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Phase-fixed double-group 3-Γ symbols. III. Real 3-Γ symbols and coupling coefficients for the dihedral double groups

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For the infinite dihedral double group D_∞^* and the finite dihedral double groups D_2^* through D_6^*; D_8^*; D_{10}^*; and D_{12}^*, we present various choices of standard unitary irreducible matrix representations and discuss properties of corresponding 3-Γ symbols. The presentation follows a recent exposition of the general theory of 3-Γ symbols and coupling coefficients [1] and a companion description of general features of double groups and their irreps and 3-Γ symbols [2].

Key words: dihedral double groups—real phase-fixed three-gamma symbols and coupling coefficients—standard irreducible matrix representations—complex conjugation of matrix representations by inner and outer automorphisms

1. Introduction

Following a general paper on the theory of 3-Γ symbols [1] and another paper specifically dealing with properties of such quantities for double groups [2], we shall now set up basis functions for various choices of standard matrix irreps of the title groups and discuss the 3-Γ symbols generated by these basis functions ([2], Sect. 4), with the reservation that explicit calculations of complete sets of 3-Γ symbols only have been performed for the groups D_2^* through D_6^*; D_8^*; D_{10}^*; and D_{12}^*; and only selected examples from this material have been included in this paper.

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Apart from their immediate relevance for applications, the dihedral double groups deserve the attention we give them here for the following reasons:

(i) They are simpler to handle in some respects than the tetrahedral, octahedral, and icosahedral groups to be treated in subsequent papers (they are multiplicity-free and have no irreps of dimension greater than two), but nevertheless they exhibit several of the complicating features we have discussed in the general papers (irreps of all three Frobenius–Schur kinds ([1], Sect. 5.2; [3]) occur; sometimes secondary irrep bases ([2], Sect. 4) are needed). For the purpose of illustrating the theory they are thus a suitable starting point.

(ii) Some of the dihedral groups turn up as subgroups of the tetrahedral, octahedral and icosahedral groups and are therefore members of some of the group–subgroup hierarchies to which we may adapt the matrix irreps of those larger groups.

We start by discussing the infinite group D_∞^* which is a "parent" group for all the D_n^* (i.e. for $n=2,3,4,5,\ldots$, D_n^* is a subgroup of D_∞^*); cf. [4], or, for the point groups D_n and D_∞, [5]. We shall see that when we have discussed various choices of matrix irreps of D_∞^* and basis functions for them, we shall have done much of the work needed to construct 3-Γ symbols for the finite groups D_n^*.

The present paper is, of course, not the first one dealing with 3-Γ symbols for dihedral groups. Pertinent comments on the literature will be made partly as we proceed, partly in Sect. 7.

2. The group D_∞^*

The group D_∞^* will here be defined as the infinite subgroup of R_3^* generated by the elements

$$C_{2\pi/\varphi}^{Z*} = \mathcal{D}^{[1/2]}(\varphi, 0, 0) = \begin{pmatrix} e^{-i\varphi/2} & 0 \\ 0 & e^{i\varphi/2} \end{pmatrix}, \qquad 0 \le \varphi < 2\pi \tag{2.1}$$

together with the element

$$C_2^{X*} = \mathcal{D}^{[1/2]}(\pi, \pi, 0) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}. \tag{2.2}$$

The elements $C_{2\pi/\varphi}^{Z*}$ are double-group elements corresponding to rotations about the Z-axis by an angle of φ, and C_2^{X*} corresponds to the rotation by π about the X-axis. See the general discussion of double groups in ([2], Sect. 2.2) or in [6].

In Table 1 we give the rep-theoretical facts on D_∞^* which are needed as a background when applying the procedure described in [2].

There are two or three natural ways to choose standard matrix irreps for D_∞^* and basis functions generating them. These are given in Table 2 and we now comment on each of them. Those parts of the table which pertain to the groups D_n^* will be dealt with in Sect. 3.

Table 1. The group D_∞^* (Rep-theoretical facts and conventions)

Irreps (Γ)	A_1	A_2	$E_\lambda (\lambda=1,2,3,\ldots)$	$E_\lambda (\lambda=\frac{1}{2},\frac{3}{2},\frac{5}{2},\ldots)$
Dimension	1	1	2	2
Frobenius–Schur classification[a]	1[st] kind	1[st] kind	1[st] kind	2[nd] kind
Vector/spin classification[b]	vector	vector	vector	spin
$\Gamma\otimes_s\Gamma$[c]	A_1	A_1	$A_1\oplus E_{2\lambda}$	$A_2\oplus E_{2\lambda}$
$\Gamma\otimes_a\Gamma$[d]	—	—	A_2	A_1
Primary j-value[e]	0	1	λ[f]	λ
Supplementary j-values[e]			none	

[a] See ([1], Sect. 5.2).
[b] See ([2], Sect. 2.1).
[c] Means "symmetric part of $\Gamma\otimes\Gamma$", cf. ([1], Sect. A.1).
[d] Means "antisymmetric part of $\Gamma\otimes\Gamma$", cf. ([1], Sect. A.1).
[e] Cf. [2], Sect. 4. All j-values are, in accordance with rule (1) given there, lowest possible, a fact which follows from the branching rules

$$D_j(R_3^*)\rightarrow\begin{cases} A_1 \text{ for } j=0\\ A_1+E_1+E_2+\cdots+E_j \text{ for } j=2,4,6,\ldots\\ A_2+E_1+E_2+\cdots+E_j \text{ for } j=1,3,5,\ldots\\ E_{1/2}+E_{3/2}+\cdots+E_j \text{ for } j=1/2,3/2,5/2,\ldots.\end{cases}$$

[f] Note that the irreps E_λ with λ odd were assigned the j-value $\lambda+1$ in [7] (see also remarks in main text).

(i) *Adaption to the hierarchy* $D_\infty^*\supset C_\infty^*$. This is the choice obtained when we just use the R_3^*-basis functions $|jm\rangle=|\lambda\lambda\rangle$ and $|\lambda-\lambda\rangle$, in this order, to generate the irrep $E_\lambda(D_\infty^*)$ for all $\lambda=1/2,1,3/2,2,\ldots$. The irrep matrices for the elements $C_{2\pi/\varphi}^{Z^*}$ are all diagonal; thus the matrix irreps are adapted to C_∞^*, the infinite commutative subgroup of D_∞^* consisting of these elements. The 3-Γ symbols generated by these basis functions are all real, because the basis functions are, in particular, real linear combinations of the $|jm\rangle$ ([2], Sect. 4). [Indeed, all 3-Γ symbols here are just suitably normalized 3-j symbols.] Actually, one may easily check that ([2], Eq. (4.4.1)) with $R_0=C_2^{Y^*}=\mathscr{D}^{[1/2]}(0,\pi,0)$ is satisfied by this choice, so that the particularly nice formalism of ([1], Sect. 5.5) applies. It is easy to make a listing of the types of 3-Γ symbols occurring for this choice of standards, and we have done this in Table 3.

The 3-Γ symbols obey the "selection rule"

$$\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}\neq 0\Rightarrow\gamma_1+\gamma_2+\gamma_3=0 \tag{2.3}$$

due to the C_∞-adaptation ([2], Section 3.5). Furthermore, the relation

$$\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ -\gamma_1 & -\gamma_2 & -\gamma_3\end{pmatrix}=(-1)^{j(\Gamma_1)+j(\Gamma_2)+j(\Gamma_3)}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix} \tag{2.4}$$

Table 2

(i) The present standard matrix irreps and basis functions for the group hierarchies $D_\infty^* \supset C_\infty^*$ and $D_n^* \supset C_n^*$

Irrep[h]	Component[l]	Basis function	[f]$C_{2\pi/\varphi}^{Z*}$	C_2^{X*}	[g]C_2^{Y*}
A_1	0	$\|00\rangle$	1	1	1
A_2	0	$\|10\rangle$	1	-1	-1
[a]B_1	$n/2$	$\sqrt{1/2}[\|n/2 \quad n/2\rangle + (-1)^{n/2}\|n/2 \quad -n/2\rangle]$	-1	1	$(-1)^{n/2}$
[a]B_2	$-n/2$	$\sqrt{1/2}[\|n/2 \quad n/2\rangle + (-1)^{n/2+1}\|n/2 \quad -n/2\rangle]$	-1	-1	$(-1)^{n/2+1}$
[b]R_1	[c]r	$\sqrt{1/2}[\|n/2 \quad n/2\rangle + (-1)^{n/2+1/2}\|n/2 \quad -n/2\rangle]$	-1	$-i$	—
[b]R_2	[c]r	$\sqrt{1/2}[\|n/2 \quad n/2\rangle + (-1)^{n/2-1/2}\|n/2 \quad -n/2\rangle]$	-1	i	—
[d]E_λ	$\begin{cases} \lambda \\ -\lambda \end{cases}$	$\|\lambda \quad \lambda\rangle$ $\|\lambda \quad -\lambda\rangle$	$\begin{pmatrix} e^{-i\lambda\varphi} & 0 \\ 0 & e^{i\lambda\varphi} \end{pmatrix}$	$\begin{pmatrix} 0 & i^{2\lambda} \\ i^{2\lambda} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & (-1)^{2\lambda} \\ 1 & 0 \end{pmatrix}$
[d,e]E_λ	$\begin{cases} \lambda \\ -\lambda \end{cases}$	$(-1)^n\|n-\lambda \quad -(n-\lambda)\rangle$ $\|n-\lambda \quad n-\lambda\rangle$	$\begin{pmatrix} e^{-i\lambda\varphi} & 0 \\ 0 & e^{i\lambda\varphi} \end{pmatrix}$	$\begin{pmatrix} 0 & i^{2\lambda} \\ i^{2\lambda} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & (-1)^{2\lambda} \\ 1 & 0 \end{pmatrix}$

(ii) The present standard matrix irreps and basis functions[k] for the group hierarchies $D_\infty^* \supset C_2^*$ and $D_n^* \supset C_2^*$

Irrep[k]	Component[l]	Basis function	[f]$C_{2\pi/\varphi}^{Z*}$	C_2^{X*}	[g]C_2^{Y*}
A_2	1	same as in (i)			
[a]B_1	0				
[a]B_2	1				
[d,i]E_λ	$\begin{cases} 0 \\ 1 \end{cases}$	$\sqrt{1/2}[(-1)^\lambda\|\lambda\lambda\rangle + \|\lambda -\lambda\rangle]$ $\sqrt{1/2}[(-1)^{\lambda+1}\|\lambda\lambda\rangle + \|\lambda -\lambda\rangle]$	$\begin{pmatrix} \cos\lambda\varphi & i\sin\lambda\varphi \\ i\sin\lambda\varphi & \cos\lambda\varphi \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} (-1)^\lambda & 0 \\ 0 & (-1)^{\lambda+1} \end{pmatrix}$
[d,i,e]E_λ	$\begin{cases} 0 \\ 1 \end{cases}$	$\sqrt{1/2}[\|n-\lambda \quad n-\lambda\rangle + (-1)^{n-\lambda}\|n-\lambda \quad -(n-\lambda)\rangle]$ $\sqrt{1/2}[\|n-\lambda \quad n-\lambda\rangle + (-1)^{n-\lambda+1}\|n-\lambda \quad -(n-\lambda)\rangle]$	$\begin{pmatrix} \cos\lambda\varphi & i\sin\lambda\varphi \\ i\sin\lambda\varphi & \cos\lambda\varphi \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} (-1)^\lambda & 0 \\ 0 & (-1)^{\lambda+1} \end{pmatrix}$
[d,j]E_λ	$\begin{cases} 1/2 \\ -1/2 \end{cases}$	$\sqrt{1/2}[(-1)^{\lambda+1/2}\|\lambda\lambda\rangle + \|\lambda -\lambda\rangle]$ $\sqrt{1/2}[(-1)^{\lambda-1/2}\|\lambda\lambda\rangle + \|\lambda -\lambda\rangle]$	$\begin{pmatrix} \cos\lambda\varphi & i\sin\lambda\varphi \\ i\sin\lambda\varphi & \cos\lambda\varphi \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} 0 & (-1)^{\lambda-1/2} \\ (-1)^{\lambda+1/2} & 0 \end{pmatrix}$

(iii) Alternative matrix irreps for the group hierarchies $D^*_\infty \supset C^*_2$ and $D^*_n \supset C^*_2$

Irrep	Component[l]	[f] $C^{Z*}_{2\pi/\varphi}$	C^{X*}_2	[g] C^{Y*}_2
[d,i] E_λ	$\begin{cases} 0 \\ 1 \end{cases}$	$\begin{pmatrix} \cos\lambda\varphi & -\sin\lambda\varphi \\ \sin\lambda\varphi & \cos\lambda\varphi \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} (-1)^\lambda & 0 \\ 0 & (-1)^{\lambda+1} \end{pmatrix}$
[d,j] E_λ	$\begin{cases} 1/2 \\ -1/2 \end{cases}$	$\begin{pmatrix} \cos\lambda\varphi & -\sin\lambda\varphi \\ \sin\lambda\varphi & \cos\lambda\varphi \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} 0 & i^{2\lambda+2} \\ i^{2\lambda} & 0 \end{pmatrix}$

[a] These irreps only present in D^*_n for n even.
[b] These irreps only present in D^*_n for n odd.
[c] Regarding these component designations, see main text.
[d] In D^*_∞, $\lambda = 1/2, 1, 3/2, 2, \ldots$; in D^*_n, $\lambda = 1/2, 1, \ldots, n/2 - 1/2$.
[e] Secondary basis; only in D^*_n and for 2λ even.
[f] For D^*_n, read $\varphi = 2\pi/n$.
[g] With the present conventions, this is not an element of D^*_n for n odd.
[h] In D^*_2, A_1 is called A, A_2 is called B_1, and B_1 is called B_3.
[i] For 2λ even.
[j] For 2λ odd.
[k] In this table, A_1, R_1, and R_2 are left out, since the entries would be completely identical to those given in (i).
[l] Except for R_1 and R_2, the component γ is always a number chosen so that the eigenvalue of the function is $e^{-i\gamma\varphi}$ under $C^{Z*}_{2\pi/\varphi}$ in case (i) and $e^{-i\gamma 2\pi/2}$ under C^{X*}_2 in cases (ii) and (iii).

Table 3

Types of 3-Γ symbols for $D^*_\infty \supset C^*_\infty$ [a]

$$\begin{pmatrix} A_1 & A_1 & A_1 \\ 0 & 0 & 0 \end{pmatrix}^{e,d} = 1; \quad \begin{pmatrix} A_2 & A_1 & A_2 \\ 0 & 0 & 0 \end{pmatrix}^{e};$$

$$\begin{pmatrix} E_\lambda & A_1 & E_\lambda \\ \lambda & 0 & -\lambda \end{pmatrix}^{e/o}; \quad \begin{pmatrix} E_\lambda & A_2 & E_\lambda \\ \lambda & 0 & -\lambda \end{pmatrix}^{o/e};$$

$$\begin{pmatrix} E_\lambda & E_{2\lambda} & E_\lambda \\ \lambda & -2\lambda & \lambda \end{pmatrix}^{e}, \quad \begin{pmatrix} E_\lambda & E_{2\lambda} & E_\lambda \\ -\lambda & 2\lambda & -\lambda \end{pmatrix}^{e,b};$$

$$\begin{pmatrix} E_\lambda & E_\mu & E_{\lambda+\mu} \\ \lambda & \mu & -(\lambda+\mu) \end{pmatrix}^{c}, \quad \begin{pmatrix} E_\lambda & E_\mu & E_{\lambda+\mu} \\ -\lambda & -\mu & \lambda+\mu \end{pmatrix}^{c,b};$$

$$\begin{pmatrix} E_\lambda & E_\mu & E_{\lambda-\mu} \\ \lambda & -\mu & \mu-\lambda \end{pmatrix}^{f}, \quad \begin{pmatrix} E_\lambda & E_\mu & E_{\lambda-\mu} \\ -\lambda & \mu & \lambda-\mu \end{pmatrix}^{f,b}, \lambda > \mu$$

[a] The table applies to choice (i) of Table 2. Note the selection rule (2.3). Of course this table tells, *independently of choice of standards for the irreps,* which irrep triples can have non-zero triple coefficients.

[b] Relations exist between the 3-Γ symbols within each of these three pairs: see Eq. (2.4).

[c] Even if $(-1)^{2\lambda+2\mu} = 1$, odd otherwise.

[d] See ([2], Sect. 4.4).

[e] Even.

[e/o] Even for λ an integer, odd otherwise.

[o/e] Odd for λ an integer, even otherwise.

[f] Even if $(-1)^{2\lambda} = 1$, odd otherwise.

is valid, owing to (2.3) and the form

$$\mathbb{\Gamma}(C_2^{Y*})_{\gamma\gamma'} = (-1)^{j(\Gamma)-\gamma'}\delta(\gamma, \gamma') \tag{2.5}$$

of the irrep matrices for the element C_2^{Y*} (cf. again [2], Sect. 3.5). In (2.4) and (2.5), the symbol $j(\Gamma_i)$ denotes the primary j-value for Γ_i as defined in Table 1.

(ii) *Adaption to the hierarchy* $D^*_\infty \supset C^*_2$. By C^*_2 we shall here mean the subgroup of D^*_∞ generated by the element C_2^{X*}. Thus, for this choice of standard matrix irreps $\mathbb{\Gamma}$ the matrix $\mathbb{\Gamma}(C_2^{X*})$ is always diagonal. *Note that the irrep component designations are now chosen on the basis of these generator matrices.*

The present matrix irreps have the "symmetric generator irrep matrices" – property and thus allow real 3-Γ symbols ([2], Sect. 3.2). Indeed, the standard basis functions given in Table 2 for this hierarchy are all real linear combinations of the $|jm\rangle$ functions and thus generate real 3-Γ symbols ([2], Sect. 4.4). Eq. (4.4.1) of [2] still holds with $R_0 = C_2^{Y*}$ and therefore also the formalism of ([1], Sect. 5.5).

Observe that the 3-Γ symbols for this choice obey the "selection rule"

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} \neq 0 \Rightarrow \gamma_1 + \gamma_2 + \gamma_3 = 0 \text{ or } 2 \tag{2.6}$$

because of the C^*_2-adaption.

(iii) *Adaption to the hierarchy* $D_\infty^* \supset C_2^*$, *variant.* For the vector irreps of D_∞^*, these matrix irreps are identical, except for a renaming of group elements, to the ones used for D_∞ in [7]. It may easily be checked that they have the property that if a triple $\Gamma_1\Gamma_2\Gamma_3$ has non-zero fix-vectors, then the matrices

$$\Gamma_1 \otimes \Gamma_2 \otimes \Gamma(C_{2\pi/\varphi}^{Z*}) \quad \text{and} \quad \Gamma_1 \otimes \Gamma_2 \otimes \Gamma_3(C_2^{Y*})$$

are all real (use the fact, [2], Sect. 2.1, that such triples always contain an even number of spin irreps). From this we may conclude that these matrix forms of the irreps allow real 3-Γ symbols to be chosen ([2], Sect. 3.2). Indeed, it may be seen that changing the basis functions of (ii) by the prescription

$$|\Gamma\gamma\rangle_{(\mathrm{iii})} = \alpha^{2\gamma}|\Gamma\gamma\rangle_{(\mathrm{ii})} \tag{2.7}$$

where $\alpha = \exp(i\pi/4)$, gives basis functions generating the (iii)-matrix irreps and simultaneously generating real 3-Γ symbols for all triples. In fact, the 3-Γ symbols generated, when following our procedure, from the basis functions defined by (2.7) satisfy the relation

$$\begin{aligned}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_{(\mathrm{iii})} &= \alpha^{(2\gamma_1+2\gamma_2+2\gamma_3)}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_{(\mathrm{ii})}\\ &= i^{(\gamma_1+\gamma_2+\gamma_3)}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma_3\\ \gamma_1 & \gamma_2 & \gamma_3\end{pmatrix}_{(\mathrm{ii})},\end{aligned} \tag{2.8}$$

where the phase factor in the latter expression is seen from (2.6) to be always 1 or −1. Eq. (2.6) is of course, then, also satisfied by the variant 3-Γ symbols. In view of (2.8) it is never necessary to tabulate or even calculate the variant 3-Γ symbols separately.

One may now, using any desired choice of basis functions for D_∞^* among the above ones, generate any desired portion of the infinitely many 3-Γ symbols for D_∞^*. We shall not tabulate such 3-Γ symbols separately, but some of them appear below as 3-Γ symbols for some of the subgroups D_n^* of D_∞^*.

[Kibler and Grenet [8] have given explicit formulas, in terms of 3-*j* symbols for SU(2), for all general types of *f* coefficients (a choice of coefficients closely related to coupling coefficients) corresponding to a particular choice of $(\mathrm{SU}(2) \supset D_\infty^*)$-adapted basis functions. Their standard irreducible matrix representations of D_∞^* are a mixture of our choices (i) and (ii) with some additional sign changes.]

3. The groups D_n^*, $n = 2, 3, 4, 5, \ldots$

For each integer $n \geq 2$ we shall define here D_n^* as the subgroup of D_∞^* (and thus of R_3^*) generated by C_2^{X*} and C_n^{Z*}.

Table 4 gives the rep-theoretical information on the groups D_n^* needed in the following. What we shall have to discuss here is the assignment of *j*-values and basis functions to the irreps of D_n^*, cf. ([2], Sect. 4.4).

Table 4. The groups D_n^* (rep-theoretical facts and conventions)

Irreps (Γ)	A_1	[m] A_2	[c,m] B_1	[c,m] B_2	[d] R_1	[d] R_2	E_λ ; $\lambda = 1, 2, \ldots$	[e] E_λ ; $\lambda = 1/2, 3/2, \ldots$
Dimension	1	1	1	1	1	1	2	2
Frobenius–Schur classification[a]	1st kind				3rd kind		1st kind	2nd kind
Vector/spin classification[b]	vector				spin		vector	spin
$\Gamma \otimes_s \Gamma$[f]	A_1	A_1	A_1	A_1	A_2	A_2	$A_1 \oplus E_{2\lambda}$ if $1 \le \lambda < n/4$ [j,m] $A_1 \oplus B_1 \oplus B_2$ if $\lambda = n/4$ $A_1 \oplus E_{n-2\lambda}$ if $n/4 < \lambda < n/2$	$A_2 \oplus E_{2\lambda}$ if $1/2 \le \lambda < n/4$ [k,m] $A_2 \oplus B_1 \oplus B_2$ if $\lambda = n/4$ $A_2 \oplus E_{n-2\lambda}$ if $n/4 < \lambda < n/2$
$\Gamma \otimes_a \Gamma$[g]	—	—	—	—	—	—	A_2	A_1
D_∞^*-irreps yielding Γ on restriction to D_n^*	A_1	A_2	E_μ $\mu \equiv n/2 \pmod n$				E_μ, $\mu \equiv \lambda \pmod n$ or $\mu \equiv n - \lambda \pmod n$	
D_∞^*-irreps yielding Γ on restriction to D_n^*	E_μ, $\mu \equiv n$ (mod n)							
Primary j-value[h,i]	0	1	$n/2$				λ	λ
Supplementary j-value	none						$n - \lambda$	none

[a] See ([1], Sect. 5.2). [b] See ([2], Sect. 2.1). [c] This irrep is only present in D_n^* for n even.
[d] This irrep is only present in D_n^* for n odd. Other notations for R_1, R_2 are ρ_1, ρ_2 ([18], App. 2) and A′, B′ [10][l].
[e] Other notations for E_λ with $\lambda = 1/2, 3/2, \ldots$: E′, E″ etc. ([18], App. 2); E'_λ [10]; and Γ_λ [8][l].
[f] Means "symmetric part of $\Gamma \otimes \Gamma$", cf. ([1], Sect. A.1). [g] Means "antisymmetric part of $\Gamma \otimes \Gamma$", cf. ([1], Sect. A.1). [h] Cf. ([2], Sect. 4).
[i] Note that the irreps E_λ with $\lambda = 1, 3, 5, \ldots$ were assigned the primary j-value $\lambda + 1$ in [7] (see also remarks in main text).
[j] Only becomes effective when $4 | n$. [k] Only becomes effective when $4 \nmid n$.
[l] Butler [15] uses an intricate system of boldface numerals as irrep labels; these numbers coincide sometimes, but not always, with our primary j-value.
[m] See [h] of legend to Table 2.

All primary j-values are simply as low as possible, in accordance with rule (1) in ([2], Sect. 4). The interesting thing to note is the assignment of *secondary* j-values to all irreps $E_\lambda(D_n^*)$ of the first kind. However, a general discussion of the necessity of two sets of basis functions for these irreps and the reason for choosing the particular j-values given in Table 4 will be deferred to Sect. 4. This is done for the sake of clarity, and a reader who wishes to do so may read Sect. 4 before proceeding in the present section.

Basis functions for D_n^* with the j-values thus selected are chosen according to three different schemes, corresponding to the three choices of standard matrix irreps and basis functions for D_∞^* in Sect. 2. Prescriptions for this are given in each part of Table 2; the following general features may be noted:

The standard form of the irreps $\mathbb{E}_\lambda(D_n^*)$, $1/2 \leq \lambda < n/2$, is in each case simply the matrix irrep obtained by restricting $\mathbb{E}_\lambda(D_\infty^*)$ to D_n^* and the basis functions may thus be taken over directly as those for $\mathbb{E}_\lambda(D_\infty^*)$.

The one-dimensional irreps B_1, B_2 and R_1, R_2 are given in Table 2; in D_2^*, A_1, A_2, B_1, and B_2 are called A, B_1, B_3, and B_2, respectively. Basis functions are always made out of the $E_{n/2}(D_\infty^*)$ set, with free phases fixed according to the principles given in ([2], Sect. 4.4). The easiest cases to consider here are (ii) and (iii), where $E_{n/2}(D_\infty^*)$ has a matrix form which directly blocks out as $B_1 \oplus B_2$, resp. $R_1 \oplus R_2$, upon restriction to D_n^*.

A problem only arises for the (first-kind) irreps $E_\lambda(D_n^*)$ with λ integer which, as mentioned, have to be assigned secondary bases. Given n and λ and a particular choice among (i)–(iii), the irrep $E_{n-\lambda}(D_\infty^*)$ will yield, on restriction to D_n^*, an irrep equivalent to $E_\lambda(D_n^*)$, but generally with a different matrix form than the one fixed as the standard above. Interchanging the D_∞^* basis functions for $E_{n-\lambda}$ *and/or* changing the sign of one of the functions gives, however, in each case the correct matrix form.

Summing up, case (i) involves matrix irreps of D_n^* adapted to C_n^* (the subgroup generated by C_n^{Z*}), while those of cases (ii) and (iii) are $(D_n^* \supset C_2^*)$-adapted. Note that *the irrep component designations are chosen accordingly.* The mutually complex conjugate third-kind irreps $R_1(D_n^*)$ and $R_2(D_n^*)$, n odd, have the non-numerical component designation "r"; the reason for using such a symbol was given in ([2], Sect. 3.4). For the purpose of checking with the selection rules (3.1) and (3.2) below, the component translations $R_1 r = n/2$, $R_2 r = -n/2$ in case (i) and $R_1 r = 1/2$, $R_2 r = -1/2$ in cases (ii) and (iii) may be used. The basis functions prescribed in Table 2 for the groups D_n^* generate real 3-Γ symbols.

It may furthermore be checked that for D_n^*, n even, Eq. (4.4.1) of [2] is satisfied so that the formalism of ([1], Sect. 5.5) applies.

The 3-Γ symbols of choice (i) satisfy, because of the adaption to C_n^*, the "selection rule"

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} \neq 0 \Rightarrow \gamma_1 + \gamma_2 + \gamma_3 \equiv 0 \pmod{n} \tag{3.1}$$

([2], Sect. 3.5). Those of choices (ii) and (iii) satisfy the rule

$$\begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} \neq 0 \Rightarrow \gamma_1 + \gamma_2 + \gamma_3 \equiv 0 \pmod 2). \tag{3.2}$$

Note. Consider the groups D_n^* with n odd. For all of the choices (i)–(iii), the matrix representing $C_2^{X^*}$ in the irreps E_λ is imaginary when λ is equal to half an odd integer. This is of course unavoidable when one insists that it be diagonal, since its eigenvalues are i and $-i$. However, in the C_n^*-adaptation situation, the irreps E_λ may for all λ be chosen in a matrix form with $C_2^{X^*}$ represented by the matrix

$$\begin{pmatrix} 0 & (-1)^{2\lambda} \\ 1 & 0 \end{pmatrix} \tag{3.3}$$

and $C_2^{Z^*}$ by the same diagonal matrix as in Table 2(i). On the other hand it is easily seen that in such a situation not all 3-Γ symbols can be real. (The idea is to demonstrate that certain standard matrix irrep triples $\Gamma_1\Gamma_2\Gamma_3$ will have a purely imaginary matrix for $\Gamma_1(C_2^{X^*})\otimes\Gamma_2(C_2^{X^*})\otimes\Gamma_3(C_2^{X^*})$ and to realize that an imaginary matrix cannot have a real fix-vector). If one is, nevertheless, interested in this variant form of the irreps, one need not tabulate separate basis functions or 3-Γ symbols. The relation

$$|\Gamma\gamma\rangle_{\text{variant}} = \alpha^{-2\gamma}|\Gamma\gamma\rangle_{(\text{i})}, \tag{3.4}$$

where α is $\exp(i\pi/4)$, provides basis functions generating them, and the generated 3-Γ symbols differ from the ones known in case (i) just by the phase factor $i^{-(\gamma_1+\gamma_2+\gamma_3)}$. This phase factor is always one of the numbers $1, -1, i$, and $-i$ so that the variant 3-Γ symbols are either real or purely imaginary. (The whole discussion in this note may be compared with the one surrounding Eqs. (2.7) and (2.8) above.)

4. Secondary bases for the irreps E_λ of D_n^*, $n = 3, 4, 5, \ldots$

Suppose $n \geq 3$ is given and E_λ is one of the first-kind two-dimensional (and thus vector-type ([2], Sect. 2.1)) irreps of D_n^*. Then λ is an integer with $0 < \lambda < n/2$, and therefore $(n-\lambda)/2$ is either an integer or half an odd integer and satisfies $n/4 < (n-\lambda)/2 < n/2$. There is thus a two-dimensional irrep $E_{(n-\lambda)/2}$ of D_n^*, and consideration of Table 4 shows that the tensor product $E_{(n-\lambda)/2}\otimes E_{(n-\lambda)/2}$ contains $E_{n-2(n-\lambda)/2} = E_\lambda$ and thus (see, for example, the reasoning in [1], Sect. A.1) that $E_{(n-\lambda)/2}E_{(n-\lambda)/2}E_\lambda$ has non-zero fix-vectors. However, using the primary bases for $E_{(n-\lambda)/2}$ and E_λ gives only zero triple coefficients for $E_{(n-\lambda)/2}E_{(n-\lambda)/2}E_\lambda$. This fact is easily appreciated if one recalls that these bases are also bases for the D_∞^*-irreps with the same designations and that (Table 3) in D_∞^*, triple coefficients for $E_{(n-\lambda)/2}E_{(n-\lambda)/2}E_\lambda$ are necessarily zero (because $\lambda \neq 2(n-\lambda)/2$ under our present assumptions). The procedure of ([2], Sect. 4.4) then tells us to assign a secondary basis to one of the irreps in the triple $E_{(n-\lambda)/2}E_{(n-\lambda)/2}E_\lambda$. Now, if $\lambda = (n-\lambda)/2$, i.e. if $\lambda = n/3$, then all three irreps are identical, and we conclude that E_λ must be assigned a secondary basis. If $(n-\lambda)/2 \neq \lambda$, rule (9) in ([2], Sect. 4.4) concerning triples containing two and only two identical irreps also says that E_λ is the one to be assigned a secondary basis. Thus, in any case E_λ has to be assigned a secondary basis, and since λ and $n \geq 3$ were chosen arbitrarily, we have seen that we shall *always have to assign* $E_\lambda(D_n^*)$ *a secondary as well as a primary basis.* The above reference to D_∞^* suggests the secondary j-value $j = n - \lambda$ for E_λ, and since this is also the next-to-lowest j-value assignable to $E_\lambda(D_n^*)$, it is in accordance with the prescriptions of [2] to choose a secondary $E_\lambda(D_n^*)$-basis with $j = n - \lambda$. So this is what we have done, as already described above. It turns out that with our assignments of basis functions we can generate all 3-Γ symbols for the groups D_2^*, D_3^*, D_4^*, D_5^*, D_6^*, D_8^*, D_{10}^*, and D_{12}^*, which we believe to be at present the only D_n^*-groups of direct interest in chemistry, and which are the only ones for which we have carried through the actual calculation of 3-Γ symbols. (The reason for the inclusion of D_8^*, D_{10}^* and D_{12}^* is that, by the definitions in ([2], Sect. 2.2), these groups are the double groups of D_{4d}, D_{5h}, and D_{6d}, respectively).

The question now arising of *when* to use primary and *when* to use secondary bases for the $E_\lambda(D_n^*)$ requires some commenting and we shall supply such a discussion by going through some selected examples. For those D_n^*-groups which we have investigated, secondary bases are only needed in connection with irrep triples of the form $E_{\lambda_1}E_{\lambda_2}E_{\lambda_3}$. We shall distinguish the following situations:

1° All three λ's different, $\lambda_1 \neq \lambda_2 \neq \lambda_3 \neq \lambda_1$: For some of these cases, no secondary bases are needed. An example of this is $E_1E_2E_3$ in D_8^*. Consider however, e.g. $E_3E_4E_5$ in D_{12}^*. Since none of the numbers 3, 4, and 5 is the sum or difference of the remaining two, consideration of D_∞^*-irrep triples (Table 3) shows that using the primary bases for all three irreps just gives zero triple coefficients. However, if any one of the three is assigned its secondary basis and the remaining two their primary bases, non-zero triple coefficients are generated. (Cf. the fact that

$$\begin{aligned} &E_9(D_\infty^*) \rightarrow E_3(D_{12}^*) \\ &E_8(D_\infty^*) \rightarrow E_4(D_{12}^*) \\ &E_7(D_\infty^*) \rightarrow E_5(D_{12}^*) \end{aligned} \tag{4.1}$$

and that each of the D_∞^*-triples $E_9E_4E_5$, $E_3E_8E_5$ and $E_3E_4E_7$ has non-zero fix-vectors.) Rule (10) in ([2], Sect. 4.4) then tells us, of the three possibilities, to use for E_5 its secondary basis (since $3+4+7 < 3+8+5 < 9+4+5$). Evidently the rule is always decisive when three different λ's are involved.

2° Two equal λ's and the third one different, say $\lambda_1 = \lambda_3 \neq \lambda_2$: Again, sometimes the primary bases are sufficient. An example is $E_1E_2E_1$ in D_5^*. When $\lambda_1 + \lambda_3 \neq \lambda_2$, however, a secondary basis is needed and by the discussion above it is E_{λ_2} which is to be assigned its secondary basis. For example, $E_{3/2}E_1E_{3/2}$ in D_4^* is associated with the j-triple 3/2 3 3/2 and $E_4E_2E_4$ in D_{10}^* is associated with the j-triple 484.

3° All three λ's equal, $\lambda_1 = \lambda_2 = \lambda_3 = \lambda$: This situation by Table 4 only occurs for $\lambda = n/3$ (in groups D_n^* where n is a multiple of 3). A triple of this type has, as we know, always multiplicity 1 and is thus simple phase ([1], Sect. 3.2); since E_λ occurs in $E_\lambda \otimes_s E_\lambda$ (Table 4), its fix-vectors are necessarily fully symmetric ([1], Sect. 3.2 and Sect. A.1) so that 3-Γ symbols for $E_\lambda E_\lambda E_\lambda$ are *even*. Since the D_∞^*-irrep triple $E_\lambda E_\lambda E_\lambda$ has only zero triple coefficients, we have to assign the secondary basis with $j = n - \lambda = 2\lambda$ to E_λ in one of the three positions. The only problem is whether the position of the secondary basis is of consequence for the resulting 3-Γ symbols for $E_\lambda E_\lambda E_\lambda$. This turns out *not* to be the case, that is, the transformed 3-*j* symbols involved satisfy the relations:

$$\begin{pmatrix} 2\lambda & \lambda & \lambda \\ E_\lambda\gamma_1 & E_\lambda\gamma_2 & E_\lambda\gamma_3 \end{pmatrix} = \begin{pmatrix} \lambda & 2\lambda & \lambda \\ E_\lambda\gamma_1 & E_\lambda\gamma_2 & E_\lambda\gamma_3 \end{pmatrix} = \begin{pmatrix} \lambda & \lambda & 2\lambda \\ E_\lambda\gamma_1 & E_\lambda\gamma_2 & E_\lambda\gamma_3 \end{pmatrix}. \tag{4.2}$$

Let us prove just the first equality: since $2\lambda + \lambda + \lambda = 4\lambda$ which is an even number, the 3-*j* symbols are even ([1], Sect. 6) so that

$$\begin{pmatrix} 2\lambda & \lambda & \lambda \\ E_\lambda\gamma_1 & E_\lambda\gamma_2 & E_\lambda\gamma_3 \end{pmatrix} = \begin{pmatrix} \lambda & 2\lambda & \lambda \\ E_\lambda\gamma_2 & E_\lambda\gamma_1 & E_\lambda\gamma_3 \end{pmatrix}; \tag{4.3}$$

and since any $E_\lambda(D_n^*)E_\lambda(D_n^*)E_\lambda(D_n^*)$ fix-vector as stated above is symmetric, we further have

$$\begin{pmatrix} \lambda & 2\lambda & \lambda \\ E_\lambda\gamma_2 & E_\lambda\gamma_1 & E_\lambda\gamma_3 \end{pmatrix} = \begin{pmatrix} \lambda & 2\lambda & \lambda \\ E_\lambda\gamma_1 & E_\lambda\gamma_2 & E_\lambda\gamma_3 \end{pmatrix}, \tag{4.4}$$

as desired. Compare with the discussion of the triple TTT in [9].

Notes. (1) The prescriptions given above for primary and secondary basis functions for irreps of D_n^* are of course applicable for all n; however, for a group D_n^* not among the ones we have checked, we – in principle – do not know whether non-zero triple coefficients may be generated for all triples by using these basis functions. All we can say is that no "D_∞^* – selection rule" tells anything about the possible vanishing of the generated triple coefficients. Possibly a general investigation of this question is not complicated, but we have not at the moment pursued the subject any further.

(2) It should be noted that the assignment of basis functions to the irreps E_λ with λ integer in the present paper differs in several respects from that made in [7] in connection with the groups D_n: In the first place, our present procedure tells us to always assign $j = \lambda$ as the primary j-value, whereas $j = \lambda + 1$ was used for λ odd in [7]. Secondly, we here use different j-values for primary and secondary bases, whereas in [7], as an example, E_1 of D_3 was assigned a primary as well as a secondary basis with $j = 2$. Thus, even in the cases where we here choose the same standard matrix irreps for a given D_n^* as we did in [7] (choice (iii), see Sect. 2), phase differences are to be expected between the present 3-Γ symbols and those of [7].

(3) The only previous attempt at a *general* treatment of 3-Γ symbols for dihedral double groups *using basis functions* is [10]. However, no *explicit* discussion is given of the necessity of secondary sets of basis functions and of the use of such sets. Also, it is easy to show that with the standard matrix irreps used by those

authors, some 3-Γ symbols for D_n^* with n odd *must* come out to be non-real. (Cf. note in Sect. 3 above.)

5. Examples: 3-Γ symbols for $D_3^* \supset C_3^*$ and for $D_3^* \supset C_2^*$

The tables of 3-Γ symbols for the D_n^* groups which we have generated on the basis of the above discussion are too numerous and voluminous to be all included in the present paper. However, a couple of examples will convey most of the general features. We have chosen to display in Table 5 the 3-Γ symbols for $D_3^* \supset C_3^*$ (choice (i) above) and $D_3^* \supset C_2^*$ (choice (ii)); as far as we know, this is the first presentation of all-real sets of 3-Γ symbols for D_3^*.

We note the following features which illustrate general points made in [1] and [2] or above:

(a) We see that for $D_3^* \supset C_2^*$, there are generally more allowed component triples (see the irrep triples $E_1A_1E_1$ and $E_{1/2}E_1E_{1/2}$) than for $D_3^* \supset C_3^*$, cf. the selection rule (3.2) which is weaker than (3.1).

Table 5

3-Γ symbols for D_3^* generated by the basis functions of Table 2

(i) $D_3^* \supset C_3^*$

$$\begin{pmatrix} A_1 & A_1 & A_1 \\ 0 & 0 & 0 \end{pmatrix} = 1; \quad \begin{pmatrix} A_2 & A_1 & A_2 \\ 0 & 0 & 0 \end{pmatrix} = -1; \quad \begin{pmatrix} R_1 & A_1 & R_2 \\ r & 0 & r \end{pmatrix} = 1;$$

even; even; odd; $A=-1$

$$\begin{pmatrix} E_1 & A_1 & E_1 \\ 1 & 0 & -1 \end{pmatrix} = \sqrt{1/2}; \quad \begin{pmatrix} E_{1/2} & A_1 & E_{1/2} \\ 1/2 & 0 & -1/2 \end{pmatrix} = -\sqrt{1/2};$$

even; odd

$$\begin{pmatrix} E_1 & A_2 & E_1 \\ 1 & 0 & -1 \end{pmatrix} = -\sqrt{1/2}; \quad \begin{pmatrix} E_{1/2} & A_2 & E_{1/2} \\ 1/2 & 0 & -1/2 \end{pmatrix} = \sqrt{1/2};$$

odd; even

$$\begin{pmatrix} R_1 & A_2 & R_1 \\ r & 0 & r \end{pmatrix} = 1; \quad \begin{pmatrix} R_2 & A_2 & R_2 \\ r & 0 & r \end{pmatrix} = -1;$$

even; even

$E_{1/2}$	E_1	$E_{1/2}$	3-Γ
1/2	−1	1/2	$-\sqrt{1/2}$
−1/2	1	−1/2	$-\sqrt{1/2}$

even

E_1	$E_{1/2}$	R_1	3-Γ
1	1/2	r	$+\sqrt{1/2}$
−1	−1/2	r	$-\sqrt{1/2}$

odd; $A=-1$

E_1	$E_{1/2}$	R_2	3-Γ
1	1/2	r	$-\sqrt{1/2}$
−1	−1/2	r	$-\sqrt{1/2}$

odd; $A=+1$

E_1	E_1	E_1	3-Γ
1	1	1	$-\sqrt{1/2}$
−1	−1	−1	$\sqrt{1/2}$

even; $A=-1$

Table 5.—cont.

3-Γ symbols for D_3^* generated by the basis functions of Table 2

(ii) $D_3^* \supset C_2^*$

$$\begin{pmatrix} A_1 & A_1 & A_1 \\ 0 & 0 & 0 \end{pmatrix} = 1; \quad \begin{pmatrix} A_2 & A_1 & A_2 \\ 0 & 0 & 0 \end{pmatrix} = -1; \quad \begin{pmatrix} R_1 & A_1 & R_2 \\ r & 0 & r \end{pmatrix} = +1;$$

even; even; odd; $A=-1$

$$\begin{pmatrix} E_1 & A_1 & E_1 \\ 0 & 0 & 0 \end{pmatrix} = -\begin{pmatrix} E_1 & A_1 & E_1 \\ 1 & 0 & 1 \end{pmatrix} = -\sqrt{1/2}; \quad \begin{pmatrix} E_{1/2} & A_1 & E_{1/2} \\ 1/2 & 0 & -1/2 \end{pmatrix} = \sqrt{1/2};$$

even; odd

$$\begin{pmatrix} E_1 & A_2 & E_1 \\ 0 & 1 & 1 \end{pmatrix} = \sqrt{1/2}; \quad \begin{pmatrix} R_1 & A_2 & R_1 \\ r & 1 & r \end{pmatrix} = 1; \quad \begin{pmatrix} R_2 & A_2 & R_2 \\ r & 1 & r \end{pmatrix} = -1;$$

odd; even; even

$$-\begin{pmatrix} E_{1/2} & A_2 & E_{1/2} \\ 1/2 & 1 & 1/2 \end{pmatrix} = \begin{pmatrix} E_{1/2} & A_2 & E_{1/2} \\ -1/2 & 1 & -1/2 \end{pmatrix} = \sqrt{1/2};$$

even

$E_{1/2}$	E_1	$E_{1/2}$	3-Γ
1/2	0	−1/2	1/2
1/2	1	1/2	−1/2
−1/2	1	−1/2	−1/2

even

E_1	$E_{1/2}$	R_1	3-Γ
0	−1/2	r	$-\sqrt{1/2}$
1	1/2	r	$-\sqrt{1/2}$

odd; $A=-1$

E_1	$E_{1/2}$	R_2	3-Γ
0	1/2	r	$-\sqrt{1/2}$
1	−1/2	r	$-\sqrt{1/2}$

odd; $A=+1$

E_1	E_1	E_1	3-Γ
0	0	0	1/2
0	1	1	1/2

even; $A=-1$

(b) We note that $(A_1A_1A_1/000) = +1$ in both cases and recall that consequences of this relation were mentioned in ([2], Sect. 4.4).

(c) We have given the one by one Derome–Sharp $\mathbb{A}$ matrix ([1], Sect. 5.4) for some of the triples as a number A. We note that for $R_1A_1R_2$ we have an illustration of (4.4.7) of [2] and for $E_1E_{1/2}R_1$ an illustration of (A.5.7) of [1]; in these cases, a negative A *must* occur within our set of conventions. This is true even for $E_1E_1E_1$, a triple of first-kind irreps. If we keep the present matrix irreps, the only way to obtain $A=+1$ for $E_1E_1E_1$ would be to multiply the basis functions by a non-real complex phase. The A matrices may in all cases be calculated from the 3-Γ symbols given in the table. For example, for $D_3^* \supset C_2^*$ we have, giving all details,

$$\begin{pmatrix} \bar{E}_1 & \bar{E}_{1/2} & \bar{R}_1 \\ 0 & -1/2 & r \end{pmatrix} = \begin{pmatrix} \bar{E}_1 & \bar{E}_{1/2} & R_2 \\ 0 & -1/2 & r \end{pmatrix} = -\begin{pmatrix} E_1 & \bar{E}_{1/2} & R_2 \\ 0 & -1/2 & r \end{pmatrix}$$
$$= -\begin{pmatrix} E_1 & E_{1/2} & R_2 \\ 0 & 1/2 & r \end{pmatrix} = -\begin{pmatrix} E_1 & E_{1/2} & R_1 \\ 0 & -1/2 & r \end{pmatrix} \tag{5.1}$$

from which it is seen that $A=-1$ for $E_1E_{1/2}R_1$. In the calculation (5.1) we used, twice, the conjugation formulae developed in ([1], Sect. 5.3).

(d) To illustrate further our formalism, we demonstrate the construction of coupling coefficients according to ([1], Sect. 5.3): for $D_3^* \supset C_2^*$ we get

$$\begin{aligned}
&\langle E_1 1 E_{1/2} 1/2 | R_2 r\rangle \\
&= \pi(E_1E_{1/2}\bar{R}_2)\pi(E_1A_1\bar{E}_1)\,\mathrm{sign}\,(\bar{R}_2A_1R_2)\sqrt{\dim R_2}\begin{pmatrix} \bar{E}_1 & \bar{E}_{1/2} & R_2 \\ 1 & 1/2 & r \end{pmatrix} \\
&= \pi(E_1E_{1/2}R_1)\pi(E_1A_1E_1)\,\mathrm{sign}\,(R_1A_1R_2)\begin{pmatrix} \bar{E}_1 & \bar{E}_{1/2} & R_2 \\ 1 & 1/2 & r \end{pmatrix} \\
&= (-1)(+1)(+1)\begin{pmatrix} \bar{E}_1 & \bar{E}_{1/2} & R_2 \\ 1 & 1/2 & r \end{pmatrix} \\
&= -\begin{pmatrix} \bar{E}_1 & \bar{E}_{1/2} & R_2 \\ 1 & 1/2 & r \end{pmatrix} = -(+1)(-1)\begin{pmatrix} E_1 & E_{1/2} & R_2 \\ 1 & -1/2 & r \end{pmatrix} = -\sqrt{1/2}; \qquad (5.2)
\end{aligned}$$

here we used ([1], Eqs. (5.3.15) and (5.3.14)); ([1], Eq. (5.3.13)); Table 5 of this paper in connection with ([1], Eq. (5.3.5)); and Table 5 once more.

[See again note (3) in Sect. 4. In addition, [11] gives a set of what is called symmetry coupling coefficients for D_3^*, generated by specified basis functions. Some of the coefficients are non-real. It is claimed that 3-Γ symbols cannot be constructed. A secondary basis is provided for $E_1(D_3^*)$, but no closer discussion of the use of it is given.]

6. Further material available

If there is a subgroup D_m^* of D_n^* with $m<n$, then one may choose standard matrix irreps of D_n^* which upon restriction to D_m^* yield the irreps of *that* group in the standard $D_m^* \supset C_m^*$ or $D_m^* \supset C_2^*$ form discussed above. These matrix irreps of D_n^* will generally not be identical to any of those met with in cases (i)–(iii), but will be closely related to them. We have prepared basis functions and 3-Γ symbols for the following hierarchies of this kind:

$$\begin{aligned}
&D_4^* \supset D_2^* \supset C_2^*\ \text{(i)}, \qquad D_4^* \supset D_2^* \supset C_2^*\ \text{(ii)} \\
&D_6^* \supset D_3^* \supset C_3^* \\
&D_6^* \supset D_3^* \supset C_2^* \\
&D_6^* \supset D_2^* \supset C_2^*\ \text{(i)}, \qquad D_6^* \supset D_2^* \supset C_2^*\ \text{(ii)}.
\end{aligned} \qquad (6.1)$$

All of these symmetry hierarchies may rather obviously be of practical relevance, but the two $D_6^* \supset D_3^*$ hierarchies are of interest from a fundamental point of view as well. It has recently been proved [12] that the existence of real coupling coefficients for a certain set of matrix irreps of a given group – or, equivalently (use arguments given in Appendix A of [13]) real 3-Γ symbols – implies that there is a (unique) automorphism of the group (homomorphic one-to-one mapping of the group onto itself) carrying all the matrix irreps into their complex conjugates. For all the basis function sets represented by (6.1), the automorphism just mentioned is the *inner* automorphism $R \to C_2^{Y^*} R (C_2^{Y^*})^{-1}$. (In fact, in this material, Eq. (4.4.1) of [2] is always satisfied with $R_0 = C_2^{Y^*}$ and the formalism of ([1], Sect. 5.5) applies). For D_3^* which possess irreps of the third kind, an irrep-conjugating automorphism must be outer (and so the above one is). The situation we are describing with $D_3^* \subset D_6^*$ is analogous to the one encountered with the tetrahedral double group [9] and the imbedding of it in the octahedral double group in [14].

7. Further remarks on the literature

Information equivalent to sets of 3–Γ symbols for various dihedral double-group hierarchies may be extracted from the tables in [15]. The method used in [15] is radically different from the one described here (cf. our remarks in [2]) and in particular does not involve basis functions. Information on matrix irreps and basis functions is difficult to extract from [15] and [16]. The paper [17] deals with $D_{4d} \supset D_4 \supset C_4$ (or rather their double groups; cf. [2], Sect. 2.2) by Butler's method.

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References

1. Damhus, T., Harnung, S. E., Schäffer, C. E.: paper I in this series
2. Same, paper II in the series
3. Damhus, T.: Linear Algebra Appl. **32**, 125 (1980)
4. Sivardière, J.: Phys. Stat. Sol. (b) **107**, 117 (1981)
5. Artmann, B.: Math.-Phys. Semesterber. (Univ. Giessen) **24**, 20 (1977)
6. Damhus, T.: Double groups as symmetry groups for spin-orbit coupling Hamiltonians, submitted to Match
7. Harnung, S. E., Schäffer, C. E.: Struct. Bond. **12**, 201 (1972)
8. Kibler, M. R., Grenet, G.: Int. J. Quant. Chem. **11**, 359 (1977)
9. Damhus, T., Harnung, S. E., Schäffer, C. E.: paper IV in this series
10. Golding, R. M., Newmarch, J. D.: Molec. Phys. **33**, 1301 (1977)
11. König, E., Kremer, S.: Theoret. Chim. Acta (Berl.) **32**, 27 (1973)
12. Bickerstaff, R. P., Damhus, T.: Int. J. Quantum Chem. (in press)
13. Damhus, T.: J. Math. Phys. **22**, 7 (1981)
14. Damhus, T., Harnung, S. E., Schäffer, C. E.: paper V in this series
15. Butler, P. H.: Point group symmetry applications. New York: Plenum Press 1981
16. Butler, P. H., Reid, M. F.: J. Phys. A **12**, 1655 (1979)
17. Prasad, L. S. R. K., Bharati, K.: J. Phys. A. **13**, 781 (1980)
18. Griffith, J. S.: The theory of transition metal ions. Cambridge: University Press 1971; first impression 1961

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