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Phase-fixed double-group 3-Γ symbols. IV. Real 3-Γ symbols and coupling coefficients for the group hierarchies $T^* \supset C_3^*$ and $T^* \supset C_2^*$

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We present sets of real 3-Γ symbols which correspond to explicitly given irreducible matrix representations for the two double group hierarchies $T^* \supset C_3^*$ and $T^* \supset C_2^*$. They fit into the formalism exposed in a previous paper [1] on the general theory of 3-Γ symbols and coupling coefficients and illustrate much of the discussion in a subsequent one [2] treating the particular properties of the double groups.

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

1. Introduction

Continuing the series [1–3] of papers devoted to the establishment of real, phase-fixed ([2], Sect. 4) 3-Γ symbols ([1], Sect. 4) for all the double groups ([2], Sect. 2), in this paper we treat the tetrahedral double group T^*.

Of course, many systems with tetrahedral symmetry have, in fact, full T_d symmetry so that one is likely to use T_d (which is isomorphic to the octahedral group O) or its double group T_d^* (which is defined to be O^*, cf. [2], Sect. 2) in analyzing these systems. There are, however, some systems which have an (approximate) T_h symmetry [4, 5], and since T_h^* is defined to be $T^* \times C_i$ ([2], Sect. 2), the group T^* becomes relevant in such cases. Although rare, some systems also exist with pure T symmetry [6] or very nearly that symmetry [7].

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Furthermore, the tetrahedral double group is distinguished by being easy to overview (a set of 3-Γ symbols may be tabulated on a single page), while at the same time exhibiting several complicating rep-theoretical features (it is non-ambivalent, indeed has irreps of all three Frobenius–Schur kinds ([1], Sect. 5.2; or [8]) like did the groups D_n^* with n odd [3], and it is furthermore non-multiplicity-free). We therefore find it justified to give it here a rather detailed treatment.

Table 1 contains the general information on T^* which we shall need here. Further properties may be found in [9] and [10] and in the literature referred to in ([2], Sect. 2). Frobenius [11] was probably the first to give the character table.

The tetrahedral double group may be generated by elements C_3^* and C_2^* corresponding to a three-fold and a two-fold rotation, respectively, around axes forming an angle of Arccos $(\sqrt{1/3})$ with each other. There are thus two natural group–subgroup hierarchies to which one may adapt the matrix irreps of T^*, namely, $T^* \supset C_3^*$ and $T^* \supset C_2^*$. We shall now discuss these two main cases separately

Table 1. The tetrahedral double group T^* (rep-theoretical facts and conventions)

	A	C_1	C_2	T	E_1	E_2	E_3
	[b]A	E		T	E′	E″	E‴
	[c]Γ_1	Γ_3	Γ_2	Γ_4		U′	
Irreps[a] (Γ)	[d]A_1	C	B	T	E′	E″	E‴
Dimension	1	1	1	3	2	2	2
Frobenius–Schur classification[e]	1st kind	3rd kind		1st kind	2nd kind	3rd kind	
Vector/spin-classification[f]		vector				spin	
$\Gamma \otimes_s \Gamma^{g,i}$	A	C_1	C_2	$A \oplus C_1 \oplus C_2 \oplus T$	T	T	T
$\Gamma \otimes_A \Gamma^{h,i}$	—	—	—	T	A	A	A
Primary j-value[j]	0	2	2	1	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{3}{2}$
Secondary j-value[j]	—	—	—	2	—	—	—

[a] At the top is given our present notation for the irreps. Note that the totally symmetric irrep (1_{T^*} in the notation of [1]) is denoted A.
[b] Notation of [4, 20, 22] (except for "A" instead of "A_1").
[c] Additional notation of [22].
[d] Notation of [19]. Still another notation is the one used in Butler's book [16].
[e] See ([1], Sect. 5.2).
[f] See ([2], Sect. 2.1).
[g] Means "symmetric part of $\Gamma \otimes \Gamma$".
[h] Means "antisymmetric part of $\Gamma \otimes \Gamma$".
[i] See ([1], Sect. A.1).
[j] See discussion in ([2], Sect. 4).
Note that C_1, C_2 and E_2, E_3 form pairs of mutually complex conjugate irreps. The distinctions between C_1 and C_2 and between E_2 and E_3 are actually not meaningful in an abstract context; the correlations of notation are made on the basis of the convention that "C_3" of [22] is "C_3^*" of the present work and that "C_3" of [19], which uses *clockwise* rotations, is $(C_3^{Z*})^{-1}$ of the present work

(possible adaptation to $T^* \supset D_2^* \supset C_2^*$ will also be touched upon in Sect. 4). Some recent literature on tetrahedral symmetry coefficients will be commented upon in Sect. 5.

2. Matrix irreps and 3-Γ symbols for $T^* \supset C_3^*$

Fig. 1 shows how we choose to place the coordinate system in connection with this hierarchy. The three-fold axis is along the Z-axis and the two-fold axis lies in the XZ-plane. In this way, the above mentioned generators of T^* are

$$C_3^{Z*} = \mathscr{D}^{[1/2]}(2\pi/3, 0, 0)$$

and (2.1)

$$C_2^* = \mathscr{D}^{[1/2]}(0, \text{Arccos}\,(-1/3), \pi).$$

Regarding our definitions of double groups and notation for their elements, see ([2], Sect. 2) or [12].

This placement of the tetrahedron in the coordinate system or, rather, this way of placing the coordinate system relative to the axes of the rotations generating the tetrahedral group, is chosen for two reasons. Firstly, it allows very simple expressions for basis functions generating real 3-Γ symbols (see below). Secondly, it is convenient for correlation with the octahedron as we (partly from other considerations) choose to place *that* in connection with the hierarchy $O^* \supset C_3^*$ in [13].

Table 2 then gives our standard matrix irreps for $T^* \supset C_3^*$. Note that the matrix forms of E_2 and E_3 are *mutually complex conjugate* when the pairwise identical components are taken in the same order; this is, of course, trivially also true of C_1 and C_2.

All generator irrep matrices are symmetric; this ensures that these standard irreps allow *real* 3-Γ symbols to be chosen ([2], Sect. 3.2). Indeed, the standard basis functions we suggest in Table 3 are all *real* linear combinations of the $|jm\rangle$ functions and thus generate real 3-Γ symbols ([2], Sect. 4), as seen in Table 4. We have made use of the observations in ([2], Sect. 4.5) in choosing that relative orientation of the coordinate system and the axes of the tetrahedral generators which leads to the simplest expression for the basis functions. Remaining free phases have been chosen in accordance with the rules in ([2], Sect. 4).

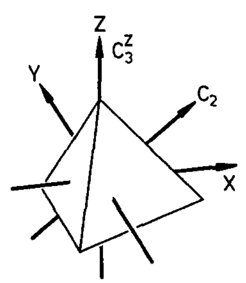

Fig. 1. Placement of the coordinate system relative to the axes of the tetrahedral generators as used in Sect. 2 for the hierarchy $T^* \supset C_3^*$. The two-fold rotation about the axis denoted here C_2 has euler angles (0, Arccos $(-1/3)$, π)

Table 2. Standard matrix irreps for $T^* \supset C_3^*$

Γ	components[a]	$\Gamma(C_3^{Z*})$	$\Gamma(C_2^*)$
A	0	1	1
C_1	c	$e^{-i2\pi/3}$	1
C_2	c	$e^{i2\pi/3}$	1
T	$\begin{cases} 1 \\ 0 \\ -1 \end{cases}$	$\begin{pmatrix} e^{-i2\pi/3} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i2\pi/3} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{3} & -\frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{pmatrix}$
E_1	$\begin{cases} \frac{1}{2} \\ -\frac{1}{2} \end{cases}$	$\begin{pmatrix} e^{-i\pi/3} & 0 \\ 0 & e^{i\pi/3} \end{pmatrix}$	$\begin{bmatrix} -i\sqrt{\frac{1}{3}} & -i\sqrt{\frac{2}{3}} \\ -i\sqrt{\frac{2}{3}} & i\sqrt{\frac{1}{3}} \end{bmatrix}$
E_2	$\begin{cases} a \\ b \end{cases}$	$\begin{bmatrix} e^{-i\pi/3} & 0 \\ 0 & -1 \end{bmatrix}$	$\begin{bmatrix} i\sqrt{\frac{1}{3}} & i\sqrt{\frac{2}{3}} \\ i\sqrt{\frac{2}{3}} & -i\sqrt{\frac{1}{3}} \end{bmatrix}$
E_3	$\begin{cases} a \\ b \end{cases}$	$\begin{bmatrix} e^{i\pi/3} & 0 \\ 0 & -1 \end{bmatrix}$	$\begin{bmatrix} -i\sqrt{\frac{1}{3}} & -i\sqrt{\frac{2}{3}} \\ -i\sqrt{\frac{2}{3}} & i\sqrt{\frac{1}{3}} \end{bmatrix}$

[a] A numerical component γ means "eigenvalue $e^{-i\gamma 2\pi/3}$ under C_3^{Z*}". The third-kind irrep components may be translated to numerical ones by the rules $C_1 c = 1$; $C_2 c = -1$; $E_2 a = \frac{1}{2}$; $E_3 a = -\frac{1}{2}$; $E_2 b = \frac{3}{2}$; $E_3 b = -\frac{3}{2}$ (cf. [2], Sect. 3.4). The two generators are defined in (2.1) in the main text.

Table 3. Basis functions for $T^* \supset C_3^*$

$\vert 0\,\mathrm{A}\,0\rangle = \vert 0\,0\rangle$	
$\vert \frac{1}{2}\,\mathrm{E}_1\,\frac{1}{2}\rangle = \vert \frac{1}{2}\,\frac{1}{2}\rangle$	
$\vert \frac{1}{2}\,\mathrm{E}_1\,\frac{1}{2}\rangle = \vert \frac{1}{2}\,-\frac{1}{2}\rangle$	
$\vert 1\,\mathrm{T}\,1\rangle = \vert 1\,1\rangle$	$\vert 2\,\mathrm{T}\,1\rangle = \sqrt{\frac{1}{3}}\vert 2\,1\rangle + \sqrt{\frac{2}{3}}\vert 2\,-2\rangle$
$\vert 1\,\mathrm{T}\,0\rangle = \vert 1\,0\rangle$	$\vert 2\,\mathrm{T}\,0\rangle = -\vert 2\,0\rangle$
$\vert 1\,\mathrm{T}\,-1\rangle = \vert 1\,-1\rangle$	$\vert 2\,\mathrm{T}\,-1\rangle = -\sqrt{\frac{2}{3}}\vert 2\,2\rangle + \sqrt{\frac{1}{3}}\vert 2\,-1\rangle$
$\vert \frac{3}{2}\,\mathrm{E}_2\,a\rangle = \vert \frac{3}{2}\,\frac{1}{2}\rangle$	
$\vert \frac{3}{2}\,\mathrm{E}_2\,b\rangle = \sqrt{\frac{1}{3}}\vert \frac{3}{2}\,\frac{3}{2}\rangle - \sqrt{\frac{2}{3}}\vert \frac{3}{2}\,-\frac{3}{2}\rangle$	
$\vert \frac{3}{2}\,\mathrm{E}_3\,a\rangle = -\vert \frac{3}{2}\,-\frac{1}{2}\rangle$	
$\vert \frac{3}{2}\,\mathrm{E}_3\,b\rangle = \sqrt{\frac{2}{3}}\vert \frac{3}{2}\,\frac{3}{2}\rangle + \sqrt{\frac{1}{3}}\vert \frac{3}{2}\,-\frac{3}{2}\rangle$	
$\vert 2\,\mathrm{C}_1\,c\rangle = +\sqrt{\frac{2}{3}}\vert 2\,1\rangle - \sqrt{\frac{1}{3}}\vert 2\,-2\rangle$	
$\vert 2\,\mathrm{C}_2\,c\rangle = +\sqrt{\frac{1}{3}}\vert 2\,2\rangle + \sqrt{\frac{2}{3}}\vert 2\,-1\rangle$	

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 is a T^*-irrep and γ a component of Γ. The functions generate the matrix irreps given in Table 2.

Table 4. 3-Γ symbols for $T^* \supset C_3^*$

A	A	A	3-Γ	(even)
0	0	0	+1	

C_1	C_1	C_1	3-Γ	(even)
c	c	c	+1	

C_2	C_2	C_2	3-Γ	(even)
c	c	c	−1	

T	A	T	3-Γ	(even)
1	0	−1	$+\sqrt{1/3}$	
0	0	0	$-\sqrt{1/3}$	

E_1	A	E_1	3-Γ	(odd)
1/2	0	−1/2	$-\sqrt{1/2}$	

T	C_1	T	3-Γ	(even)
1	c	1	$-\sqrt{1/3}$	
−1	c	0	$-\sqrt{1/3}$	

$A(TC_1T) = -1$

E_2	C_1	E_2	3-Γ	(odd)
a	c	b	$-\sqrt{1/2}$	

E_3	C_2	E_3	3-Γ	(odd)
a	c	b	$+\sqrt{1/2}$	

E_1	C_2	E_2	3-Γ	(even)
1/2	c	a	$\sqrt{1/2}$	
−1/2	c	b	$\sqrt{1/2}$	

$A(E_1C_2E_2) = +1$

E_1	T	E_2	3-Γ	(odd)
1/2	1	b	$+\sqrt{1/3}$	
1/2	−1	a	$-\sqrt{1/6}$	
−1/2	0	a	$-\sqrt{1/3}$	
−1/2	−1	b	$+\sqrt{1/6}$	

$A(E_1TE_2) = +1$

T	T	T	3-Γ	(odd)
1	0	−1	$-\sqrt{1/6}$	

T	T	T	3-Γ	(even)
1	1	1	$\sqrt{2/9}$	
1	0	−1	$-\sqrt{1/18}$	
0	0	0	$-\sqrt{2/9}$	
−1	−1	−1	$-\sqrt{2/9}$	

$\mathbb{A}$(TTT)	odd	even
odd	1	0
even	0	−1

C_1	A	C_2	3-Γ	(even)
c	0	c	−1	

E_2	A	E_3	3-Γ	(odd)
a	0	a	$-\sqrt{1/2}$	
b	0	b	$-\sqrt{1/2}$	

E_1	T	E_1	3-Γ	(even)
1/2	−1	1/2	$-\sqrt{1/3}$	
1/2	0	−1/2	$+\sqrt{1/6}$	
−1/2	1	−1/2	$-\sqrt{1/3}$	

E_2	T	E_2	3-Γ	(even)
a	1	b	$\sqrt{1/6}$	
b	0	b	$-\sqrt{1/3}$	
a	−1	a	$+\sqrt{1/3}$	

$A(E_2TE_2) = +1$

E_2	T	E_3	3-Γ	(even)
a	1	b	$-\sqrt{1/3}$	
a	0	a	$+\sqrt{1/6}$	
b	0	b	$-\sqrt{1/6}$	
b	−1	a	$+\sqrt{1/3}$	

By the general argument given in ([2], Sect. 3.5), 3-Γ symbols for $T^* \supset C_3^*$ satisfy the "selection rule"

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta \neq 0 \Rightarrow \gamma_1 + \gamma_2 + \gamma_3 \equiv 0 \ (\mathrm{mod}\ 3), \tag{2.2}$$

provided one makes the translations of the non-numerical components of the third-kind irreps given in Table 2.

For some of the triples, the Derome–Sharp $\mathbb{A}$ matrix ([1], Sect. 5.4) for the 3-Γ symbols generated here has been given (when one-dimensional, just as a number A). This has allowed a slight compactification of the table of 3-Γ symbols, since for example

$$\begin{pmatrix} \bar{\mathrm{E}}_1 & \bar{\mathrm{T}} & \mathrm{E}_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} = \begin{pmatrix} \bar{\mathrm{E}}_1 & \bar{\mathrm{T}} & \bar{\mathrm{E}}_2 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} = A(\mathrm{E}_1\mathrm{TE}_2)\begin{pmatrix} \mathrm{E}_1 & \mathrm{T} & \mathrm{E}_2 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} \tag{2.3}$$

so that for the evaluation of $(\mathrm{E}_1\mathrm{TE}_3/\gamma_1\gamma_2\gamma_3)$ one may use the tabulated $(\mathrm{E}_1\mathrm{TE}_2/\gamma_1\gamma_2\gamma_3)$'s together with the conjugating matrices for E_1 and T, i.e., the 3-Γ symbols for the triples $\mathrm{E}_1\mathrm{AE}_1$ and TAT. In some cases, of course, no space would be saved by giving the $\mathbb{A}$ matrix; examples are the triples $\mathrm{C}_1\mathrm{C}_1\mathrm{C}_1$ and $\mathrm{E}_2\mathrm{C}_1\mathrm{E}_2$.

The triple TTT will be discussed separately in Sect. 3.

An example of the calculation of a coupling coefficient according to the conventions in [1] will illustrate further the use of Table 4:

$$\begin{aligned} \langle \mathrm{E}_2 a \mathrm{E}_3 b | \bar{\mathrm{T}} 1 \rangle &= \pi(\mathrm{E}_2\mathrm{E}_3\mathrm{T})\pi(\mathrm{E}_2\mathrm{AE}_3)\ \mathrm{sign}\ (\mathrm{TA}\bar{\mathrm{T}})\sqrt{3}\begin{pmatrix} \mathrm{E}_3 & \mathrm{E}_2 & \bar{\mathrm{T}} \\ a & b & 1 \end{pmatrix} \\ &= -\sqrt{3}\begin{pmatrix} \mathrm{E}_3 & \mathrm{E}_2 & \bar{\mathrm{T}} \\ a & b & 1 \end{pmatrix} \\ &= -\sqrt{3}\begin{pmatrix} \mathrm{E}_2 & \mathrm{E}_3 & \bar{\mathrm{T}} \\ b & a & 1 \end{pmatrix} \\ &= -\sqrt{3}\begin{pmatrix} \mathrm{E}_2 & \mathrm{E}_3 & \mathrm{T} \\ b & a & -1 \end{pmatrix} = -1. \end{aligned} \tag{2.4}$$

Here we used first the definition of ([1], Eq. (5.3.15)), then the fact that the 3-Γ symbols $(\mathrm{E}_2\mathrm{E}_3\bar{\mathrm{T}}/\gamma_1\gamma_2\gamma_3)$ are *even*, then an analog of ([1], Eq. (5.3.10)), then Table 4 to find the actual value of $(\mathrm{TAT}/-1\ 0\ {+1})$ for the conjugation and finally Table 4 again for $(\mathrm{E}_2\mathrm{E}_3\mathrm{T}/b\ a\ -1)$.

3. The multiplicity triple TTT

It may be seen from the lower part of Table 1 that j-values have been assigned to the irreps of T^* in accordance with the procedure of ([2], Sect. 4). The interesting T^*-irrep triple in this connection is TTT which has multiplicity 2 and which we shall now comment upon. This discussion applies to the $T^* \supset C_3^*$ case as well as to the $T^* \supset C_2^*$ case otherwise treated below in Sect. 4. Using the primary basis functions for T three times gives T^*-adapted 3-j symbols of the form

$$\begin{pmatrix} 1 & 1 & 1 \\ \mathrm{T}\gamma_1 & \mathrm{T}\gamma_2 & \mathrm{T}\gamma_3 \end{pmatrix}. \tag{3.1}$$

These numbers form a fully antisymmetric fix-vector and hence a set of *odd* symbols $(\mathrm{TTT}/\gamma_1\gamma_2\gamma_3)_o$ for TTT (normalization is of course unnecessary here). Using the secondary j-value, 2, in, say, the second position gives T^*-adapted 3-j symbols of the form

$$\begin{pmatrix} 1 & 2 & 1 \\ \mathrm{T}\gamma_1 & \mathrm{T}\gamma_2 & \mathrm{T}\gamma_3 \end{pmatrix}. \tag{3.2}$$

These 3-j symbols turn out to form a non-zero set. From ([2], Eq. (4.6.2)) we see that the $(111/\mathrm{T}\gamma_1\mathrm{T}\gamma_2\mathrm{T}\gamma_3)$'s and the $(121/\mathrm{T}\gamma_1\mathrm{T}\gamma_2\mathrm{T}\gamma_3)$'s make up mutually orthogonal fix-vectors for TTT. Since TTT has multiplicity 2 and we just saw that there is an (at least) one-dimensional space of fully antisymmetric fix-vectors, it is – as already stated earlier – simple phase and we conclude from Table 1 that there is also a one-dimensional space of fully symmetric fix-vectors orthogonal to the antisymmetric ones (cf. [1], Sects. 3.2 and A.1). In all we conclude that with the normalization constant N defined by

$$N = \left[\sum_{\gamma_1,\gamma_2,\gamma_3} \left| \begin{pmatrix} 1 & 2 & 1 \\ \mathrm{T}\gamma_1 & \mathrm{T}\gamma_2 & \mathrm{T}\gamma_3 \end{pmatrix} \right|^2 \right]^{-1/2}, \tag{3.3}$$

we get a set of *even* 3-Γ symbols $(\mathrm{TTT}/\gamma_1\gamma_2\gamma_3)_e$ for TTT by the definition

$$\begin{pmatrix} \mathrm{T} & \mathrm{T} & \mathrm{T} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_e = N \begin{pmatrix} 1 & 2 & 1 \\ \mathrm{T}\gamma_1 & \mathrm{T}\gamma_2 & \mathrm{T}\gamma_3 \end{pmatrix}. \tag{3.4}$$

Furthermore, invoking the even character of the $(T \supset C_3^*)$-adapted 121 3-j symbols as well as the even character of the 3-Γ symbols (3.4) themselves, we see that each of the following definitions give the same TTT 3-Γ symbols:

$$\begin{aligned} \begin{pmatrix} \mathrm{T} & \mathrm{T} & \mathrm{T} \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_e &= N \begin{pmatrix} 2 & 1 & 1 \\ \mathrm{T}\gamma_1 & \mathrm{T}\gamma_2 & \mathrm{T}\gamma_3 \end{pmatrix} \\ &= N \begin{pmatrix} 1 & 2 & 1 \\ \mathrm{T}\gamma_1 & \mathrm{T}\gamma_2 & \mathrm{T}\gamma_3 \end{pmatrix} \\ &= N \begin{pmatrix} 1 & 1 & 2 \\ \mathrm{T}\gamma_1 & \mathrm{T}\gamma_2 & \mathrm{T}\gamma_3 \end{pmatrix}. \end{aligned} \tag{3.5}$$

(In principle, we could of course have done without these identities, but it is evidently convenient that one does not have to remember on which of the three positions to use the secondary j-value).

It could be argued that the even 3-Γ symbols for TTT should have been defined by normalizing T^*-adapted even 3-j symbols of the form

$$\begin{pmatrix} 2 & 2 & 2 \\ \mathrm{T}\gamma_1 & \mathrm{T}\gamma_2 & \mathrm{T}\gamma_3 \end{pmatrix}, \tag{3.6}$$

since then it would have been *evident* that the correct permutational properties were obtained, and there would have been no problems concerning the placement of the secondary j-value. However, we do want to stick to rule (10) of ([2], Sect. 4) regarding minimum values of $j_1+j_2+j_3$, and it turns out that the 222 definition gives 3-Γ symbols with opposite sign of the above ones (a situation which obviously cannot be remedied by real phase changes on the T^* basis functions). (Compare discussion of the triple VVV in the icosahedral group [14]).

For both our sets of 3-Γ symbols, the Derome–Sharp $\mathbb{A}$ matrix for the triple TTT ([1], Sect. 5.4) is

$$\mathbb{A}(\mathrm{TTT}) = \begin{array}{c|cc} & \text{odd} & \text{even} \\ \hline \text{odd} & 1 & 0 \\ \text{even} & 0 & -1 \end{array}\;. \tag{3.7}$$

Not having the unit matrix here is one of the prices we (willingly) pay in order to have all-real sets of 3-Γ symbols; cf. also discussion in Sect. 5 below.

4. Matrix irreps and 3-Γ symbols for $T^* \supset C_2^*$

Fig. 2 shows the placement of the coordinate system used here. The two-fold rotation generator is C_2^{Z*}; the three-fold axis lies in the XZ-plane. In this way we may choose as generators

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

and (4.1)

$$-C_3^* = \mathscr{D}^{[1/2]}(7\pi/4,\ \pi/2,\ 11\pi/4).$$

The latter generator choice necessitates a comment. The three-fold rotation C_3 about the axis singled out on Fig. 2 has Euler angles $(7\pi/4, \pi/2, 3\pi/4)$ (see, e.g. [12]). The corresponding elements of T^* are, by the conventions of ([2], Sect. 2)

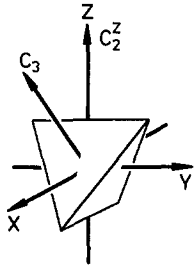

Fig. 2. Placement of the coordinate system as used for $T^* \supset C_2^*$ in Sect. 4. The counterclockwise rotation about the axis denoted here C_3 has Euler angles $(7\pi/4, \pi/2, 3\pi/4)$

or [12],

$$C_3^* = \mathscr{D}^{[1/2]}(7\pi/4,\ \pi/2, 3\pi/4)$$

and

$$-C_3^* = \mathscr{D}^{[1/2]}(7\pi/4,\ \pi/2, 11\pi/4).$$

The latter element is the one yielding the same character values of the T^*-irreps as $C_3^{Z^*}$ discussed in Sect. 2 and is therefore a natural choice among the two. Since the double groups as defined here always contain matrices $\boldsymbol{R}^*$ together with their negatives $-\boldsymbol{R}^*$, it is of course immaterial for the resulting copy of T^* which three-fold generator we choose.

Table 5 gives our standard C_2^*-adapted matrix irreps for T^* and Table 6 our choice of standard basis functions generating these irreps. Note that the irreps again have the "symmetric generator matrices"-property ([2], Sect. 3.2) ensuring the existence of real triple coefficients and that the basis functions are, indeed, real linear combinations of the $|jm\rangle$ so that they do generate real 3-Γ symbols. The general remarks made in Sect. 2 regarding choice of coordinate system and fixation of basis functions apply here again.

This time the "selection rule" on the 3-Γ symbols is

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta \neq 0 \Rightarrow \gamma_1 + \gamma_2 + \gamma_3 \equiv 0 \ (\mathrm{mod}\ 2), \tag{4.2}$$

again provided the components of the third-kind irreps are "translated" according to Table 4.

Table 5. Standard matrix irreps for $T^* \supset C_2^*$

Γ	components	$\Gamma(C_2^{Z^*})$	$\Gamma(-C_3^*)$
A	0	1	1
C_1	c	1	$e^{-i2\pi/3}$
C_2	c	1	$e^{i2\pi/3}$
T	$\begin{cases} 1 \\ 0 \\ -1 \end{cases}$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$\begin{bmatrix} -\frac{1}{2}i & -\frac{1}{2}-\frac{1}{2}i & -\frac{1}{2} \\ -\frac{1}{2}-\frac{1}{2}i & 0 & \frac{1}{2}-\frac{1}{2}i \\ -\frac{1}{2} & \frac{1}{2}-\frac{1}{2}i & \frac{1}{2}i \end{bmatrix}$
E_1	$\begin{cases} \frac{1}{2} \\ -\frac{1}{2} \end{cases}$	$\begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}$	$\begin{bmatrix} \frac{1}{2}-\frac{1}{2}i & -i\sqrt{1/2} \\ -i\sqrt{1/2} & \frac{1}{2}+\frac{1}{2}i \end{bmatrix}$
E_2	$\begin{cases} a \\ b \end{cases}$	$\begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}$	$\sqrt{1/2}\begin{bmatrix} e^{-i11\pi/12} & e^{i5\pi/6} \\ e^{i5\pi/6} & e^{-i5\pi/12} \end{bmatrix}$
E_3	$\begin{cases} a \\ b \end{cases}$	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$	$\sqrt{1/2}\begin{bmatrix} e^{i11\pi/12} & e^{-i5\pi/6} \\ e^{-i5\pi/6} & e^{i5\pi/12} \end{bmatrix}$

A numerical component γ means "eigenvalue $e^{-i\gamma\pi}$ under $C_2^{Z^*}$". The third-kind irrep components may be translated to numerical ones by the rules $C_1c = C_2c = 0$; $E_2a = E_3b = \frac{1}{2}$; $E_2b = E_3a = -\frac{1}{2}$. The two generators are defined in (4.1) in the main text.

Table 6. Basis functions for $T^* \supset C_2^*$

$\lvert 0\,\mathrm{A}\,0\rangle = \lvert 0\,0\rangle$	
$\lvert \tfrac{1}{2}\,\mathrm{E}_1\,\tfrac{1}{2}\rangle = \lvert \tfrac{1}{2}\,\tfrac{1}{2}\rangle$	
$\lvert \tfrac{1}{2}\,\mathrm{E}_1\,-\tfrac{1}{2}\rangle = \lvert \tfrac{1}{2}\,-\tfrac{1}{2}\rangle$	
$\lvert 1\,\mathrm{T}\,1\rangle = \lvert 1\,1\rangle$	$\lvert 2\,\mathrm{T}\,1\rangle = -\lvert 2\,-1\rangle$
$\lvert 1\,\mathrm{T}\,0\rangle = \lvert 1\,0\rangle$	$\lvert 2\,\mathrm{T}\,0\rangle = \sqrt{\tfrac{1}{2}}\lvert 2\,2\rangle + \sqrt{\tfrac{1}{2}}\lvert 2\,-2\rangle$
$\lvert 1\,\mathrm{T}\,-1\rangle = \lvert 1\,-1\rangle$	$\lvert 2\,\mathrm{T}\,-1\rangle = -\lvert 2\,1\rangle$
$\lvert \tfrac{3}{2}\,\mathrm{E}_2\,a\rangle = \sqrt{\tfrac{1}{2}}\lvert \tfrac{3}{2}\,\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{2}}\lvert \tfrac{3}{2}\,-\tfrac{3}{2}\rangle$	
$\lvert \tfrac{3}{2}\,\mathrm{E}_2\,b\rangle = \sqrt{\tfrac{1}{2}}\lvert \tfrac{3}{2}\,\tfrac{3}{2}\rangle - \sqrt{\tfrac{1}{2}}\lvert \tfrac{3}{2}\,-\tfrac{1}{2}\rangle$	
$\lvert \tfrac{3}{2}\,\mathrm{E}_3\,a\rangle = \sqrt{\tfrac{1}{2}}\lvert \tfrac{3}{2}\,\tfrac{3}{2}\rangle + \sqrt{\tfrac{1}{2}}\lvert \tfrac{3}{2}\,-\tfrac{1}{2}\rangle$	
$\lvert \tfrac{3}{2}\,\mathrm{E}_3\,b\rangle = \sqrt{\tfrac{1}{2}}\lvert \tfrac{3}{2}\,\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{2}}\lvert \tfrac{3}{2}\,-\tfrac{3}{2}\rangle$	
$\lvert 2\,\mathrm{C}_1\,c\rangle = -\tfrac{1}{2}\lvert 2\,2\rangle + \sqrt{\tfrac{1}{2}}\lvert 2\,0\rangle + \tfrac{1}{2}\lvert 2\,-2\rangle$	
$\lvert 2\,\mathrm{C}_2\,c\rangle = \tfrac{1}{2}\lvert 2\,2\rangle + \sqrt{\tfrac{1}{2}}\lvert 2\,0\rangle - \tfrac{1}{2}\lvert 2\,-2\rangle$	

Basis functions are given in the same form as in table 3. The functions generate the matrix irreps given in Table 5. Note that the A, E_1, and 1T functions are identical to those of Table 3 (although the component designations now have a different meaning).

Compactification of the table of 3-Γ symbols, Table 7, has again been possible by giving Derome–Sharp $\mathbb{A}$ matrices ([1], Sect. 5.4).

As a final comment we point to the fact that the dihedral group D_2^* [3] is an intermediate group between T^* and C_2^*, that is, we have $T^* \supset D_2^* \supset C_2^*$. It is therefore a natural question whether we could put the restriction on out matrix irreps that they be also D_2^*-adapted. This turns out to involve some complications, however:

One problem is that strict adaptation to D_2^* would violate our fundamental requirement that mutually conjugate third-kind irreps should occur in matrix forms which are precisely complex conjugates of one another. To see this, consider the subduction relations

$$\begin{aligned} &\mathrm{E}_2(T^*) \to \mathrm{E}_{1/2}(D_2^*) \\ &\mathrm{E}_3(T^*) \to \mathrm{E}_{1/2}(D_2^*). \end{aligned} \tag{4.3}$$

If $\mathrm{E}_2(T^*)$ and $\mathrm{E}_3(T^*)$ have matrix forms $\mathbb{E}_2$ and $\mathbb{E}_3$ with $\bar{\mathbb{E}}_2 = \mathbb{E}_3$, then we have, in particular, $\overline{(\mathbb{E}_2 \downarrow D_2^*)} = (\mathbb{E}_3 \downarrow D_2^*)$; but this means that $\mathrm{E}_{1/2}(D_2^*)$ occurs in two *different* matrix forms (since $\mathrm{E}_{1/2}(D_2^*)$ is of the second kind and thus cannot have a matrix form which is equal to its complex conjugate). And the difference does not just amount to a permutation of the components of $\mathbb{E}_3 \downarrow D_2^*$ (which might have been acceptable), because $\mathrm{E}_{1/2}(D_2^*)$ has only *anti*symmetric conjugation matrices.

Another thing is that it has been proved [15–17] that real 3-Γ symbols may *not* be chosen corresponding to $(T^* \supset D_2^* \supset C_2^*)$-adapted irreps. Nevertheless, we

Table 7. 3-Γ symbols for $T^* \supset C_2^*$

C_1	C_1	C_1	3-Γ	(even)
c	c	c	-1	

C_2	C_2	C_2	3-Γ	(even)
c	c	c	-1	

C_1	A	C_2	3-Γ	(even)
c	0	c	$+1$	

T	C_1	T	3-Γ	(even)
1	c	1	$1/2$	
1	c	-1	$\sqrt{1/12}$	
0	c	0	$\sqrt{1/3}$	
-1	c	-1	$-1/2$	

$A(\mathrm{TC_1T}) = +1$

E_2	C_1	E_2	3-Γ	(odd)
a	c	b	$\sqrt{1/2}$	

E_3	C_2	E_3	3-Γ	(odd)
a	c	b	$\sqrt{1/2}$	

E_1	T	E_2	3-Γ	(odd)
$1/2$	1	a	$-1/2$	
$1/2$	0	b	$-\sqrt{1/6}$	
$1/2$	-1	a	$-\sqrt{1/12}$	
$-1/2$	1	b	$-\sqrt{1/12}$	
$-1/2$	0	a	$-\sqrt{1/6}$	
$-1/2$	-1	b	$+1/2$	

$A(\mathrm{E_1TE_2}) = -1$

T	T	T	3-Γ	(even)
1	1	0	$\sqrt{1/6}$	
-1	-1	0	$\sqrt{1/6}$	

$\mathbb{A}$(TTT)	odd	even
odd	1	0
even	0	-1

E_2	A	E_3	3-Γ	(odd)
a	0	a	$\sqrt{1/2}$	
b	0	b	$\sqrt{1/2}$	

E_1	C_2	E_2	3-Γ	(odd)
$1/2$	c	b	$\sqrt{1/2}$	
$-1/2$	c	a	$-\sqrt{1/2}$	

$A(\mathrm{E_1C_2E_2}) = -1$

E_2	T	E_2	3-Γ	(even)
a	1	a	$-1/2$	
a	-1	a	$\sqrt{1/12}$	
a	0	b	$\sqrt{1/6}$	
b	1	b	$\sqrt{1/12}$	
b	-1	b	$+1/2$	

$A(\mathrm{E_2TE_2}) = +1$

E_2	T	E_3	3-Γ	(even)
b	1	a	$-\sqrt{1/3}$	
a	0	a	$\sqrt{1/6}$	
b	0	b	$-\sqrt{1/6}$	
a	-1	b	$\sqrt{1/3}$	

Those 3-Γ symbols which are generated by one or more of A, E_1, and 1T basis functions are identical to the corresponding ones in Table 4 (cf. legend to Table 6) and have been left out here (this concerns the triples AAA, $(\mathrm{TTT})_o$, TAT, $\mathrm{E_1AE_1}$, and $\mathrm{E_1TE_1}$).

have prepared a set of basis functions according to the rules set out in ([2], Sect. 4) which are ($T^* \supset D_2^* \supset C_2^*$)-adapted *except* for the above reservation, i.e. which satisfy $\bar{\mathbb{E}}_2(T^*) = \mathbb{E}_3(T^*)$ and thus feature two different matrix forms of $E_{1/2}(D_2^*)$. These functions generate 3-Γ symbols – many of which are certainly neither purely real or purely imaginary – obeying our general formalism [1]. This material is available from the authors upon request.

5. Concluding remarks

We have seen that real 3-Γ symbols exist for suitable choices of matrix irreps of T^* with each of the subgroup-adaptions $T^* \supset C_3^*$ and $T^* \supset C_2^*$. We have thus illustrated in particular the existence of real 3-Γ symbols (and coupling coefficients) for T, the tetrahedral group, a fact which follows from a general theorem proved in ([18], Sect. VI), as noted there.

[It has recently been proved [17] that the existence of real 3-Γ symbols (and thus real coupling coefficients, cf. arguments given in Appendix A of [18]) for a set of matrix irreps of a finite group implies that there is a (unique) automorphism of the group carrying all the matrix irreps into their complex conjugates. For the tetrahedral group or double group, such an automorphism is necessarily *outer* because the group has irreps of the third Frobenius–Schur kind (cf. discussions in [8] and [18]). The automorphism is, in both the present T^* cases, describable as the mapping

$$R \to C_2^{Y^*} R (C_2^{Y^*})^{-1}$$

of T^* onto itself. The R_3^*-element $C_2^{Y^*} = \mathscr{D}^{[1/2]}(0, \pi, 0)$ is not an element of T^*.

In [13], we imbed T^* in the octahedral double group O^* which there contains $C_2^{Y^*}$ and thereby have the above mapping as an *inner* automorphism of O^*.]
Golding and Newmarch [19] have given V coefficients (which are also 3-Γ symbols) for $T^* \supset C_3^*$. Their matrix irreps are less simple than those of Table 2 and their E″ and E‴ are not mutually complex conjugate. Their V coefficients are not all real. They achieve a slight reduction in tabulation of 3-Γ symbols in comparison with the present treatment, but on the other hand the user has to learn additional conventions associated with a "time-reversal operator". A secondary basis is given for the irrep T, but there is no discussion of the use of it. There are some errors in their tables.

Lulek [20] gives T^*-adapted 3-j symbols ($3j\Gamma\gamma$ symbols). These are not all real. No information is given on standard form of matrix irreps. (Using the basis functions given in [20], however, we have obtained the matrix irreps. They are adapted to $T^* \supset C_2^*$; E_2 and E_3 are not mutually complex conjugate). Butler [21, 16] has given material equivalent to non-real sets of 3-Γ symbols for T^*. The construction process used in those works is not based on matrix irreps or basis functions which are regarded as rather inferior aspects. This has as a consequence that exact information on these matters is difficult to extract from [16].

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