicities associated with the triples VVV, VUV, $\mathrm{WT_1W}$, $\mathrm{WT_2W}$, WUW, WVW, XUW, and XVW necessitate the assignment of two j-values to $\mathrm{T_1}$, $\mathrm{T_2}$, and U and three j-values to V.

Table 3

ⓐ Subduction relations $R_3^* \to I^*$	ⓑ j-value assigned to irreps of I^*
$D_0 \to A$	A 0
$D_{1/2} \to E_1$	T_1 1 (primary), 5
$D_1 \to T_1$	T_2 3 (primary), 5
$D_{3/2} \to X$	U 3 (primary), 4
$D_2 \to V$	V 2 (primary), 4, 5
$D_{5/2} \to W$	E_1 $\frac{1}{2}$
$D_3 \to U \oplus T_2$	E_2 $\frac{7}{2}$
$D_{7/2} \to W \oplus E_2$	X $\frac{3}{2}$
$D_4 \to V \oplus U$	W $\frac{5}{2}$
$D_5 \to V \oplus T_1 \oplus T_2$	

See main text, Sect. 2. For a partial continuation of Table 3a, see [36]

As pointed out in ([2], Sect. 4.3), it is necessary to check that transformed 3-j symbols generated by basis functions corresponding to our primary and supplementary j-values actually may be renormalized to give subgroup 3-Γ symbols by ([2], Eq. (4.3.6)).

For all multiplicity triples discussed here, the remarks of ([2], Sect. 4.6) show that using the primary and supplementary j-values of Table 3b leads to mutually orthogonal sets of triple coefficients. E.g., the transformed 3-j symbols

$$\begin{pmatrix} 3/2 & 3 & 5/2 \\ X\gamma_1 & U\gamma_2 & W\gamma_3 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 3/2 & 4 & 5/2 \\ X\gamma_1 & U\gamma_2 & W\gamma_3 \end{pmatrix}$$

form mutually orthogonal non-vanishing sets which are, consequently, used for the construction of two mutually orthogonal sets of 3-Γ symbols of the type $(XUW/\gamma_1\gamma_2\gamma_3)$, one *odd* ($3/2+3+5/2$ is odd) and one *even* ($3/2+4+5/2$ is even), cf. [2, Eq. (4.3.7)]. Similar remarks apply to the triples WT_1W, WT_2W, WUW, WVW, and XVW, and for these six triples there are no further problems. Note that for the triple WVW with multiplicity three, we get two sets of odd 3-Γ symbols and one set of even 3-Γ symbols.

For the triple UUU, there is a problem similar to (but in a way simpler than) the one we met in connection with the triples $E_\lambda E_\lambda E_\lambda$, $\lambda = n/3$, in the dihedral double groups D_n^* with n equal to a multiple of 3 ([3], Sect. 4). The transformed 3-j symbols

$$\begin{pmatrix} 3 & 3 & 3 \\ U\gamma_1 & U\gamma_2 & U\gamma_3 \end{pmatrix}$$

make up a simultaneously symmetric and antisymmetric fix-vector for UUU ([1], Sect. 3.2) and thus vanish. (Thus we have an instance of "conflicting symmetries" [30].) Instead, the 3-Γ symbols $(UUU/\gamma_1\gamma_2\gamma_3)$ are constructed from transformed 3-j symbols of the form $(343/U\gamma_1U\gamma_2U\gamma_3)$, and it may further be checked that the secondary j-value $j=4$ may just as well be chosen in the first or third position.

Table 4. Triples of j-values used in the construction of 3-Γ symbols for I^*-irrep triples necessitating the use of supplementary j-values

I^*-irrep triple	j-value triple
U U U	334
V V V	222, 224
V U V	232, 242
W T_1 W	$\frac{5}{2}\,1\,\frac{5}{2}, \frac{5}{2}\,5\,\frac{5}{2}$
W T_2 W	$\frac{5}{2}\,3\,\frac{5}{2}, \frac{5}{2}\,5\,\frac{5}{2}$
W U W	$\frac{5}{2}\,3\,\frac{5}{2}, \frac{5}{2}\,4\,\frac{5}{2}$
W V W	$\frac{5}{2}\,2\,\frac{5}{2}, \frac{5}{2}\,4\,\frac{5}{2}, \frac{5}{2}\,5\,\frac{5}{2}$
W X U	$\frac{5}{2}\,\frac{3}{2}\,3, \frac{5}{2}\,\frac{3}{2}\,4$
W X V	$\frac{5}{2}\,\frac{3}{2}\,2, \frac{5}{2}\,\frac{3}{2}\,4$

Finally, the triple VVV has dim $\mathscr{F}_s = 2$, and the j-triples 222 and 224 yield mutually orhogonal, symmetric fix-vectors; it may be shown to be immaterial where the $j=4$ is placed.

[If we had not set up the rule of minimum $j_1 + j_2 + j_3$ ([2], Sect. 4.4), there would have been other possibilities for the construction of 3-Γ symbols for VVV with the use of j-values from Table 3b. The triple pairs 442, 444 and 552, 554 both give an orthogonal set of VVV fix-vectors; however, each of these four fix-vectors is a linear combination with complicated coefficients of both of the two fix-vectors derived from 222 and 224. In particular, one cannot use 444 together with 222 if one wants an orthogonal pair, even though this would have been attractive because one could have skipped the argument concerning the position of the secondary j-value. Cf. discussion of the tetrahedral triple TTT ([4], Sect. 3).

Butler's separations of the multiplicities in I^* [26] are, in general, not necessarily the same as ours. They do not seem to be explicitly specified in [26], but in principle the tables there enable a retrieval of "3-*jm* factors" and thus information equivalent to the coefficients in linear combinations like the ones just discussed for VVV.]

Table 4 summarizes the j-triples thus selected for the I^*-triples involving irreps necessitating supplementary j-values. For all other triples, 3-Γ symbols are constructed by using only primary j-values.

3. Basis functions and 3-Γ symbols adapted to $I^* \supset C_5^*$

3.1. Choice of a generating set for the icosahedral double group

There are many ways to choose a set of generators and relations between them so that they define the group I^*, i.e. the group has many *presentations*, ([11, 14]; [31], Chap. 11), some of which are highly symmetrical [32] (although maybe not suited for all specific practical purposes [33]). Here we shall choose the rotation C_5 of $2\pi/5$ around the Z axis and the two-fold rotation C_2 with axis in the

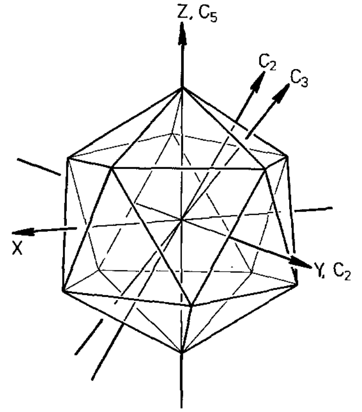

Fig. 1. A regular icosahedron placed in a Cartesian coordinate system in such a way that the Z axis is a five-fold symmetry axis and the Y axis is a two-fold symmetry axis with the positive part intersecting an icosahedron edge which forms a Δ pair (defines a right-hand screw) together with the Z axis. As generators for the icosahedral group we here choose C_5 and C_2 with the axes shown. These generators satisfy $C_2C_5 = C_3^{-1}$, where the three-fold symmetry axis in question is also marked on the figure, and thus the relations $C_5^5 = C_2^2 = (C_2C_5)^3 = E$, i.e. we have the presentation of the icosahedral group given by Bolza and discussed by Littlewood [46].

Note that the regular icosahedron of course has full symmetry $I_h = I \times S_2$, whereas we have above only been interested in the double group I^* of the proper rotation group I. The double group I_h^* has been defined ([2], Sect. 2.2; [34]).

XZ-plane and direction cosines $\alpha_x = -5^{-1/4}\Phi^{-1/2}$, $\alpha_y = 0$, $\alpha_z = 5^{-1/4}\Phi^{-1/2}$ for its axis (where Φ is the golden number $(1+5^{1/2})/2$) as generators of the pure rotation group I (See Fig. 1); we may then choose the corresponding double-group elements

$$C_5^* = \mathscr{D}^{[1/2]}(2\pi/5, 0, 0)$$

and

$$C_2^* = \mathscr{D}^{[1/2]}(\pi, \operatorname{Arccos}(\sqrt{1/5}), 0) \tag{3.1}$$

as generators of I^*, whereby I^* is fully specified as a group of 2×2 matrices (cf. [2], Sect. 2 or [34]). With this choice, the R_3^*-element

$$C_2^{Y*} = \mathscr{D}^{[1/2]}(0, \pi, 0), \tag{3.2}$$

corresponding to a rotation of π around the Y axis, also becomes an element of I^*. This will be of interest to us later on.

The above choice of a geometric set-up for the icosahedron will be motivated in the next subsection.

3.2. Basis functions and 3-Γ symbols for $I^* \supset C_5^*$

Our starting point was the functions given by McLellan [6]. With McLellan's choice, the R_3^*-element $C_2^{X*} = \mathscr{D}^{[1/2]}(\pi, \pi, 0)$, corresponding to a rotation of π around the X axis, is an element of I^*. Our first modification of those functions was made in order to achieve the "conjugation of standard irreps by a fixed group element" situation described in ([1], Sect. 5.5). Thus we had the situation that for any standard matrix irrep Γ, the matrix $\Gamma(C_2^{X*})$ was a conjugation matrix for Γ and, in particular, we knew now that all-real sets of 3-Γ symbols could be chosen corresponding to our standard matrix irreps. However, the basis functions themselves were of a less pleasing appearance. We then made use of the observations made in ([2], Sect. 4.5) and rotated the coordinate system (or, alternatively expressed, rotated the axes of the icosahedral generators relatively to the coordinate system) so as to obtain some much simpler basis functions yielding the same matrix irreps and transformed 3-j symbols. Now the element C_2^{Y*} had the rôle formerly played by C_2^{X*}. After some phase changes made in accordance with the rules given in ([2], Sect. 4.4), we arrived at the basis functions given in Table 5.

Our generator C_2 is situated with respect to our X axis as was McLellan's "C" with respect to his Y axis.

[There are, in fact, two geometrically distinct ways of choosing a coordinate system with the Z axis as a five-fold axis in a regular icosahedron and the Y axis as a two-fold axis of the same icosahedron: that icosahedron edge which intersects the positive part of the Y axis forms a chiral skew line pair together with the Z axis and this may be either a Δ pair or a Λ pair [35]; for the present basis

Table 5. Basis functions for $I^* \supset C_5^*$. The coordinate system used is discussed in Sects. 3.1 and 3.2 of the main text. The basis functions are given in the form $|j\Gamma\gamma\rangle = \sum_m s(jm, j\Gamma\gamma)|jm\rangle$ (cf. [2], Eq. (4.3.2)), where Γ denotes an irrep of I^* and γ a component of Γ. The functions generate matrix irreps of I^* with the properties given in Table 6

$\|0\,\mathrm{A}\,0\rangle = \|0\,0\rangle$	$\|3\,\mathrm{T}_2\,{+2}\rangle = \sqrt{\tfrac{3}{5}}\,\|3\,{+2}\rangle - \sqrt{\tfrac{2}{5}}\,\|3\,{-3}\rangle$
$\|\tfrac{1}{2}\,\mathrm{E}_1\,{+\tfrac{1}{2}}\rangle = \|\tfrac{1}{2}\,{+\tfrac{1}{2}}\rangle$	$\|3\,\mathrm{T}_2\,0\rangle = \|3\,0\rangle$
$\|\tfrac{1}{2}\,\mathrm{E}_1\,{-\tfrac{1}{2}}\rangle = \|\tfrac{1}{2}\,{-\tfrac{1}{2}}\rangle$	$\|3\,\mathrm{T}_2\,{-2}\rangle = \sqrt{\tfrac{2}{5}}\,\|3\,{+3}\rangle + \sqrt{\tfrac{3}{5}}\,\|3\,{-2}\rangle$
$\|1\,\mathrm{T}_1\,{+1}\rangle = \|1\,{+1}\rangle$	$\|3\,\mathrm{U}\,{+2}\rangle = \sqrt{\tfrac{2}{5}}\,\|3\,{+2}\rangle + \sqrt{\tfrac{3}{5}}\,\|3\,{-3}\rangle$
$\|1\,\mathrm{T}_1\,0\rangle = \|1\,0\rangle$	$\|3\,\mathrm{U}\,{+1}\rangle = \|3\,1\rangle$
$\|1\,\mathrm{T}_1\,{-1}\rangle = \|1\,{-1}\rangle$	$\|3\,\mathrm{U}\,{-1}\rangle = \|3\,{-1}\rangle$
$\|\tfrac{3}{2}\,\mathrm{X}\,{+\tfrac{3}{2}}\rangle = \|\tfrac{3}{2}\,{+\tfrac{3}{2}}\rangle$	$\|3\,\mathrm{U}\,{-2}\rangle = -\sqrt{\tfrac{3}{5}}\,\|3\,{+3}\rangle + \sqrt{\tfrac{2}{5}}\,\|3\,{-2}\rangle$
$\|\tfrac{3}{2}\,\mathrm{X}\,{+\tfrac{1}{2}}\rangle = \|\tfrac{3}{2}\,{+\tfrac{1}{2}}\rangle$	$\|\tfrac{7}{2}\,\mathrm{E}_2\,{+\tfrac{3}{2}}\rangle = \sqrt{\tfrac{7}{10}}\,\|\tfrac{7}{2}\,{+\tfrac{3}{2}}\rangle + \sqrt{\tfrac{3}{10}}\,\|\tfrac{7}{2}\,{-\tfrac{7}{2}}\rangle$
$\|\tfrac{3}{2}\,\mathrm{X}\,{-\tfrac{1}{2}}\rangle = \|\tfrac{3}{2}\,{-\tfrac{1}{2}}\rangle$	$\|\tfrac{7}{2}\,\mathrm{E}_2\,{-\tfrac{3}{2}}\rangle = -\sqrt{\tfrac{3}{10}}\,\|\tfrac{7}{2}\,{+\tfrac{7}{2}}\rangle + \sqrt{\tfrac{7}{10}}\,\|\tfrac{7}{2}\,{-\tfrac{3}{2}}\rangle$
$\|\tfrac{3}{2}\,\mathrm{X}\,{-\tfrac{3}{2}}\rangle = \|\tfrac{3}{2}\,{-\tfrac{3}{2}}\rangle$	$\|4\,\mathrm{U}\,{+2}\rangle = -\sqrt{\tfrac{14}{15}}\,\|4\,{+2}\rangle - \sqrt{\tfrac{1}{15}}\,\|4\,{-3}\rangle$
$\|2\,\mathrm{V}\,{+2}\rangle = \|2\,{+2}\rangle$	$\|4\,\mathrm{U}\,{+1}\rangle = \sqrt{\tfrac{7}{15}}\,\|4\,{+1}\rangle + \sqrt{\tfrac{8}{15}}\,\|4\,{-4}\rangle$
$\|2\,\mathrm{V}\,{+1}\rangle = \|2\,{+1}\rangle$	$\|4\,\mathrm{U}\,{-1}\rangle = \sqrt{\tfrac{8}{15}}\,\|4\,{+4}\rangle - \sqrt{\tfrac{7}{15}}\,\|4\,{-1}\rangle$
$\|2\,\mathrm{V}\,0\rangle = \|2\,0\rangle$	$\|4\,\mathrm{U}\,{-2}\rangle = -\sqrt{\tfrac{1}{15}}\,\|4\,{+3}\rangle + \sqrt{\tfrac{14}{15}}\,\|4\,{-2}\rangle$
$\|2\,\mathrm{V}\,{-1}\rangle = \|2\,{-1}\rangle$	$\|4\,\mathrm{V}\,{+2}\rangle = \sqrt{\tfrac{1}{15}}\,\|4\,{+2}\rangle - \sqrt{\tfrac{14}{15}}\,\|4\,{-3}\rangle$
$\|2\,\mathrm{V}\,{-2}\rangle = \|2\,{-2}\rangle$	$\|4\,\mathrm{V}\,{+1}\rangle = -\sqrt{\tfrac{8}{15}}\,\|4\,{+1}\rangle + \sqrt{\tfrac{7}{15}}\,\|4\,{-4}\rangle$
$\|\tfrac{5}{2}\,\mathrm{W}\,{+\tfrac{5}{2}}\rangle = \|\tfrac{5}{2}\,{+\tfrac{5}{2}}\rangle$	$\|4\,\mathrm{V}\,0\rangle = \|4\,0\rangle$
$\|\tfrac{5}{2}\,\mathrm{W}\,{+\tfrac{3}{2}}\rangle = \|\tfrac{5}{2}\,{+\tfrac{3}{2}}\rangle$	$\|4\,\mathrm{V}\,{-1}\rangle = -\sqrt{\tfrac{7}{15}}\,\|4\,{+4}\rangle - \sqrt{\tfrac{8}{15}}\,\|4\,{-1}\rangle$
$\|\tfrac{5}{2}\,\mathrm{W}\,{+\tfrac{1}{2}}\rangle = \|\tfrac{5}{2}\,{+\tfrac{1}{2}}\rangle$	$\|4\,\mathrm{V}\,{-2}\rangle = \sqrt{\tfrac{14}{15}}\,\|4\,{+3}\rangle + \sqrt{\tfrac{1}{15}}\,\|4\,{-2}\rangle$
$\|\tfrac{5}{2}\,\mathrm{W}\,{-\tfrac{1}{2}}\rangle = \|\tfrac{5}{2}\,{-\tfrac{1}{2}}\rangle$	$\|5\,\mathrm{T}_1\,{+1}\rangle = \sqrt{\tfrac{3}{10}}\,\|5\,{+1}\rangle - \sqrt{\tfrac{7}{10}}\,\|5\,{-4}\rangle$
$\|\tfrac{5}{2}\,\mathrm{W}\,{-\tfrac{3}{2}}\rangle = \|\tfrac{5}{2}\,{-\tfrac{3}{2}}\rangle$	$\|5\,\mathrm{T}_1\,0\rangle = -\sqrt{\tfrac{7}{50}}\,\|5\,{+5}\rangle - \sqrt{\tfrac{18}{25}}\,\|5\,0\rangle + \sqrt{\tfrac{7}{50}}\,\|5\,{-5}\rangle$
$\|\tfrac{5}{2}\,\mathrm{W}\,{-\tfrac{5}{2}}\rangle = \|\tfrac{5}{2}\,{-\tfrac{5}{2}}\rangle$	$\|5\,\mathrm{T}_1\,{-1}\rangle = \sqrt{\tfrac{7}{10}}\,\|5\,{+4}\rangle + \sqrt{\tfrac{3}{10}}\,\|5\,{-1}\rangle$
	$\|5\,\mathrm{T}_2\,{+2}\rangle = \sqrt{\tfrac{3}{5}}\,\|5\,{+2}\rangle + \sqrt{\tfrac{2}{5}}\,\|5\,{-3}\rangle$
	$\|5\,\mathrm{T}_2\,0\rangle = \sqrt{\tfrac{9}{25}}\,\|5\,{+5}\rangle - \sqrt{\tfrac{7}{25}}\,\|5\,0\rangle - \sqrt{\tfrac{9}{25}}\,\|5\,{-5}\rangle$
	$\|5\,\mathrm{T}_2\,{-2}\rangle = -\sqrt{\tfrac{2}{5}}\,\|5\,{+3}\rangle + \sqrt{\tfrac{3}{5}}\,\|5\,{-2}\rangle$
	$\|5\,\mathrm{V}\,{+2}\rangle = -\sqrt{\tfrac{2}{5}}\,\|5\,{+2}\rangle + \sqrt{\tfrac{3}{5}}\,\|5\,{-3}\rangle$
	$\|5\,\mathrm{V}\,{+1}\rangle = \sqrt{\tfrac{7}{10}}\,\|5\,{+1}\rangle + \sqrt{\tfrac{3}{10}}\,\|5\,{-4}\rangle$
	$\|5\,\mathrm{V}\,0\rangle = -\sqrt{\tfrac{1}{2}}\,\|5\,{+5}\rangle - \sqrt{\tfrac{1}{2}}\,\|5\,{-5}\rangle$
	$\|5\,\mathrm{V}\,{-1}\rangle = \sqrt{\tfrac{3}{10}}\,\|5\,{+4}\rangle - \sqrt{\tfrac{7}{10}}\,\|5\,{-1}\rangle$
	$\|5\,\mathrm{V}\,{-2}\rangle = \sqrt{\tfrac{3}{5}}\,\|5\,{+3}\rangle + \sqrt{\tfrac{2}{5}}\,\|5\,{-2}\rangle$

Table 6. Properties of the standard matrix irreps for $I^* \supset C_5^*$. See Sect. 3 of main text. The two elements $\boldsymbol{C}_5^{Z*}$ and $\boldsymbol{C}_2^{Y*}$ actually only generate the subgroup D_5^* of I^*, but the irrep matrices of the generator $\boldsymbol{C}_2^*$ (Sect. 3.1) were of such a complicated appearance that they were not of much interest except for their symmetry (Sect. 3.2).

Explanation of table: "diag" means diagonal, "bidiag" bidiagonal; thus, e.g.,

$$\operatorname{diag}[\bar{\omega}', \omega'] = \begin{pmatrix} \bar{\omega}' & 0 \\ 0 & \omega' \end{pmatrix} \text{ and } \operatorname{bidiag}[1, -1, 1, -1] = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

The component designations are taken over from McLellan [6]; their significance is seen when considering the $\boldsymbol{C}_5^{Z*}$-matrices

Irrep Γ	Components (as column indices)	($\boldsymbol{C}_5^{Z*}$)	($\boldsymbol{C}_2^{Y*}$)	($\boldsymbol{C}_2^*$)
T_1	$(1, 0, -1)$	$\operatorname{diag}[\bar{\omega}, 1, \omega]$	$\operatorname{bidiag}[1, -1, 1]$	s, r
T_2	$(2, 0, -2)$	$\operatorname{diag}[\bar{\omega}^2, 1, \omega^2]$	$\operatorname{bidiag}[-1, -1, -1]$	s, r
U	$(2, 1, -1, -2)$	$\operatorname{diag}[\bar{\omega}^2, \bar{\omega}, \omega, \omega^2]$	$\operatorname{bidiag}[-1, 1, 1, -1]$	s, r
V	$(2, 1, 0, -1, -2)$	$\operatorname{diag}[\bar{\omega}^2, \bar{\omega}, 1, \omega, \omega^2]$	$\operatorname{bidiag}[1, -1, 1, -1, 1]$	s, r
E_1	$(\frac{1}{2}, -\frac{1}{2})$	$\operatorname{diag}[\bar{\omega}', \omega']$	$\operatorname{bidiag}[1, -1]$	s, i
E_2	$(\frac{3}{2}, -\frac{3}{2})$	$\operatorname{diag}[(\bar{\omega}')^3, (\omega')^3]$	$\operatorname{bidiag}[1, -1]$	s, i
X	$(\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2})$	$\operatorname{diag}[(\bar{\omega}')^3, \bar{\omega}', \omega', (\omega')^3]$	$\operatorname{bidiag}[1, -1, 1, -1]$	s, i
W	$(\frac{5}{2}, \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2})$	$\operatorname{diag}[(\bar{\omega}')^5, (\bar{\omega}')^3, \bar{\omega}', \omega', (\omega')^3, (\omega')^5]$	$\operatorname{bidiag}[1, -1, 1, -1, 1, -1]$	s, i

$\omega' = \exp(i2\pi/10)$; $\omega = (\omega')^2$; s = symmetric; r = real; i = purely imaginary functions, it is a Δ pair. The other possibility would correspond to basis functions generally modified by powers of $e^{-i2\pi/5}$ when expressed in terms of the $|jm\rangle$ (cf. [2], Sect. 4.5) and thus having much more complicated expressions than the present ones.

The positive part of McLellan's X axis must have intersected an edge forming a Λ pair with the Z axis.

A similar phenomenon was described by Boyle & Schäffer [36] for coordinate systems formed by three icosahedral two-fold axes.]

Some of the properties of the matrix irreps generated by these basis functions may be seen in Table 6. It is seen, in particular, that these matrix irreps have the "symmetric generator matrices"-property and thus allow *real* 3-Γ symbols ([2], Sect. 3.2). Indeed, the basis functions in Table 5 are all real linear combinations of the $|jm\rangle$ functions and thus generate real icosahedral 3-Γ symbols by the procedure outlined in ([2], Sect. 4).

The irreps and 3-Γ symbols satisfy the relations

$$\begin{pmatrix} \Gamma & A & \Gamma \\ \gamma & 0 & \gamma' \end{pmatrix} = (\dim \Gamma)^{-1/2} \Gamma(C_2^{Y*})_{\gamma\gamma'}$$
$$= (\dim \Gamma)^{-1/2} \delta(-\gamma, \gamma')(-1)^{j(\Gamma)-\gamma'}. \tag{3.2.1}$$

We recall that the 3-Γ symbols in (3.2.1) are the elements of the matrices we have chosen as *conjugating matrices* for the standard matrix irreps ([1], Sect. 5). Here and in the following $j(\Gamma)$ denotes the primary j-value assigned to Γ in Table 3b. Note that we here have a particular example of the general relation ([2], (3.3.1)). Some consequences of relations (3.2.1) will now be pointed out.

Firstly, because of the first equation in (3.2.1), the particularly convenient formalism of ([1], Sect. 5.5) applies. We recall that this means that all 3-Γ symbols may be chosen real; all Derome–Sharp $\mathbb{A}$ matrices ([1], Sect. 5.4) are unit matrices, i.e. the formula

$$\begin{pmatrix} \bar{\Gamma}_1 & \bar{\Gamma}_2 & \bar{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta = \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta \tag{3.2.2}$$

holds generally; and that $\mathbb{B}$ matrices ([1], Sect. 5.4) are given by $\mathbb{B}^i(\Gamma_1\Gamma_2\Gamma_3)_{\alpha\beta} = \pi(\Gamma_i A \Gamma_i)\delta(\alpha, \beta)$ so that, e.g.

$$\begin{pmatrix} \bar{\Gamma}_1 & \bar{\Gamma}_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta = \pi(\Gamma_3 A \Gamma_3) \begin{pmatrix} \Gamma_1 & \Gamma_2 & \bar{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta \tag{3.2.3}$$

is generally valid. Furthermore, the conventional relation between coupling coefficients and 3-Γ symbols, discussed in ([1], Sect. 5.3), assumes the simple form

$$\langle \Gamma_1\gamma_1\Gamma_2\gamma_2 | \beta\Gamma_3\gamma_3 \rangle$$
$$= \pi(\Gamma_1\Gamma_2\Gamma_3\beta)\pi(\Gamma_2 A \Gamma_2)\sqrt{\dim \Gamma_3} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \bar{\Gamma}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta. \tag{3.2.4}$$

Table 7. Some selected 3-Γ symbols for $I^* \supset C_5^*$ generated by the basis functions of Table 5. The multiplicity index β contains information on the permutational characteristic of the 3-Γ symbols; thus $\beta = o$, $o1$, *or* $o2$ indicates *odd* 3-Γ symbols and $\beta = e$, $e1$ or $e2$ *even* 3-Γ symbols. The triples of j-values used for the construction of 3-Γ symbols can be found in Table 4; thus, the $(\mathrm{WVW}/\gamma_1\gamma_2\gamma_3)_{o1}$ 3-Γ symbols correspond to $(j_1, j_2, j_3) = (\frac{5}{2}, 2, \frac{5}{2})$, whereas the $o2$ and e labels for WVW correspond to $(\frac{5}{2}, 4, \frac{5}{2})$ and $(\frac{5}{2}, 5, \frac{5}{2})$, respectively

γ_1	γ_2	γ_3	$\begin{pmatrix} \mathrm{V} & \mathrm{V} & \mathrm{V} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_{e1}$
2	0	−2	$+\sqrt{\frac{2}{35}}$
2	−1	−1	$-\sqrt{\frac{3}{35}}$
1	0	−1	$+\sqrt{\frac{1}{70}}$
0	0	0	$-\sqrt{\frac{2}{35}}$

γ_1	γ_2	γ_3	$\begin{pmatrix} \mathrm{V} & \mathrm{V} & \mathrm{V} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_{e2}$
2	2	1	$+\sqrt{\frac{7}{75}}$
2	0	−2	$+\sqrt{\frac{1}{350}}$
2	−1	−1	$+\sqrt{\frac{4}{525}}$
1	0	−1	$+\sqrt{\frac{8}{175}}$
0	0	0	$+\sqrt{\frac{18}{175}}$

γ_1	γ_2	γ_3	$\begin{pmatrix} \mathrm{X} & \mathrm{U} & \mathrm{W} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_{o}$
$\frac{1}{2}$	2	$\frac{5}{2}$	$+\sqrt{\frac{3}{32}}$
$-\frac{1}{2}$	−2	$\frac{5}{2}$	$-\sqrt{\frac{1}{24}}$
$-\frac{3}{2}$	−1	$\frac{5}{2}$	$+\sqrt{\frac{1}{32}}$
$\frac{3}{2}$	2	$\frac{3}{2}$	$-\sqrt{\frac{9}{160}}$
$-\frac{1}{2}$	−1	$\frac{3}{2}$	$+\sqrt{\frac{49}{480}}$
$\frac{1}{2}$	−2	$\frac{3}{2}$	$-\sqrt{\frac{1}{120}}$
$-\frac{3}{2}$	1	$\frac{1}{2}$	$+\sqrt{\frac{9}{80}}$
$\frac{1}{2}$	−1	$\frac{1}{2}$	$-\sqrt{\frac{1}{240}}$
$\frac{3}{2}$	−2	$\frac{1}{2}$	$+\sqrt{\frac{1}{20}}$

γ_1	γ_2	γ_3	$\begin{pmatrix} \mathrm{X} & \mathrm{U} & \mathrm{W} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_{e}$
$\frac{3}{2}$	1	$\frac{5}{2}$	$-\sqrt{\frac{2}{15}}$
$\frac{1}{2}$	2	$\frac{5}{2}$	$-\sqrt{\frac{1}{160}}$
$-\frac{1}{2}$	−2	$\frac{5}{2}$	$-\sqrt{\frac{1}{40}}$
$-\frac{3}{2}$	−1	$\frac{5}{2}$	$-\sqrt{\frac{1}{480}}$
$\frac{3}{2}$	2	$\frac{3}{2}$	$-\sqrt{\frac{1}{96}}$
$\frac{1}{2}$	−2	$\frac{3}{2}$	$-\sqrt{\frac{1}{8}}$
$-\frac{1}{2}$	−1	$\frac{3}{2}$	$-\sqrt{\frac{1}{32}}$
$\frac{3}{2}$	−2	$\frac{1}{2}$	$-\sqrt{\frac{1}{12}}$
$\frac{1}{2}$	−1	$\frac{1}{2}$	$-\sqrt{\frac{1}{16}}$
$-\frac{3}{2}$	1	$\frac{1}{2}$	$+\sqrt{\frac{1}{48}}$

γ_1	γ_2	γ_3	$\begin{pmatrix} \mathrm{W} & \mathrm{V} & \mathrm{W} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_{o1}$
$\frac{5}{2}$	0	$-\frac{5}{2}$	$-\sqrt{\frac{5}{84}}$
$\frac{5}{2}$	−1	$-\frac{3}{2}$	$+\sqrt{\frac{1}{14}}$
$\frac{5}{2}$	−2	$-\frac{1}{2}$	$-\sqrt{\frac{1}{28}}$
$\frac{3}{2}$	0	$-\frac{3}{2}$	$-\sqrt{\frac{1}{420}}$
$\frac{3}{2}$	−1	$-\frac{1}{2}$	$-\sqrt{\frac{1}{35}}$
$\frac{3}{2}$	−2	$\frac{1}{2}$	$+\sqrt{\frac{9}{140}}$
$\frac{1}{2}$	0	$-\frac{1}{2}$	$+\sqrt{\frac{4}{105}}$

γ_1	γ_2	γ_3	$\begin{pmatrix} \mathrm{W} & \mathrm{V} & \mathrm{W} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_{e}$
$\frac{5}{2}$	2	$\frac{1}{2}$	$-\sqrt{\frac{2}{75}}$
$\frac{5}{2}$	1	$\frac{3}{2}$	$+\sqrt{\frac{3}{100}}$
$\frac{5}{2}$	0	$\frac{5}{2}$	$+\sqrt{\frac{1}{10}}$
$\frac{5}{2}$	−1	$-\frac{3}{2}$	$+\sqrt{\frac{1}{300}}$
$\frac{5}{2}$	−2	$-\frac{1}{2}$	$+\sqrt{\frac{1}{150}}$
$\frac{3}{2}$	2	$\frac{3}{2}$	$-\sqrt{\frac{1}{15}}$
$\frac{3}{2}$	−1	$-\frac{1}{2}$	$+\sqrt{\frac{1}{30}}$
$\frac{3}{2}$	−2	$\frac{1}{2}$	$+\sqrt{\frac{1}{30}}$
$\frac{1}{2}$	−1	$\frac{1}{2}$	$+\sqrt{\frac{1}{15}}$

γ_1	γ_2	γ_3	$\begin{pmatrix} \mathrm{W} & \mathrm{V} & \mathrm{W} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_{o2}$
$\frac{5}{2}$	2	$\frac{1}{2}$	$-\sqrt{\frac{7}{75}}$
$\frac{5}{2}$	1	$\frac{3}{2}$	$-\sqrt{\frac{7}{150}}$
$\frac{5}{2}$	0	$-\frac{5}{2}$	$-\sqrt{\frac{1}{140}}$
$\frac{5}{2}$	−1	$-\frac{3}{2}$	$-\sqrt{\frac{8}{525}}$
$\frac{5}{2}$	−2	$-\frac{1}{2}$	$-\sqrt{\frac{3}{700}}$
$\frac{3}{2}$	0	$-\frac{3}{2}$	$-\sqrt{\frac{9}{140}}$
$\frac{3}{2}$	−1	$-\frac{1}{2}$	$-\sqrt{\frac{4}{105}}$
$\frac{3}{2}$	−2	$\frac{1}{2}$	$-\sqrt{\frac{1}{420}}$
$\frac{1}{2}$	0	$-\frac{1}{2}$	$-\sqrt{\frac{1}{35}}$

(In (3.2.3) and (3.2.4), the permutational characteristic (transposition phase) $\pi(\Gamma_1\Gamma_2\Gamma_3\beta)$ is +1 if the 3-Γ symbols $(\Gamma_1\Gamma_2\Gamma_3/\gamma_1\gamma_2\gamma_3)_\beta$ are *even* and -1 if they are *odd* ([1], Sect. 4).)

Secondly, the fix-vector property of 3-Γ symbols ([1], Sects. 3 and 4) together with the second equation in (3.2.1) leads [2, Sect. 3.5] to the following general internal relation between 3-Γ symbols for a given triple $\Gamma_1\Gamma_2\Gamma_3$:

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ -\gamma_1 & -\gamma_2 & -\gamma_3 \end{pmatrix}_\beta = (-)^{j(\Gamma_1)+j(\Gamma_2)+j(\Gamma_3)-\gamma_1-\gamma_2-\gamma_3} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta . \tag{3.2.5}$$

Eqs. (3.2.1) together with ([1], Sects. 5.3.1–5.3.2) show that conjugations are generally carried out by the formla

$$\begin{pmatrix} \cdots & \bar{\Gamma} & \cdots \\ & \gamma & \end{pmatrix} = (-1)^{j(\Gamma)-\gamma} \begin{pmatrix} \cdots & \Gamma & \cdots \\ & -\gamma & \end{pmatrix}. \tag{3.2.6}$$

Because of the C_5^*-adaption, the 3-Γ symbols also satisfy ([2], Sect. 3.5) the "selection rule"

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta \neq 0 \Rightarrow \gamma_1+\gamma_2+\gamma_3 \equiv 0 \pmod 5. \tag{3.2.7}$$

Space limitations prevent us from giving a full tabulation of the 3-Γ symbols generated by the basis functions of Table 5. Besides, we actually think that the most important thing about the present paper is that we describe *how* a set of 3-Γ symbols with the above properties may be generated (most naturally by a computer, maybe even only internally in computer programs when they are to be used). Large tables as required here are bound to contain errors (if not reproduced directly from the computer-output). However, for illustration purposes, we give in Table 7 the 3-Γ symbols just for the triples VVV, XUW, WVW (all multiplicity triples; one, three, and two irreps involved, respectively, and multiplicities two, two, and three, respectively). The table has been condensed by the use of formula (3.2.5); for example, although $(\mathrm{XUW}/-1/2\ \ -2\ \ -5/2)_o$ is not in the table, we find there $(\mathrm{XUW}/1/2\ \ 2\ \ 5/2)_o$, and (3.2.5) then gives

$$\begin{aligned} \begin{pmatrix} \mathrm{X} & \mathrm{U} & \mathrm{W} \\ -1/2 & -2 & -5/2 \end{pmatrix}_o &= (-1)^{3/2+3+5/2-1/2-2-5/2} \begin{pmatrix} \mathrm{X} & \mathrm{U} & \mathrm{W} \\ 1/2 & 2 & 5/2 \end{pmatrix}_o \\ &= \begin{pmatrix} \mathrm{X} & \mathrm{U} & \mathrm{W} \\ 1/2 & 2 & 5/2 \end{pmatrix}_o = \sqrt{3/32}. \end{aligned} \tag{3.28}$$

We have used here "o" (for odd) as an abbreviation for "$3/2+3+5/2$".

[Using more or less the same basis functions as McLellan, Golding [25], König and Kremer [27], and Pooler [9] obtained "symmetry coupling coefficients" for I^*, 3-Γ symbols for I, and "3-*jm* symbols" for I, respectively. In all cases, non-real (but then purely imaginary) coefficients occur. All three expositions involve complicating concepts of either "minus'ing" [25, 37] or "time-reversal" [27, 9]. Pooler seems to use j-values much the same way as we have done above, although he criticizes the very similar (but disguised) use Golding makes of them. We would like to emphasize that these j-values do not introduce any information which is extraneous to the icosahedral Wigner–Racah algebra; they are just a convenient way of representing information *within* that algebra. (Of course the *reason* that they work lies in the relations with the rotation group.)

The tables of [25] were checked on a computer by the present authors; some errors were found (one is pointed out in [9]).]

4. Adaption to other subgroup hierarchies

There is quite a number of icosahedral subgroup hierarchies to which one might adapt the icosahedral matrix irreps other than $I^* \supset C_5^*$ discussed above. Butler [26, 38], Boyle [21, 36, 10], and the present authors [36, 39] have each worked with one or several of these. The general impression emerging from these investigations is that basis functions and 3-Γ symbols become much more complicated and the whole formalism less elegant than was the case with $I^* \supset C_5^*$. In some cases, 3-Γ symbols cannot all be chosen real.

We shall now briefly summarize what is known about these other cases.

4.1. Further pentagonal hierarchies

It is a rather trivial matter to modify the basis functions of Table 5 so that they become adapted to either of the hierarchies $I^* \supset D_5^* \supset C_5^*$ or $I^* \supset D_5^* \supset C_2^*$ (cf. [3]). For none of these we have been able to avoid non-real 3-Γ symbols. In fact, it has recently been *proved* [40] that strict adaption to $I^* \supset D_5^*$ excludes the possibility of having all coupling coefficients real, and this is equivalent to stating that not all 3-Γ symbols can be chosen real (the latter follows from arguments given in [41]).

If one relaxes the requirement of D_5^*-adaptation just for the two third-kind spin irreps R_1 and R_2 (see definition in [3]) and combines them to a reducible two-dimensional rep, one may establish basis functions and *real* 3-Γ symbols obeying a formalism almost as elegant as the one described above for $I^* \supset C_5^*$. Since the results are so similar, they will not be reproduced here, but copies of the complete material thus produced are available from the present authors upon request.

4.2. Trigonal hierarchies

The following trigonal hierachies may be envisaged:

$$\begin{aligned} &I^* \supset C_3^* \\ &I^* \supset T^* \supset C_3^* \\ &I^* \supset D_3^* \supset C_3^* \\ &I^* \supset D_3^* \supset C_2^*. \end{aligned} \tag{4.2.1}$$

It was proved in [40] that strict adaption of matrix irreps to $I^* \supset D_3^*$ or to $I^* \supset T^*$ makes it impossible to have all coupling coefficients (or all 3-Γ symbols) real. In fact, this is not even possible for $I \supset T$. For $I^* \supset T^* \supset C_3^*$, we have previously proved [39] that real 3-Γ symbols did not exist. That proof was based on actual numbers from a trial calculation, whereas the arguments in [40] are of a more global group-theoretic nature.

The hierarchy $I^* \supset T^* \supset C_3^*$ is relevant for the kind of systems discussed in [6, 7, 42].

We do not at the present time have any results for an adaption to $I^* \supset C_3^*$ without adaption to T^* or D_3^* also.

4.3. Diagonal and further tetrahedral hierarchies

The remaining hierarchies terminating with C_2^* are

$$\begin{aligned} &I^* \supset C_2^* \\ &I^* \supset D_2^* \supset C_2^* \\ &I^* \supset T^* \supset C_2^* \\ &I^* \supset T^* \supset D_2^* \supset C_2^*. \end{aligned} \tag{4.3.1}$$

For the hierarchies involving T^*, a full set of real 3-Γ symbols does not exist; as noted above, this is even true for $I \supset T$, the proof being given in [40].

We have constructed some basis functions adapted to $I^* \supset D_2^* \supset C_2^*$ which are also *almost* T^*-adapted, their only default in this respect being that the tetrahedral third-kind irreps C_1, C_2, E_2, and E_3 [4] have been mixed to form a reducible two-dimensional rep E with a real matrix form equivalent to $C_1 \oplus C_2$ and a reducible 4-dimensional rep with a (non-real) matrix form equivalent to $E_2 \oplus E_3$. These basis functions have the conjugation property of ([1], Eq. (4.4.1)) ("irrep conjugation by a fixed group element"). Thus real 3-Γ symbols obeying the formalism of ([1], Sect. 5.5) may be chosen and are indeed generated by these basis functions. However, many of the 3-Γ symbols have a very complicated algebraic form, e.g. one obtains

$$\begin{pmatrix} \mathrm{E} & \mathrm{W} & \mathrm{T} \\ \mathrm{E}_1(T^*)\mathrm{E}_{1/2}(D_2^*)1/2 & \beta\mathrm{E}_1(T^*)\mathrm{E}_{1/2}(D_2^*)1/2 & \mathrm{T}(T^*)\mathrm{B}_3(D_2^*)x \end{pmatrix}$$
$$= \sqrt{9/256} + \sqrt{5/2304} - \sqrt{3/256} + \sqrt{5/768}. \tag{4.3.2}$$

On the other hand, this hierarchy may be a relevant one for the study of, e.g. hexanitrato-rare-earth ions of the form $[M(NO_3)_6]^{3-}$ having T_h symmetry [42] and approximate icosahedral symmetry, so the material may be of interest and we hope to finish this work in the near future.

If we stay with the $I^*(\supset T^*) \supset D_2^* \supset C_2^*$-material just mentioned and restrict attention to the vector irreps, we are effectively just studying the icosahedral pure rotation group I in an adaption to $I(\supset T) \supset D_2 \supset C_2$. Here the 3-Γ symbols have at most two terms (compare with the four terms in (4.3.2) above), and the basis functions may be expressed simply in terms of either the standard real spherical harmonics or cubic harmonics. Thus a rather satisfactory "real algebra" emerges which is a continuation of the treatment of the crystallographic point groups given in [43]. One possible choice of irrep matrices corresponding to this adaption has been published in [10]. It is our intention to make this material the subject of a separate publication.

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