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Clebsch–Gordan coefficients for the corepresentations of Shubnikov point groups: II. Cubic groups

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Abstract. On the basis of the generalised Racah lemma for the corepresentations (coreps) of antiunitary groups, a general method is given for the calculation of Clebsch–Gordan coefficients (CGC) for the coreps of all 90 antiunitary Shubnikov magnetic point groups. Tables of basic functions, compatibility tables, multiplication tables and CGC for single and double coreps of all antiunitary, cubic point groups for odd and even basis (with respect to space inversion) are presented. The tables are necessary for problems in solid state spectroscopy and crystal field theory (selection rules, Wigner–Eckart theorem).

1. Introduction

As was shown by Wigner (1959), the operator of time inversion θ and all its combinations with unitary operators are antiunitary. The groups of unitary and antiunitary operators are known as antiunitary groups. Under the action of such group elements all quantum mechanical quantities transform by Wigner corepresentations (coreps), not by the ordinary representations. A detailed presentation of the coreps theory and its applications in solid state physics are given in the books of Bradley and Cracknell (1972) and Cracknell (1974). For a more efficient application of antiunitary groups and their coreps in a number of quantum mechanical problems, it is necessary to reconsider the theory of irreducible tensorial sets (algebra of Racah) for the case of coreps. The main component of this theory is the Clebsch–Gordan coefficient (CGC) for the coreps. This was discussed for the first time by Kotzev (1972, 1974), Aviran and Litvin (1973), Rudra (1974), Sacata (1974) and van den Broek (1979), whose results were in good agreement with those of Kotzev (1972). Another approach to the CGC calculation was given by Dirl (1980), who assumed that convenient CGC for the normal subgroup of the antiunitary group were given (a historical review could be found in Rudra and Sikdar (1976) and Kotzev and Aroyo (1980)). In recent papers (Rudra and Sikdar 1976, 1977) there were reports about the calculation of the CGC for the Shubnikov point groups, but only in the case of even, under space inversion, basic functions (the tables were not contained in Rudra and Sikdar (1976, 1977)). A new, more effective method for the calculation of the CGC for the coreps, based on the generalised Racah lemma, was suggested by Kotzev and Aroyo (1977) (see also Kotzev and Aroyo (1977, 1978a, b, c, 1979) where the CGC for the coreps of all 90 antiunitary Shubnikov point groups, for single and double valued coreps in the case of even and odd (under space inversion) basic functions, were calculated and tabulated). Unfortunately these editions are in insufficient circulation and they remain difficult of access for a great number of

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specialists. The aim of this paper is to systematise the results of Kotzev and Aroyo (1978a, 1979) and to make the CGC for the coreps of antiunitary cubic groups more accessible.

2. Method of calculation

The CGC for the coreps of antiunitary groups are the matrix elements

$$[\alpha_1 a_1 \alpha_2 a_2 | \alpha \rho_\alpha a] = U^{\alpha_1 \alpha_2}_{a_1 a_2, \alpha \rho_\alpha a} \tag{1}$$

of a unitary matrix $U^{\alpha_1\alpha_2}$ which reduces the inner Kronecker product of the irreducible coreps D^{α_1} and D^{α_2} to a block diagonal form. The index $\rho_\alpha = 1, \ldots, C^{\alpha_1\alpha_2}_\alpha$ specifies the equivalent D^α which are contained $C^{\alpha_1\alpha_2}_\alpha$ times in the reduction of $D^{\alpha_1} \boxtimes D^{\alpha_2}$. The matrices $U^{\alpha_1\alpha_2}$ are chosen in such a way that all $D^{\alpha\rho_\alpha}$ ($\rho_\alpha = 1, \ldots, C^{\alpha_1\alpha_2}_\alpha$) identically coincide, i.e. $D^{\alpha\rho_\alpha} = D^\alpha$. The generalised Racah lemma (Kotzev and Aroyo 1977, 1980), which concerns the relation between the CGC $U^{\alpha_1\alpha_2}$ for the group A and the corresponding coefficients $U^{\beta_1\beta_2}$ for a subgroup $B \subset A$, has the following matrix form:

$$\left(\bigoplus_{\beta_i \in \alpha_i} U^{\beta_1\beta_2} \right) = \bar{U}^{\alpha_1\alpha_2} (X^{\alpha_1\alpha_2})^{-1} \tag{2a}$$

where

$$\bar{U}^{\alpha_1\alpha_2} = (S^{\alpha_1} \boxtimes S^{\alpha_2})^{-1} U^{\alpha_1\alpha_2} \left(\bigoplus_{\alpha\rho_\alpha} S^\alpha \right). \tag{2b}$$

Here S^α are the subduction matrices of the coreps D^α in their subduction to the group $B \subset A$; the matrix $\bar{U}^{\alpha_1\alpha_2}$ contains the CGC for $D^{\alpha_1} \boxtimes D^{\alpha_2}$, but in a new basis; $X^{\alpha_1\alpha_2}$ is the matrix of the so-called isoscalar factors. The main difference from the classical Racah lemma (Racah 1949) is that in the case of coreps all isoscalar factors should be real, and so $X^{\alpha_1\alpha_2}$ is orthogonal. A proof of this statement and a more detailed exposé of this method can be found in Kotzev and Aroyo (1977, 1980).

All 122 Shubnikov (magnetic) point groups are subgroups of the full orthogonal group O(3), supplemented with time inversion—$\infty\infty\bar{1}1'$—$O(3) \otimes \Theta$, where $\Theta = \{1, \theta\}$. There are three types of Shubnikov point groups—32 ordinary point groups, 32 grey point groups and 58 black and white point groups. For the sake of convenience in physical applications, the CGC are calculated both for even (Kotzev and Aroyo 1978a, b, c) and odd (Kotzev and Aroyo 1979) basic functions. The choice of the basic functions for the grey groups coincides with the functions given in Leushin (1968), and for the black and white groups the functions are derived by the method given in Kotzev and Aroyo (1977).

Every even (odd) function Φ^α_a (Ψ^α_a) transforms as the ath component of the irreducible corep D^α, and is a linear combination of the form

$$\Phi^{\alpha\tau_\alpha}_a \equiv |(j+)\alpha\tau_\alpha a\rangle = \sum_m \varphi^{j+}_m S^{j+}_{m,\alpha\tau_\alpha a}, \tag{3a}$$

$$\Psi^{\alpha\tau_\alpha}_a \equiv |(j-)\alpha\tau_\alpha a\rangle = \sum_m \psi^{j-}_m S^{j-}_{m,\alpha\tau_\alpha a}, \tag{3b}$$

where the functions

$$\varphi^{j+}_m \equiv |jm\rangle, \qquad m = j, j-1, \ldots, -j, \tag{4a}$$

$$\psi^{j-}_m \equiv |\bar{j}m\rangle \qquad m = j, j-1, \ldots, -j, \tag{4b}$$

form a basis of an even (positive) irreducible corep D^{j+} (4a), or of an odd (negative) irreducible corep D^{j-} (4b) of the generalised full orthogonal group $O(3)\otimes\Theta$, and they transform as eigenfunctions of the operator of angular momentum. The functions are chosen in such a way that

$$C^z_n|jm\rangle = \exp(2\pi i m/n)|jm\rangle, \tag{5a}$$

$$C^z_n|\bar{j}m\rangle = \exp(2\pi i m/n)|\bar{j}m\rangle, \tag{5b}$$

$$I|jm\rangle = |jm\rangle, \tag{6a}$$

$$I|\bar{j}m\rangle = -|\bar{j}m\rangle, \tag{6b}$$

$$\theta|jm\rangle = (-1)^{j-m}|j-m\rangle, \tag{7a}$$

$$\theta|\bar{j}m\rangle = (-1)^{j-m}|\bar{j}-m\rangle. \tag{7b}$$

As was shown by Kotzev (1972, see also Kotzev and Aroyo 1978a) the CGC for the coreps of $O(3)\otimes\Theta$ coincide with the well known Wigner coefficients $(j_1m_1j_2m_2|jm)$,

$$[j_1m_1j_2m_2|j1m] \equiv (j_1m_1j_2m_2|jm). \tag{8}$$

To reduce the volume of the calculation, the antiunitary double point groups are arranged in 21 isomorphic sets (table 1). The groups in every row of the table are isomorphic with the exception of the last one. It is a centrosymmetrical group, which is related to the proper rotation group (first column) of the set.

The CGC for the coreps of the Shubnikov point groups can be calculated with the help of the generalised Racah lemma, either directly from (8), i.e. using the Wigner coefficients as starting coefficients for every group, or by a successive descent down the subgroup chain:

$$O(3)\otimes\Theta \supset G\otimes\Theta \supset \cdots \supset C_1. \tag{9}$$

In our calculations we have used the second method, which proves to be more efficient, for proper rotation groups. (So, the coefficients (8) are starting coefficients for the groups $O\otimes\Theta$ and $D_6\otimes\Theta$ only.) Naturally for such groups, $G_0 \subset SO(3)\otimes\Theta$, where $G_0 = G1'$ or $G(H)$, the choice of even or odd basis is of no significance.

The calculation of the CGC for the coreps of the other groups in the isomorphic sets is carried out according to the following scheme.

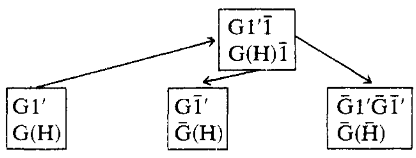

Figure 1. Calculation of CGC.

We should note that not only are the matrices of the coreps of all isomorphic groups equivalent, but they identically coincide. To each set of isomorphic groups is related a centrosymmetrical group $G\bar{1} = G_0\otimes C_i$, $C_i = \{E, I\}$ (fourth column of table 1), whose coreps are in a direct correspondence with the coreps of the group of proper rotations (first column), there being two irreducible coreps (even $D^{\alpha+}$ and odd $D^{\alpha-}$) of $G1'\bar{1}$ or $G(H)\bar{1}$ for each one of the proper rotation group.

The even coreps are such that

$$D^{\alpha+}(R)=D^{\alpha}(R), \qquad R\in \mathrm{G}_0, \tag{10a}$$
$$D^{\alpha+}(IR)=D^{\alpha}(R),$$

while the odd satisfy

$$D^{\alpha-}(R)=D^{\alpha}(R), \qquad R\in \mathrm{G}_0, \tag{10b}$$
$$D^{\alpha-}(IR)=-D^{\alpha}(R), \qquad R\in \mathrm{G}_0,$$

where D^{α} are the coreps of the group $\mathrm{G}_0\subset \mathrm{G}_0\otimes \mathrm{C}_i$.

The reduction matrices ensuring the transitions $(D^{\alpha}\uparrow \mathrm{G}\bar{1})=D^{\alpha+}$ or $(D^{\alpha}\uparrow \mathrm{G}\bar{1})=D^{\alpha-}$ are identity matrices. From the Racah lemma it follows that $X^{\alpha_1\alpha_2}$ is also an identity matrix. Using the generalised Racah lemma (as it gives the relation between CGC of a group and its subgroups, the lemma can be used for the determination of the CGC of the supergroup, starting with the coefficients of its subgroups), having in mind that $C_{\alpha}^{\alpha_1\alpha_2}$ for these groups are the same as for the groups before supplementing with the inversion, except that

$$D^{\alpha_1\pm}\boxtimes D^{\alpha_2\pm}=\bigoplus_{\alpha} C_{\alpha}^{\alpha_1\alpha_2}D^{\alpha+}, \tag{11a}$$

$$D^{\alpha_1\mp}\boxtimes D^{\alpha_2\pm}=\bigoplus_{\alpha} C_{\alpha}^{\alpha_1\alpha_2}D^{\alpha-}, \tag{11b}$$

and supposing that $\rho_{\alpha+}=\rho_{\alpha-}=\rho_{\alpha}$, we obtain the following relations:

$$[\alpha_1 a_1\alpha_2 a_2|\alpha\rho_{\alpha}a]=[\alpha_1^{\pm}a_1\alpha_2^{\pm}a_2|\alpha^{+}\rho_{\alpha+}a]=[\alpha_1^{\mp}a_1\alpha_2^{\pm}a_2|\alpha^{-}\rho_{\alpha-}a]. \tag{12}$$

For the groups of $\mathrm{G}\bar{1}'$, $\bar{\mathrm{G}}(\mathrm{H})$ (second column of table 1) and $\bar{\mathrm{G}}1'$, $\bar{\mathrm{G}}\bar{1}'$, $\bar{\mathrm{G}}(\bar{\mathrm{H}})$ (third column of table 1) types, which include inversion axes and inversion planes of symmetry, but do not contain the inversion I itself, we can use again the generalised Racah lemma, with CGC of the corresponding centrosymmetrical group as starting coefficients (these groups are subgroups of the related centrosymmetrical group) (figure 1). The form of the coefficients for these groups depends on the choice of the functions with respect to the space inversion. We will note that if both of the functions are even $\Phi_{a_1}^{\alpha_1}\Phi_{a_2}^{\alpha_2}$ or odd $\Psi_{a_1}^{\alpha_1}\Psi_{a_2}^{\alpha_2}$, their product decomposes into even functions. If one of the functions is odd, and the other even, then the product decomposes into odd functions. In all the cases the products $\Phi_{a_1}^{\alpha_1}\Phi_{a_2}^{\alpha_2}$; $\Psi_{a_1}^{\alpha_1}\Psi_{a_2}^{\alpha_2}$; $\Phi_{a_1}^{\alpha_1}\Psi_{a_2}^{\alpha_2}$; $\Psi_{a_1}^{\alpha_1}\Phi_{a_2}^{\alpha_2}$ transform by the equivalent coreps $D^{\alpha_1}\boxtimes D^{\alpha_2}$, which is written symbolically in the form

$$\alpha_1^{\mathrm{e}}\times\alpha_2^{\mathrm{e}}\sim\alpha_1^{\mathrm{o}}\times\alpha_2^{\mathrm{o}}\sim\alpha_1^{\mathrm{e}}\times\alpha_2^{\mathrm{o}}\sim\alpha_1^{\mathrm{o}}\times\alpha_2^{\mathrm{e}}.$$

Here the indices 'e' and 'o' stand for even and odd choices of the basic functions. The symbols 'g' and 'u' or '+', '−' are not used because there is a possibility of perceiving these functions as basic functions of even and odd coreps $D^{\alpha\pm}$ of the centrosymmetrical groups.

For the groups of the type $\mathrm{G}\bar{1}'$ (or $\bar{\mathrm{G}}(\mathrm{H})$) which do not have improper elements in the unitary subgroup, the transitions $(D^{\alpha+}\downarrow \mathrm{G}\bar{1})'=D^{\alpha^{\mathrm{e}}}$ and $(D^{\alpha-}\downarrow \mathrm{G}\bar{1}')=D^{\alpha^{0}}$ are carried out by the reduction matrices of the type $S^{\alpha+}=E$ and $S^{\alpha-}=\mathrm{i}E$. Using the generalised Racah lemma and supposing that $\rho_{\alpha+}=\rho_{\alpha^{0}}=\rho_{\alpha^{\mathrm{e}}}$, we obtain the following relations for the CGC for $G\bar{1}'$ (or $\bar{G}(H)$) groups:

$$
\begin{aligned}
[\alpha_1^+ a_1 \alpha_2^+ a_2 | \alpha \rho_\alpha a] &= [\alpha_1^e a_1 \alpha_2^e a_2 | \alpha^e \rho_\alpha a] \\
&= -[\alpha_1^o a_1 \alpha_2^o a_2 | \alpha^e \rho_\alpha a] \\
&= [\alpha_1^o a_1 \alpha_2^e a_2 | \alpha^o \rho_\alpha a] \\
&= [\alpha_1^e a_1 \alpha_2^o a_2 | \alpha^o \rho_\alpha a]. \qquad (13)
\end{aligned}
$$

For the groups of the type $\bar{G}1'$ (or $\bar{G}\bar{1}'$, $\bar{G}(\bar{H})$), which have improper elements in the unitary subgroup, the transitions $(D^{\alpha+}\downarrow\bar{G}1') = D^{\alpha^e}$ and $(D^{\alpha-}\downarrow\bar{G}1') = D^{\alpha'^o}$, $\alpha' \neq \alpha$, are carried out by the reduction matrices $S^{\alpha+} = E$ and $S^{\alpha-} \neq E$. Again by the generalised Racah lemma, we obtain that the CGC for even bases coincide with the corresponding CGC of the related centrosymmetrical group. In the case of odd basic functions, most of the coefficients either coincide with those of even bases or differ from them by a sign. A more essential difference exists when in the decomposition of the Kronecker product of $D^{\alpha_1} \boxtimes D^{\alpha_2}$ are contained equivalent coreps, i.e. $C_\alpha^{\alpha_1\alpha_2} > 1$.

So, in the case of even bases, it is sufficient to calculate the CGC for the coreps of the double antiunitary Shubnikov groups just for 21 out of 90 groups (i.e. for the proper rotation groups, which serve as representatives of the isomorphic sets).

In the case of odd bases it is sufficient to calculate the CGC only for the groups of the third column of table 1, $\bar{G}1'$, $\bar{G}\bar{1}'$, $\bar{G}(\bar{H})$. For the other groups of the isomorphic sets the relation between the CGC of even and odd bases is trivial.

Table 1. Shubnikov point groups.

	$G1'$ $G(H)$	$G\bar{1}'$ $\bar{G}(H)$	$\bar{G}1'G1'$ $\bar{G}(\bar{H})$	$G1'\bar{1}$ $G(H)\bar{1}$
Cubic	$O\otimes\Theta$	$O_h(O)$	$T_d\otimes\Theta$ $O_h(T_d)$	$O_h\otimes\Theta$
	$T\otimes\Theta$	$T_h(T)$		$T_h\otimes\Theta$
	$O(T)$	$T_d(T)$		$O_h(T_h)$
Tetragonal	$D_4\otimes\Theta$	$D_{4h}(D_4)$	$C_{4v}\otimes\Theta D_{4h}(C_{4v}) D_{2d}\otimes\Theta D_{4h}(D_{2d})$	$D_{4h}\otimes\Theta$
	$C_4\otimes\Theta$	$C_{4h}(C_4)$	$S_4\otimes\Theta C_{4h}(S_4)$	$C_{4h}\otimes\Theta$
	$D_4(C_4)$	$C_{4v}(C_4)$	$D_{2d}(S_4)$	$D_{4h}(C_{4h})$
	$D_4(D_2)$	$D_{2d}(D_2)$	$C_{4v}(C_{2v}) D_{2d}(C_{2v})$	$D_{4h}(D_{2h})$
	$C_4(C_2)$	$S_4(C_2)$		$C_{4h}(C_{2h})$
Orthor.	$D_2\otimes\Theta$	$D_{2h}(D_2)$	$C_{2v}\otimes\Theta D_{2h}(C_{2v})$	$D_{2h}\otimes\Theta$
	$D_2(C_2)$	$C_{2v}(C_2)$	$C_{2v}(C_s)$	$D_{2h}(C_{2h})$
Monocl.	$C_2\otimes\Theta$	$C_{2h}(C_2)$	$C_s\otimes\Theta C_{2h}(C_s)$	$C_{2h}\otimes\Theta$
	$C_2(C_1)$	$C_s(C_1)$		$C_{2h}(C_i)$
Triclinic	$C_1\otimes\Theta$	$C_i(C_1)$		$C_i\otimes\Theta$
Hexagonal	$D_6\otimes\Theta$	$D_{6h}(D_6)$	$C_{6v}\otimes\Theta D_{6v}(C_{6v}) D_{3h}\otimes\Theta D_{6h}(D_{3h})$	$D_{6h}\otimes\Theta$
	$C_6\otimes\Theta$	$C_{6h}(C_6)$	$C_{3h}\otimes\Theta C_{6h}(C_{3h})$	$C_{6h}\otimes\Theta$
	$D_6(C_6)$	$C_{6v}(C_6)$	$D_{3h}(C_{3h})$	$D_{6h}(C_{6h})$
	$D_6(D_3)$	$D_{3h}(D_3)$	$C_{6v}(C_{3v}) D_{3h}(C_{3v})$	$D_{6h}(D_{3d})$
	$C_6(C_3)$	$C_{3h}(C_3)$		$C_{6h}(C_{3i})$
Trigonal	$D_3\otimes\Theta$	$D_{3d}(D_3)$	$C_{3v}\otimes\Theta D_{3d}(C_{3v})$	$D_{3d}\otimes\Theta$
	$C_3\otimes\Theta$	$C_{3i}(C_3)$		$C_{3i}\otimes\Theta$
	$D_3(C_3)$	$C_{3v}(C_3)$		$D_{3d}(C_{3i})$

Table 2. Basic functions.

$O\otimes\Theta$ $T_d\otimes\Theta$ $O_h(O)$ $O_h(T_d)$			$T_d\otimes\Theta$ $O_h(T_d)$		$T\otimes\Theta$ $T_h(T)$			$O(T)$ $T_d(T)$		
D_α	Γ_α	Φ_a^α	D_α	Ψ_a^α	D_α	Γ_α	Φ_a^α	D_α	Γ_α	Φ_a^α
$D1$	$\Gamma1=A1$	$\|00\rangle$	$D2$	$i\|\bar{0}0\rangle$	$D1$	$\Gamma1=A1$	$\|00\rangle$	$D1$	$\Gamma1=A1$	$\|00\rangle$
$D2$	$\Gamma2=A2$	$i\sqrt{1/2}(\|32\rangle-\|3\bar{2}\rangle)$	$D1$	$\sqrt{1/2}(\|\bar{3}\bar{2}\rangle-\|\bar{3}2\rangle)$						
$D3$	$\Gamma3=E$	$\|20\rangle$ $\sqrt{1/2}(\|22\rangle+\|2\bar{2}\rangle)$	$D3$	$-\sqrt{1/2}(\|\bar{2}2\rangle+\|\bar{2}\bar{2}\rangle)$ $\|\bar{2}0\rangle$	$D2$	$\Gamma2=1E$ $\Gamma3=2E$	$\|20\rangle$ $\sqrt{1/2}(\|22\rangle+\|2\bar{2}\rangle)$	$D2$ $D3$	$\Gamma2=1E$ $\Gamma3=2E$	$\sqrt{1/2}\|20\rangle-i\sqrt{1/4}(\|22\rangle+\|2\bar{2}\rangle)$ $\sqrt{1/2}\|20\rangle+i\sqrt{1/4}(\|22\rangle+\|2\bar{2}\rangle)$
$D4$	$\Gamma4=T1$	$\|11\rangle$ $\|10\rangle$ $\|1\bar{1}\rangle$	$D5$	$\|\bar{1}\bar{1}\rangle$ $i\|\bar{1}0\rangle$ $\|\bar{1}1\rangle$	$D4$	$\Gamma4=T$	$\|11\rangle$ $\|10\rangle$ $\|1\bar{1}\rangle$	$D4$	$\Gamma4=T$	$\sqrt{1/2}(\|11\rangle+\|1\bar{1}\rangle)$ $-i\sqrt{1/2}(\|11\rangle-\|1\bar{1}\rangle)$ $\|10\rangle$
$D5$	$\Gamma5=T2$	$\|21\rangle$ $i\sqrt{1/2}(\|22\rangle-\|2\bar{2}\rangle)$ $\|2\bar{1}\rangle$	$D4$	$\|\bar{2}0\rangle$ $\sqrt{1/2}(\|\bar{2}2\rangle-\|\bar{2}\bar{2}\rangle)$ $-\|\bar{2}1\rangle$						
$D6$	$\Gamma6=\bar{E}1$	$\|1/2\ 1/2\rangle$ $\|1/2\ \overline{1/2}\rangle$	$D7$	$\|\overline{1/2}\ 1/2\rangle$ $\|\overline{1/2}\ \overline{1/2}\rangle$	$D5$	$\Gamma5=\bar{E}$	$\|1/2\ 1/2\rangle$ $\|1/2\ \overline{1/2}\rangle$	$D5$	$\Gamma5=\bar{E}$	$\|1/2\ 1/2\rangle$ $\|1/2\ \overline{1/2}\rangle$
$D7$	$\Gamma7=\bar{E}2$	$\sqrt{1/6}\|5/2\ 5/2\rangle-\sqrt{5/6}\|5/2\ \overline{3/2}\rangle$ $\sqrt{5/6}\|5/2\ 3/2\rangle-\sqrt{1/6}\|5/2\ \overline{5/2}\rangle$	$D6$	$-\sqrt{1/6}\|\overline{5/2}\ 5/2\rangle+\sqrt{5/6}\|\overline{5/2}\ \overline{3/2}\rangle$ $\sqrt{5/6}\|\overline{5/2}\ 3/2\rangle-\sqrt{1/6}\|\overline{5/2}\ \overline{5/2}\rangle$						
$D8$	$\Gamma8=\bar{F}$	$\|3/2\ 3/2\rangle$ $\|3/2\ 1/2\rangle$ $\|3/2\ \overline{1/2}\rangle$ $\|3/2\ \overline{3/2}\rangle$	$D8$	$-\|\overline{3/2}\ \overline{1/2}\rangle$ $\|\overline{3/2}\ \overline{3/2}\rangle$ $\|\overline{3/2}\ 3/2\rangle$ $-\|\overline{3/2}\ 1/2\rangle$	$D6$	$\Gamma6=1\bar{F}$ $\Gamma7=2\bar{F}$	$\|3/2\ 3/2\rangle$ $\|3/2\ 1/2\rangle$ $\|3/2\ \overline{1/2}\rangle$ $\|3/2\ \overline{3/2}\rangle$	$D6$ $D7$	$\Gamma6=1\bar{F}$ $\Gamma7=2\bar{F}$	$\sqrt{1/2}(-i\|3/2\ 3/2\rangle+\|3/2\ \overline{1/2}\rangle)$ $\sqrt{1/2}(-\|3/2\ 1/2\rangle+i\|3/2\ \overline{3/2}\rangle)$ $\sqrt{1/2}(\|3/2\ 1/2\rangle+i\|3/2\ \overline{3/2}\rangle)$ $\sqrt{1/2}(i\|3/2\ 3/2\rangle+\|3/2\ \overline{1/2}\rangle)$

Table 3. Compatibility table.

D^j	0+	1+	2+	3+	1/2+	3/2+	5/2+	0−	1−	2−	3−	1/2−	3/2−	5/2−
$O_h \otimes \Theta$	1^+	4^+	$3^+ + 5^+$	$2^+ + 4^+ + 5^+$	6^+	8^+	$7^+ + 8^+$	1^-	4^-	$3^- + 5^-$	$2^- + 4^- + 5^-$	6^-	8^-	$7^- + 8^-$
$O \otimes \Theta$	1	4	3+5	2+4+5	6	8	7+8	1	4	3+5	2+4+5	6	8	7+8
$T_d \otimes \Theta$	1	4	3+5	2+4+5	6	8	7+8	2	5	3+4	1+4+5	7	8	6+8
$O_h(O)$	1	4	3+5	2+4+5	6	8	7+8	1	4	3+5	2+4+5	6	8	7+8
$O_h(T_d)$	1	4	3+5	2+4+5	6	8	7+8	2	5	3+4	1+4+5	7	8	6+8
$T_h \otimes \Theta$	1^+	4^+	$2^+ + 4^+$	$1^+ + 4^{2+}$	5^+	6^+	$5^+ + 6^+$	1^-	4^-	$2^- + 4^-$	$1^- + 4^{2-}$	5^-	6^-	$5^- + 6^-$
$T \otimes \Theta$	1	4	2+4	$1+4^2$	5	6	5+6	1	4	2+4	$1+4^2$	5	6	5+6
$T_h(T)$	1	4	2+4	$1+4^2$	5	6	5+6	1	4	2+4	$1+4^2$	5	6	5+6
$O_h(T_h)$	1^+	4^+	$2^+ + 3^+ + 4^+$	$1^+ + 4^{2+}$	5^+	$6^+ + 7^+$	$5^+ + 6^+ + 7^+$	1^-	4^-	$2^- + 3^- + 4^-$	$1^- + 4^{2-}$	5^-	$6^- + 7^-$	$5^- + 6^- + 7^-$
$O(T)$	1	4	2+3+4	$1+4^2$	5	6+7	5+6+7	1	4	2+3+4	$1+4^2$	5	6+7	5+6+7
$T_d(T)$	1	4	2+3+4	$1+4^2$	5	6+7	5+6+7	1	4	2+3+4	$1+4^2$	5	6+7	5+6+7

3. Discussion of the tables

Table 1. Shubnikov point groups. In this table are given all 90 antiunitary Shubnikov point groups classified into 21 isomorphic sets (each row of the table). Every set contains a proper rotation group (1st column), groups which contain inversion axes and inversion planes of symmetry either as antiunitary (2nd column) or unitary and antiunitary (3rd column) elements, but do not contain the space inversion I itself. To each set of isomorphic groups is related a centrosymmetrical group (4th column).

Table 2. Basic functions. In the table are given the even basic functions for the three isomorphic sets of cubic groups. Odd basic functions are given only for the groups of the third type (which include inversion axes and inversion planes of symmetry as unitary and antiunitary elements) $T_d \otimes \Theta$, $O_h(T_d)$. We have also indicated the corresponding reps of the unitary subgroups.

Table 4*a*. Multiplication table for $O \otimes \Theta$.

	1	2	3	4	5	6	7	8
1	[1]	2	3	4	5	6	7	8
2	2	[1]	3	5	4	7	6	8
3	3	3	[1+3]+2	4+5	4+5	8	8	6+7+8
4	4	5	4+5	[1+3+5]+4	2+3+4+5	6+8	7+8	$6+7+8^2$
5	5	4	4+5	2+3+4+5	[1+3+5]+4	7+8	6+8	$6+7+8^2$
6	6	7	8	6+8	7+8	[4]+1	2+5	3+4+5
7	7	6	8	7+8	6+8	2+5	[4]+1	3+4+5
8	8	8	6+7+8	$6+7+8^2$	$6+7+8^2$	3+4+5	3+4+5	$[2+4^2+5]+1+3+5$

Table 4*b*. Multiplication table for $T \otimes \Theta$.

	1	2	4	5	6
1	[1]	2	4	5	6
2	2	[1+2]+1	4^2	6	5^2+6
4	4	4^2	[1+2+4]+4	5+6	5^2+6^2
5	5	6	5+6	[4]+1	$2+4^2$
6	6	5^2+6	5^2+6^2	$2+4^2$	$[1+4^3]+1+2+4$

Table 4*c*. Multiplication table for O(T).

	1	2	3	4	5	6	7
1	[1]	2	3	4	5	6	7
2	2	[3]	1	4	6	7	5
3	3	1	[2]	4	7	5	6
4	4	4	4	[1+2+3+4]+4	5+6+7	5+6+7	5+6+7
5	5	6	7	5+6+7	[4]+1	2+4	3+4
6	6	7	5	5+6+7	2+4	[4]+3	1+4
7	7	5	6	5+6+7	3+4	1+4	[4]+2

Table 5. CGC for even bases: $\alpha_1^e \times \alpha_2^e$. ***5a.*** $O \otimes \Theta$, $O_h(\Theta)$ and $T_d \otimes \Theta$, $O_h(T_d)$ even.

2121 111−	1	3131 111	1/2	3131 311−	1/2	3132 211−i	1/2 *
3132 312	1/2	3232 111	1/2	3232 311	1/2	4141 312	1/2
4141 512 i	1/2	4142 411	1/2 *	4142 511	1/2	4143 111	1/3
4143 311	1/6	4143 412	1/2 *	4242 111−	1/3	4242 311	2/3
4243 413	1/2 *	4243 513	1/2	4343 312	1/2	4343 512 i	1/2
5151 312−	1/2	5151 512−i	1/2	5152 413 i	1/2 *	5152 513 i	1/2
5153 111−	1/3	5153 311	1/6	5153 412−	1/2 *	5252 111	1/3
5252 311	2/3	5253 411−i	1/2 *	5253 511−i	1/2	5353 312−	1/2
5353 512 i	1/2 *	6161 411	1	6162 111	1/2 *	6162 412	1/2
6262 413	1	7171 411−	1	7172 111	1/2 *	7172 412−	1/2
7272 413−	1	8181 423	5/8	8181 523−	3/8	8182 211 i	1/4
8182 312	1/4 *	8182 512 i	1/4 *	8182 522 i	1/4	8183 411	3/10
8183 421	3/40	8183 511	1/2 *	8183 521−	1/8	8184 111	1/4 *
8184 311	1/4 *	8184 412	9/20	8184 422	1/20	8282 411−	2/5
8282 421	9/40	8282 521−	3/8	8283 111−	1/4 *	8283 311	1/4 *
8283 412−	1/20	8283 422−	9/20	8284 413−	3/10	8284 423	3/40
8284 513	1/2 *	8284 523	5/40	8383 413	2/5	8383 423	9/40
8383 523	3/8	8384 211−i	1/4	8384 312	1/4 *	8384 512−i	1/4 *
8384 522 i	1/4	8484 421	5/8	8484 521	3/8	2131 312 i	*
2132 311−i	*	2141 513 i		2142 512−	1	2143 511−i	
2151 413−i		2152 412	1	2153 411 i		2161 711 i	*
2162 712 i	*	2171 611−i	*	2172 612−i	*	2181 813−i	*
2182 814 i	*	2183 811 i	*	2184 812−i	*	3141 411	1/4
3141 511−i	3/4 *	3142 412−	1	3143 413	1/4	3143 513	3/4 *
3241 413	3/4	3241 513−	1/4 *	3242 512 i	*	3243 411	3/4
3243 511	1/4 *	3151 411	3/4 *	3151 511−	1/4	3152 512	1
3153 413−	3/4 *	3153 513−	1/4	3251 413−	1/4 *	3251 513	3/4
3252 412 i	*	3253 411	1/4 *	3253 511	3/4	3161 812−	1 *
3162 813	1 *	3261 814−	1 *	3262 811	1 *	3171 814	1 *
3172 811−	1 *	3271 812−	1 *	3272 813	1 *	3181 712	1/2 *
3181 811	1/2	3182 611	1/2 *	3182 812−	1/2	3183 612−	1/2 *
3183 813−	1/2	3184 711−	1/2 *	3184 814	1/2	3281 612−	1/2 *
3281 813	1/2	3282 711	1/2 *	3282 814	1/2	3283 712−	1/2 *
3283 811	1/2	3284 611	1/2 *	3284 812	1/2	4151 211 i	1/3
4151 312	1/6 *	4151 512 i	1/2 *	4152 413 i	1/2	4152 513 i	1/2 *
4153 311	1/2 *	4153 412	1/2	4251 411−	1/2	4251 511−	1/2 *
4252 211	1/3	4252 312 i	2/3 *	4253 413−i	1/2	4253 513	1/2 *
4351 311−	1/2 *	4351 412	1/2	4352 411−i	1/2	4352 511 i	1/2 *
4353 211−i	1/3	4353 312−	1/6 *	4353 512 i	1/2 *	4161 811	1
4162 611	2/3 *	4162 812	1/3	4261 611−	1/3 *	4261 812	2/3
4262 612	1/3 *	4262 813	2/3	4361 612−	2/3 *	4361 813	1/3
4362 814	1	4171 813−	1	4172 711−	2/3 *	4172 814	1/3
4271 711	1/3	4271 814	2/3	4272 712−	1/3 *	4272 811	2/3
4371 712	2/3	4371 811	1/3	4372 812−	1	4181 711	1/6
4181 824	5/6	4182 712−	1/2	4182 811	2/5 *	4182 821−	1/10
4183 611	1/6	4183 812	8/15*	4183 822	3/10	4184 612	1/2
4184 813	2/5 *	4184 823−	1/10	4281 712−	1/3	4281 811−	3/5 *
4281 821−	1/15	4282 611−	1/3	4282 812−	1/15*	4282 822	3/5
4283 612−	1/3	4283 813	1/15*	4283 823−	3/5	4284 711−	1/3
4284 814	3/5 *	4284 824	1/15	4381 611	1/2	4381 812−	2/5 *
4381 822	1/10	4382 612	1/6	4382 813−	8/15	4382 823−	3/10
4383 711−	1/2	4383 814−	2/5 *	4383 824	1/10	4384 712	1/6
4384 821−	5/6	5161 712−	2/3	5161 811−	1/3 *	5162 812	1 *
5261 711−i	1/3	5261 814−i	2/3 *	5262 712−i	1/3	5262 811−i	2/3 *
5361 813−	1 *	5362 711−	2/3	5362 814 i	1/3 *	5171 612	2/3

Table 5*a*—continued.

5171 813	1/3 *	5172 814	1 *	5271 611 i	1/3	5271 812 i	2/3 *
5272 612−i	1/3	5272 813 i	2/3 *	5271 811−	1 *	5372 611	2/3
5372 812−	1/3 *	5181 711−	1/2 *	5181 824−	1/2 *	5182 712−	1/6 *
5182 811−	2/3	5182 821−	1/2 *	5183 611−	1/2 *	5183 822	1/2 *
5184 612	1/6 *	5184 813	2/3	5184 823−	1/6 *	5281 612−i	1/3 *
5281 813 i	1/3	5281 823 i	1/3 *	5282 711 i	1/3 *	5282 814 i	1/3
5282 824−i	1/3 *	5283 712 i	1/3 *	5283 811−i	1/3	5283 821 i	1/3 *
5284 611−i	1/3 *	5284 812−i	1/3	5284 822−i	1/3 *	5381 611−	1/6 *
5381 812	2/3	5381 822−	1/6 *	5382 612	1/2 *	5382 823	1/2 *
5383 711	1/6 *	5383 814−	2/3	5383 824−	1/6 *	5384 712	1/2 *
5384 821−	1/2 *	6171 513−	1 *	6172 211−i	1/2	6172 512−i	1/2 *
6271 211 i	1/2	6271 512−i	1/2 *	6272 511	1 *	6181 312	1/2
6181 512 i	1/2	6182 411	1/4 *	6182 511	3/4	6183 311	1/2
6183 412	1/2 *	6184 413	3/4 *	6184 513	1/4	6281 411−	3/4 *
6281 511	1/4	6282 311	1/2	6282 412−	1/2 *	6283 413−	1/4 *
6283 513	3/4	6284 312	1/2	6284 512−i	1/2	7181 311−	1/2
7181 412	1/2 *	7182 413−	3/4 *	7182 513−	1/4	7183 312	1/2
7183 512−i	1/2	7184 411	1/4 *	7184 511	3/4	7281 413−	1/4 *
7281 513	3/4	7282 312	1/2	7282 512 i	1/2	7283 411	3/4 *
7283 511−	1/4	7284 311−	1/2	7284 412−	1/2 *		

Table 5*b*. T⊗Θ, T_h(T).

2122 121−	1/2 *	4141 422	1/2	4142 423−	1/2	4243 421	1/2
4343 422−	1/2	6161 441−	3/8	6162 432	1/4 *	6162 442	1/4
6163 433−	1/2 *	6163 443	1/8	6262 443	3/8	6264 431	1/2 *
6264 441	1/8	6363 441	3/8	6364 121−	1/4	6364 432−	1/4 *
6364 442	1/4	6464 443−	3/8	6162 121	1/4	2141 423	3/4 *
2143 421	3/4 *	2241 421−	1/4 *	2242 442	1 *	2243 423−	1/4 *
5161 422	1/2	5162 423−	3/4	5164 421	1/4	5261 423−	1/4
5263 421	3/4	5264 422−	1/2				

Table 5*c*. O(T), T_d(T).

2121 311−	1	3131 211−	1	2131 111	1	4141 111−	1/3
4141 211	1/3w̲	4141 311	1/3w	4142 413−i	1/2 *	4142 423	1/2
4143 412−i	1/2 *	4143 422	1/2	4242 111−	1/3	4242 211	1/3w̲
4242 311	1/3w̲	4243 411 i	1/2 *	4243 421	1/2	4343 111−	1/3
4343 211	1/3	4343 311	1/3	5151 411	1/2	5151 412−i	1/2
5152 111	1/2 *	5152 413	1/2	5252 411	1/2	5252 412 i	1/2
6161 411−	1/2w̲	6161 412 i	1/2w	6162 311	1/2 *	6162 413	1/2
6262 411−	1/2w̲	6262 412−i	1/2w	7171 411−	1/2w	7171 412 i	1/2w̲
7172 211	1/2 *	7172 413	1/2	7272 411−	1/2w	7272 412−i	1/2w̲
2141 411	w	2142 412	w̲	2143 413−	1	2151 612	1 *
2152 611	1 *	2161 712−	1	2162 711	1	2171 511	1 *
2172 512	1 *	3141 411	w̲	3142 412	w	3143 413−	1
3151 711−	1 *	3152 712	1 *	3161 512−	1 *	3162 511−	1 *
3171 612	1	3172 611−	1	4151 512−	1/3*	4151 611	1/3w̲
4151 712	1/3w	4152 511	1/3 *	4152 612−	1/3w̲	4152 711	1/3w
4251 512 i	1/3 *	4251 611−i	1/3w	4251 712−i	1/3w̲	4252 511 i	1/3 *
4252 612−i	1/3w	4252 711 i	1/3w̲	4351 511−	1/3 *	4351 612−	1/3
4351 711	1/3	4352 512	1/3 *	4352 611	1/3	4352 712	1/3

Table 5c—continued

4161 511	1/3w	4161 612 −	1/3 *	4161 711	$1/3\underline{w}*$	4162 512 −	1/3w
4162 611	1/3 *	4162 712	$1/3\underline{w}*$	4261 511 i	$1/3\underline{w}$	4261 612 − i	1/3 *
4261 711 i	1/3w*	4262 512 i	$1/3\underline{w}$	4262 611 − i	1/3 *	4262 712 − i	1/3w*
4361 512 − i	1/3	4361 611 −	1/3 *	4361 712	1/3 *	4362 511	1/3
4362 612	1/3 *	4362 711	1/3 *	4171 512	$1/3\underline{w}$	4171 611 −	1/3w*
4171 712	1/3 *	4172 511	$1/3\underline{w}$	4171 612 − i	1/3w	4172 711 −	1/3 *
4271 512 i	1/3w	4271 611 i	$1/3\underline{w}*$	4271 712 − i	1/3 *	4272 511 i	1/3w
4272 612 − i	$1/3\underline{w}*$	4272 711 − i	1/3 *	4371 511 −	1/3	4371 612	1/3 *
4371 711 −	1/3 *	4372 512 −	1/3	4372 611	1/3 *	4372 712	1/3 *
5161 211	1/2	5161 413	1/2 *	5162 411 −	1/2w*	5162 412 i	$1/2\underline{w}*$
5261 411 −	1/2w*	5261 412 − i	$1/2\underline{w}*$	5262 211 −	1/2	5262 413	1/2 *
5171 411	$1/2\underline{w}*$	5171 412 − i	1/2w*	5172 311	1/2	5172 413	1/2 *
5271 311	1/2	5271 413 −	1/2 *	5272 411 −	$1/2\underline{w}*$	5272 412 − i	1/2w*
6171 111	1/2 *	6171 413 −	1/2	6172 411	1/2	6172 412 i	1/2
6272 411 −	1/2	6271 412 i	1/2	6272 111	1/2 *	6272 413	1/2

w = exp(i/3), $\underline{w}$ = exp(−i/3).

Table 6. CGC for odd bases: $\alpha_1^o \times \alpha_2^o$; $\alpha_1^o \times \alpha_2^e$; $\alpha_1^e \times \alpha_2^o$.

$\alpha_1\alpha_2$	$\alpha_1^o \otimes \alpha_2^o$	$\alpha_1^o \otimes \alpha_2^e$	$\alpha_1^e \otimes \alpha_2^o$	$\alpha_1\alpha_2$	$\alpha_1^o \otimes \alpha_2^o$	$\alpha_1^o \otimes \alpha_2^e$	$\alpha_1^e \otimes \alpha_2^o$
22	1	$\bar{1}$	$\bar{1}$	35	$4+\bar{5}*$	$\bar{4}+5*$	$\bar{4}*+5$
33	$1+2*+\bar{3}$	$1*+2+\bar{3}$	$\bar{1}*+\bar{2}+\bar{3}$	36	$8*$	$\bar{8}*$	$8*$
44	$1+\bar{3}+\bar{4}*+5$	$1+\bar{3}*+\bar{4}*+\bar{5}$	$1+3*+\bar{4}*+5$	37	$8*$	$\bar{8}*$	$8*$
55	$1+\bar{3}+\bar{4}*+5$	$1+\bar{3}*+4*+5$	$1+3*+4*+5$	38	$\bar{6}*+\bar{7}*+8$	$6*+7*+8$	$6*+7*+\bar{8}$
66	$1*+\bar{4}$	$1+\bar{4}*$	$\bar{1}+4*$	45	$2+\bar{3}*+4+5*$	$\bar{2}+3+4+5*$	$\bar{2}+\bar{3}+4+5*$
77	$1+\bar{4}$	$1+4*$	$\bar{1}+\bar{4}*$	46	$\bar{6}+8*$	$6+8*$	$\bar{6}*-\bar{8}$
88	$1*+2+3*+\ldots$	$\bar{1}+\bar{2}*+3*+\ldots$	$1+2*+3*+\ldots$	47	$7+8*$	$\bar{7}+8*$	$\bar{7}*-\bar{8}$
23	3	$\bar{3}$	$3*$	48	$\bar{6}*+\bar{7}*+\ldots$	$\bar{6}*+\bar{7}*+\ldots$	$\bar{6}*+\bar{7}*+\ldots$
24	$\bar{5}$	$\bar{5}$	5	56	$\bar{7}*+\bar{8}$	$\bar{7}*+\bar{8}$	$7+\bar{8}*$
25	$\bar{4}$	$\bar{4}$	4	57	$6*+\bar{8}$	$6*+\bar{8}$	$6+\bar{8}*$
26	7	$\bar{7}$	$7*$	58	$6+7+\ldots$	$6+7+\ldots$	$6+\bar{7}+\ldots$
27	6	$\bar{6}$	$6*$	67	$2+5*$	$2*+\bar{5}$	$\bar{2}*+\bar{5}$
28	$\bar{8}$	8	$8*$	68	$3+\bar{4}*+5$	$3+4+\bar{5}*$	$\bar{3}+4+\bar{5}*$
34	$\bar{4}*+5$	$4*+\bar{5}$	$\bar{4}+\bar{5}*$	78	$3+\bar{4}*+5$	$3+4+\bar{5}*$	$\bar{3}+4+\bar{5}*$

Table 3. Compatibility table. This table is concerned with the relation between the irreducible coreps of a given group and those of the various subgroups of the group. It indicates how the irreducible coreps of the generalised full orthogonal group $D^{j\pm}$ break up into the irreducible coreps of the cubic groups (as all magnetic point groups are subgroups of $O(3)\otimes\Theta$). The numbers correspond to the indices of the coreps; the upper index specifies the number of times the corep is contained in the decomposition of the corep of the supergroup.

Table 4a, b, c. Multiplication tables. The numbers correspond to the indices α_1, α_2, α of the coreps; the upper index specifies how many times the corep is contained in the decomposition of the corresponding direct product. The indices of the coreps contained in the symmetrised square of a corep are given in square brackets.

Table 5a, b, c. CGC for even bases: $\alpha_1^e \times \alpha_2^e$. In the tables we list all non-zero CGC but the trivial ones for the group in question. In some cases to save space we do not give those coefficients of the group which can be obtained simply by renumbering the corresponding coefficients of the supergroup. The coefficients which change sign under the substitution $\alpha_1 a_1 \leftrightarrow \alpha_2 a_2$ are marked by an asterisk. For the groups constructed by supplementing a group with the inversion I the CGC are also omitted. They are just those given for the group before we supplement with the space inversion (12). Because of typographical considerations, the square root signs are omitted, e.g. 31 32 211 $-\mathrm{i}\frac{1}{2}$ means $[31\ 32|211] = -\mathrm{i}\sqrt{\frac{1}{2}}$.

Table 6. CGC for odd bases: $\alpha_1^{\mathrm{o}} \times \alpha_2^{\mathrm{o}}$; $\alpha_1^{\mathrm{o}} \times \alpha_2^{\mathrm{e}}$; $\alpha_1^{\mathrm{e}} \times \alpha_2^{\mathrm{o}}$. As all CGC for the case $\alpha_1^{\mathrm{e}} \times \alpha_2^{\mathrm{e}}$ are given in table 5*a*, this table shows how the sign of the coefficient will change if one or both of the indices 'e' is substituted by 'o'.

The use of the table will be discussed by an example. The odd basic functions are given in table 2, where $I\Psi_m^j = -\Psi_m^j$. These groups are isomorphic to the group $\mathrm{O}\otimes\Theta$ and for even bases $\alpha_1^{\mathrm{e}} \times \alpha_2^{\mathrm{e}}$ all CGC are listed in table 5*a*. After the transition to the odd basis ($\alpha_i^{\mathrm{e}} \to \alpha_i^{\mathrm{o}}$) these coefficients are multiplied by ± 1. The conservation or change of the sign is indicated in table 6, where for example in the row '34' is written (the lower index denotes the corep multiplicity)

$\alpha_1\alpha_2$	$\alpha_1^{\mathrm{o}} \times \alpha_2^{\mathrm{o}}$	$\alpha_1^{\mathrm{o}} \times \alpha_2^{\mathrm{e}}$	$\alpha_1^{\mathrm{e}} \times \alpha_2^{\mathrm{o}}$
34	$\bar{4}^* + 5$	$4^* + \bar{5}$	$\bar{4} + \bar{5}^*$.

This means that $D^3 \boxtimes D^4 = D^4 \oplus D^5$ and for even bases all coefficients $[3^{\mathrm{e}}a_1\ 4^{\mathrm{e}}a_2|4^{\mathrm{e}}1a]$ and $[3^{\mathrm{e}}a_1 4^{\mathrm{e}}a_2|5^{\mathrm{e}}1a]$ are given in table 5*a*. The coefficients change sign after the transition

$$\alpha_1^{\mathrm{e}} \times \alpha_2^{\mathrm{e}} \to \alpha_1^{\mathrm{o}} \times \alpha_2^{\mathrm{o}}, \qquad \text{or} \qquad \alpha_1^{\mathrm{o}} \times \alpha_2^{\mathrm{e}}, \qquad \text{or} \qquad \alpha_1^{\mathrm{e}} \times \alpha_2^{\mathrm{o}},$$

if there is a line above the corep number α, and preserve the sign if the line is absent. The asterisk indicates that the coefficients change sign after the transition $\alpha_1 a_1 \leftrightarrow \alpha_2 a_2$. For example, we have

$$[32, 41|413] \equiv [3^{\mathrm{e}}2, 4^{\mathrm{e}}1|4^{\mathrm{e}}13] = \sqrt{\tfrac{3}{4}}, \qquad [32, 41|513] \equiv [3^{\mathrm{e}}2, 4^{\mathrm{e}}1|5^{\mathrm{e}}13] = -\sqrt{\tfrac{1}{4}},$$

and with the help of (14), we find

$$\begin{aligned}
[3^{\mathrm{e}}2, 4^{\mathrm{e}}1|4^{\mathrm{e}}13] &= -[3^{\mathrm{o}}2, 4^{\mathrm{o}}1|4^{\mathrm{e}}13] = +[4^{\mathrm{o}}1, 3^{\mathrm{o}}2|4^{\mathrm{e}}13] \\
&= +[3^{\mathrm{o}}2, 4^{\mathrm{e}}1|4^{\mathrm{o}}13] = -[4^{\mathrm{e}}1, 3^{\mathrm{o}}2|3^{\mathrm{o}}13] \\
&= -[3^{\mathrm{e}}2, 4^{\mathrm{o}}1|4^{\mathrm{o}}13] = -[4^{\mathrm{o}}1, 3^{\mathrm{e}}1|4^{\mathrm{o}}13] = \sqrt{\tfrac{3}{4}}, \\
[3^{\mathrm{e}}2, 4^{\mathrm{e}}1|5^{\mathrm{e}}13] &= +[3^{\mathrm{o}}2, 4^{\mathrm{o}}1|5^{\mathrm{e}}13] = +[4^{\mathrm{o}}1, 3^{\mathrm{o}}2|5^{\mathrm{e}}13] \\
&= -[3^{\mathrm{o}}2, 4^{\mathrm{e}}1|5^{\mathrm{o}}13] = -[4^{\mathrm{e}}1, 3^{\mathrm{o}}2|5^{\mathrm{o}}13] \\
&= -[3^{\mathrm{e}}2, 4^{\mathrm{o}}1|5^{\mathrm{o}}13] = +[4^{\mathrm{o}}1, 3^{\mathrm{e}}2|5^{\mathrm{o}}13] = -\sqrt{\tfrac{1}{4}}.
\end{aligned}$$

Only in the rows '88', '48' and '58' of table 6 are there dots, which mean that besides the coefficients indicated in these rows, in table 7 are given additional coefficients. They change in a more complicated way after the transition to odd bases (because of the repeated equivalent coreps in the Kronecker product).

Table 7. Additional CGC for $\mathrm{T_d}\otimes\Theta$, $\mathrm{O_h(T_d)}$. In this table are given the additional coefficients for the coreps of $\mathrm{T_d}\otimes\Theta$ and $\mathrm{O_h(T_d)}$. The asterisks indicate that the signs of the coefficients change after the replacement of the basic functions $\Psi_{a_1}^{\alpha_1}\Psi_{a_2}^{\alpha_2} \leftrightarrow \Psi_{a_2}^{\alpha_2}\Psi_{a_1}^{\alpha_1}$. Because of typographical considerations the square root signs are omitted, e.g. 81 82 522 $-\mathrm{i}\frac{1}{4}$ means $[81\ 82|522] = -\mathrm{i}\sqrt{\frac{1}{4}}$.

Table 7. Additional CGC for $T_d \otimes \Theta$, $O_h(T_d)$. (*a*) $T_d \otimes \Theta$, $O_h(T_d)$—$\alpha^o_1 \otimes \alpha^o_2$.

8181 413−	2/5	8181 423	9/40	8181 523	3/8	8182 512 i	1/4 *
8182 522−i	1/4	8183 411−	3/10	8183 421−	3/40	8183 511	1/2 *
8183 521	1/8	8184 412−	1/20	8184 422−	9/20	8282 421	5/8
8282 521	3/8	8283 412	9/20	8283 422−	1/20	8284 413−	3/10
8284 423−	3/40	8284 513	1/2 *	8284 523−	1/8	8383 423	5/8
8383 523−	3/8	8384 512−i	1/4 *	8384 522−i	1/4	8484 411−	2/5
8484 421	9/40	8484 521−	3/8	4181 814	2/3	4181 824	1/6 *
4182 821−	1/2 *	4183 812	2/3	4183 822−	1/6 *	4184 823−	1/2 *
4281 811−	1/3	4281 821	1/3 *	4282 812	1/3	4282 822	1/3 *
4283 813−	1/3	4283 823	1/3 *	4284 814	1/3	4284 824−	1/3 *
4381 822	1/2 *	4382 813−	2/3	4382 823	1/6 *	4383 824	1/2 *
4384 811−	2/3	4384 821−	1/6 *	5181 814−	2/5 *	5181 824−	1/10
5182 821	5/6	5183 812	2/5 *	5183 822−	1/10	5184 813−	8/15*
5184 823−	3/10	5281 813 i	1/15*	5281 823−i	3/5	5282 814−i	3/5 *
5282 824−i	1/15	5283 811 i	3/5*	5283 821 i	1/15	5284 812−i	1/15 *
5284 822 i	3/5	5381 812−	8/15*	5381 822−	3/10	5382 813	2/5 *
5382 823−	1/10	5383 824	5/6	5384 811−	2/5 *	5384 821	1/10

(*b*) $T_d \otimes \Theta$, $O_h(T_d)$—$\alpha^e_1 \otimes \alpha^o_2$.

8181 413	1/2 *	8181 423−	1/8	8181 513−	3/10	8181 523−	3/40
8182 512 i	9/20	8182 522−i	1/20	8183 421−	3/8	8183 521−	5/8
8184 412−	1/4 *	8184 422−	1/4	8281 512 i	1/20	8281 522 i	9/20
8282 411	1/2 *	8282 421	1/8	8282 511−	3/10	8282 521−	3/40
8283 412−	1/4 *	8283 422	1/4	8284 423−	3/8	8284 513	2/5
8284 523−	9/40	8381 421−	3/8	8381 511−	2/5	8381 521	9/40
8382 412−	1/4 *	8382 422	1/4	8383 413	1/2 *	8383 423	1/8
8383 513	3/10	8383 523	3/40	8384 512 i	1/20	8384 522 i	9/20
8481 412−	1/4 *	8481 422−	1/4	8482 423−	3/8	8482 523	5/8
8483 512 i	9/20	8483 522−i	1/20	8484 411	1/2 *	8484 421−	1/8
8484 511	3/10	8484 521	3/40	4181 814	8/15*	4181 824	3/10
4182 811−	2/5 *	4182 821	1/10	4183 822	5/6	4184 813−	2/5 *
4184 823	1/10	4281 811	1/15*	4281 821−	3/5	4282 812−	3/5 *
4282 822−	1/15	4283 813−	3/5 *	4283 823−	1/15	4284 814−	1/15*
4284 824	3/5	4381 812	2/5 *	4381 822−	1/10	4382 823−	5/6
4383 814	2/5*	4383 824−	1/10	4384 811−	8/15*	4384 821−	3/10
5181 824	1/2 *	5182 811−	2/3	5182 821	1/6 *	5183 822−	1/2 *
5184 813	2/3	5184 823	1/6 *	5281 813 i	1/3	5281 823−i	1/3 *
5282 814 i	1/3	5282 824 i	1/3 *	5283 811−i	1/3	5283 821−i	1/3 *
5284 812−i	1/3	5284 822 i	1/3 *	5381 812	2/3	5381 822	1/6 *
5382 823−	1/2 *	5383 814−	2/3	5383 824	1/6 *	5384 821	1/2 *

(*c*) $T_d \otimes \Theta$, $O_h(T_d)$—$\alpha^o_1 \otimes \alpha^e_2$.

4181 814−	2/3	4181 824	1/6	4182 821−	1/2 *	4183 812−	2/3
4183 822−	1/6 *	4184 823−	1/2 *	4281 811	1/3 *	4281 821	1/3 *
4282 812−	1/3	4282 822	1/3 *	4283 813	1/3	4283 823	1/3 *
4284 814−	1/3	4284 824−	1/3 *	4381 822	1/2 *	4382 813	2/3
4382 823	1/6 *	4383 824	1/2 *	4384 811	2/3	4384 821−	1/6 *
5181 814−	2/3 *	5181 824	1/10	5182 811−	8/15*	5182 821−	3/10
5183 812	2/5 *	5183 822−	1/10	5184 823	5/6	5281 813 i	3/5 *
5281 823 i	1/15	5282 814−i	1/15*	5282 824 i	3/5	5283 811 i	1/15*
5283 821−i	3/5	5284 812−i	3/5 *	5284 822−i	1/15	5381 822	5/6
5382 813	2/5 *	5382 823−	1/10	5383 814−	8/15*	5383 824−	3/10
5384 811−	2/5 *	5384 821	1/10				

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