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Clebsch–Gordan coefficients for the corepresentations of Shubnikov point groups: IV. Groups of hexagonal and trigonal systems

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Abstract. The Clebsch–Gordan coefficients for single- and double-valued corepresentations for even and odd basis functions of 35 anti-unitary Shubnikov (magnetic) point groups of hexagonal and trigonal systems have been calculated. Basis functions, multiplication tables and compatibility tables are also presented. A method based on the Racah lemma has been applied. The coefficients are necessary in solving problems of crystal field theory and solid state spectroscopy (selection rules, Wigner–Eckart theorem, etc).

1. Introduction

This paper is the last one of our series entitled 'Clebsch-Gordan coefficients (CGC) for the corepresentations (coreps) of Shubnikov point groups'. The series includes four papers in which we have tabulated CGC for single- and double-valued coreps for even and odd (under space inversion) bases of all 90 anti-unitary (AU) magnetic point groups (grey and black-and-white groups). We have also given basis function tables, multiplication tables and compatibility tables. This paper includes analogous tables for the coreps of all 35 AU point groups of the hexagonal and trigonal crystal systems.

The general theory, based on the generalisation of the Racah lemma (Kotzev and Aroyo 1977, 1978a), is given in the first part of the series (Kotzev and Aroyo 1980, hereafter referred to as I). CGC and the other auxiliary tables for the AU cubic groups are given in the second part (Kotzev and Aroyo 1981, hereafter referred to as II). In the third one (Kotzev and Aroyo 1982) we consider the groups of the tetragonal, orthorhombic, monoclinic and triclinic systems. The reader is referred to I and II for details of notations and definitions (see also Kotzev and Aroyo 1978b, c, d, 1979).

The coreps CGC calculation problem has a long history. The interest in the problem was caused by Koster's work on the Wigner–Eckart theorem for point groups (Koster 1958). One of the methods for the calculation of CGC for coreps (we should call it the 'traditional method' as it is analogous to the calculation method for Wigner coefficients (see Koster 1958)) is exposed in the papers of Kotzev (1972, 1974), Aviran and Litvin (1973), Rudra (1974) and van den Broek (1979). Sacata (1974) suggests a method which is conceptually quite similar to the traditional one. Using the same method Rudra and Sikdar (1976, 1977) have calculated CGC for 'b'- and 'c'-type coreps for even bases but the tables have not been published.

We should mention separately the series of papers by Dirl (1980), which is in fact a detailed and profound development of the calculation method discussed in the second

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part of Kotzev (1974). In Dirl's method CGC for the coreps of G(H) are derived from CGC for linear reps of the unitary subgroups $H \gtrsim G(H)$, using the Schur lemma (which is in fact an application of the Racah lemma). Some of the basic elements of Wigner–Racah algebra for grey groups are given in Newmarch and Golding (1981) but unfortunately these authors have not taken into account any papers in this field after 1974.

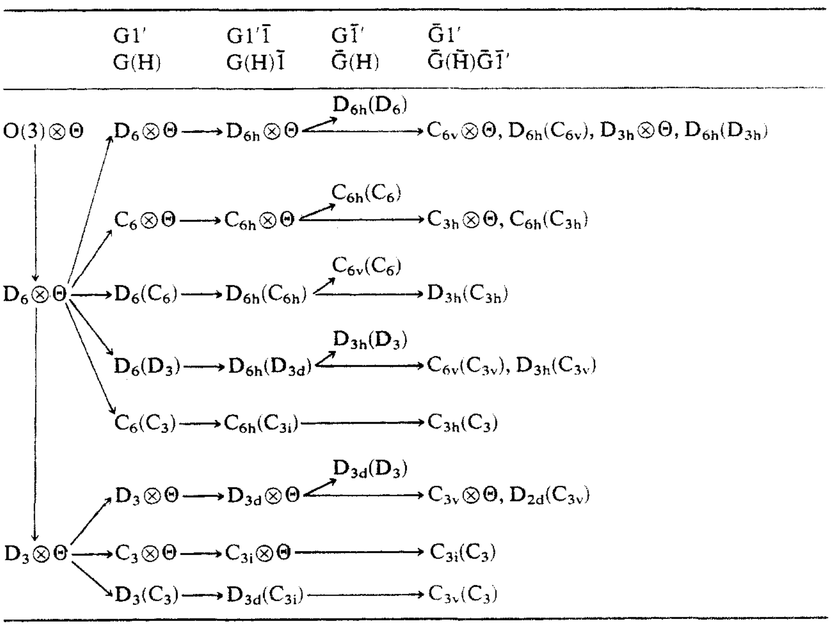
2. Calculation of the CGC

The AU double point groups from the hexagonal and trigonal systems are arranged in 8 sets (each row of table 1, see also table 1 of II). Every set contains a proper rotation group (G1′ or G(H) type in the second column of table 1), groups which contain inversion axes and planes of symmetry as AU elements only ($G\bar{1}'$ or $\bar{G}(H)$ type in the fourth column of table 1) and groups with both unitary and AU inversion axes and planes of symmetry ($\bar{G}1'$, $\bar{G}\bar{1}'$ or $\bar{G}(\bar{H})$ type in the last column of table 1). These groups are isomorphic and they do not contain the space inversion $\bar{1}$ itself. To each set of isomorphic groups is related a centrosymmetrical group ($G1'\bar{1}$ or $G(H)\bar{1}$ type in the third column of table 1). The order of the CGC calculation is shown on table 1 (follow the arrows in the table; for more details see II). The CGC for the main proper rotation groups for each system (first column of table 1) are calculated using Racah's lemma method (see I) by a successive descent down the subgroup chain

$$O(3)\otimes\Theta \supset D_6\otimes\Theta \supset D_3\otimes\Theta. \quad (1)$$

The starting coefficients are Wigner coefficients (Varshalovitch *et al* 1975) while the

Table 1. Shubnikov point groups of hexagonal and trigonal systems and calculation scheme for CGC for coreps.



starting coefficients for every set are the CGC for the corresponding proper rotation group. For such groups the choice of even or odd bases is of no significance.

For CGC of the centrosymmetrical groups, related to each isomorphic set we obtain the following relations

$$[\alpha_1 a_1 \alpha_2 a_2 | \alpha \rho_\alpha a] = [\alpha_1^{\pm} a_1 \alpha_2^{\pm} a_2 | \alpha^{+} \rho_{\alpha^+} a] = [\alpha_1^{\mp} a_1 \alpha_2^{\pm} a_2 | \alpha^{-} \rho_{\alpha^-} a] \qquad (2)$$

where $[\alpha_1 a_1 \alpha_2 a_2 | \alpha \rho_\alpha a]$ are the CGC of the corresponding proper rotation group $(\rho_\alpha = \rho_{\alpha^+} = \rho_{\alpha^-})$.

For CGC of $G\bar{1}'$ and $\bar{G}(H)$ type, we have

$$[\alpha_1^{+} a_1 \alpha_2^{+} a_2 | \alpha^{+} \rho_{\alpha^+} a] = [\alpha_1^{e} a_1 \alpha_2^{e} a_2 | \alpha^{e} \rho_{\alpha^e} a] = [\alpha_1^{e} a_1 \alpha_2^{o} a_2 | \alpha^{o} \rho_{\alpha^o} a]$$

$$= [\alpha_1^{o} a_1 \alpha_2^{e} a_2 | \alpha^{o} \rho_{\alpha^o} a] = [\alpha_1^{o} a_1 \alpha_2^{o} a_2 | \alpha^{e} \rho_{\alpha^e} a]$$

$$\rho_{\alpha^+} = \rho_{\alpha^e} = \rho_{\alpha^o} \qquad (3)$$

where $[\alpha_1^{+} a_1 \alpha_2^{+} a_2 | \alpha^{+} \rho_{\alpha^+} a]$ are the CGC for the corresponding centrosymmetrical group and the indices e and o stand for even and odd (under space inversion) basis functions, respectively.

For the groups of $\bar{G}1'$, $\bar{G}\bar{1}'$ and $\bar{G}(\bar{H})$ type, CGC for even bases coincide with those of the corresponding proper rotation group, while in the case of odd functions there exists a more complicated relation and these coefficients are given in separate tables.

So in the case of even bases it is sufficient to calculate CGC for the coreps of the proper rotation groups only. In tables 'CGC for even bases' $\alpha_1^e \times \alpha_2^e$ we list all the non-zero CGC but the trivial ones. The coefficients which change sign after the permutations $\alpha_1 a_1 \leftrightarrow \alpha_2 a_2$ are shown by an asterisk. We should mention that we consider only the permutational symmetry of the first two functions in CGC, because the symmetry becomes considerably complicated after the permutation of the third one. Similar problems and questions concerning the multiplicity problem will be discussed in a following paper. In the interest of typographical simplicity the square root signs are omitted, for example in table 5 we have

7282 311 −i1/2, which means $[7282|311] = -i\sqrt{(1/2)}$.

In the case of odd bases it is sufficient to calculate CGC for the groups of $\bar{G}1'$, $\bar{G}\bar{1}'$ and $\bar{G}(\bar{H})$ type only. For the other types of groups the relation between CGC of even and odd bases is trivial (see equations (2) and (3)). The tables 'CGC for odd bases' $\alpha_1^o \times \alpha_2^o$; $\alpha_1^o \times \alpha_2^e$; $\alpha_1^e \times \alpha_2^o$ do not show the CGC themselves but how the coefficient sign changes if one or both indices e (for even) are substituted by o (for odd). All CGC for the $\alpha_1^e \times \alpha_2^e$ case are given in an explicit form in the previous type of tables. We shall explain how to use these tables by an example. On row '57' of table 6 is written

$\alpha_1\alpha_2$	$\alpha_1^o \times \alpha_2^o$	$\alpha_1^o \times \alpha_2^e$	$\alpha_1^e \times \alpha_2^o$
57	$7+\bar{9}^*$	$\bar{7}+\bar{9}^*$	$7^*+\bar{9}$.

It means that $D_5 \otimes D_7 = D_7 \otimes D_9$. For even bases all coefficients $[5a_1\ 7a_2|71a]$ and $[5a_1\ 7a_2|91a]$ are given in table 5. These coefficients change a sign after the transition from $\alpha_1^e \times \alpha_2^e$ to $\alpha_1^o \times \alpha_2^o$, or $\alpha_1^o \times \alpha_2^e$, or $\alpha_1^e \times \alpha_2^o$ if there is a line above the corep number, and preserve the sign if the line is absent. The asterisk indicates that the coefficients change sign after the permutation $\alpha_1 a_1 \leftrightarrow \alpha_2 a_2$. In the case of repeated coreps in the product $\alpha_1 \times \alpha_2$ the subindex serves as a multiplicity index $\rho_\alpha = 1, 2, \ldots, (\alpha_1\alpha_2|\alpha)$.

Table 2. Basis functions.

$D_6\otimes\Theta$ $D_{6H}(D_6)$ $D_{3h}\otimes\Theta$ $D_{6h}(D_{3h})$ $C_{6v}\otimes\Theta$ $D_{6h}(C_{6v})$			$D_{3h}\otimes\Theta$ $D_{6h}(D_{3h})$		$C_{6v}\otimes\Theta$ $D_{6h}(C_{6v})$	
D_α	Γ_α	Φ_a^α	D_α	Ψ_a^α	D_α	Ψ_a^α
D_1	$\Gamma_1 A_1 A_1' A_1$	$\vert 00\rangle$	D_4	$\vert \bar{0}0\rangle$	D_2	$-i\vert \bar{0}0\rangle$
D_2	$\Gamma_2 A_2 A_2' A_2$	$\vert 10\rangle$	D_3	$i\vert \bar{1}0\rangle$	D_1	$i\vert \bar{1}0\rangle$
D_3	$\Gamma_3 B_1 A_1'' B_2$	$i\sqrt{(1/2)}(\vert 33\rangle-\vert 3\bar{3}\rangle)$	D_2	$\sqrt{(1/2)}(\vert \bar{3}3\rangle-\vert \bar{3}\bar{3}\rangle)$	D_4	$i\sqrt{(1/2)}(\vert \bar{3}3\rangle-\vert \bar{3}\bar{3}\rangle)$
D_4	$\Gamma_4 B_2 A_2'' B_1$	$\sqrt{(1/2)}(\vert 33\rangle+\vert 3\bar{3}\rangle)$	D_1	$\sqrt{(1/2)}(\vert \bar{3}3\rangle+\vert \bar{3}\bar{3}\rangle)$	D_3	$\sqrt{(1/2)}(\vert \bar{3}3\rangle+\vert \bar{3}\bar{3}\rangle)$
D_5	$\Gamma_5 E_1 E'' E_1$	$\vert 11\rangle$	D_6	$\vert \bar{1}\bar{1}\rangle$	D_5	$-i\vert \bar{1}1\rangle$
		$\vert 1\bar{1}\rangle$		$\vert \bar{1}1\rangle$		$i\vert \bar{1}\bar{1}\rangle$
D_6	$\Gamma_6 E_2 E' E_2$	$\vert 22\rangle$	D_5	$\vert \bar{2}\bar{2}\rangle$	D_6	$-i\vert \bar{2}2\rangle$
		$\vert 2\bar{2}\rangle$		$\vert \bar{2}2\rangle$		$i\vert \bar{2}\bar{2}\rangle$
D_7	$\Gamma_7 \bar{E}_1 \bar{E}_1 \bar{E}_1$	$\vert 1/2\ 1/2\rangle$	D_8	$-\vert \overline{1/2}\ \overline{1/2}$	D_7	$-i\vert \overline{1/2}\ 1/2\rangle$
		$\vert 1/2\ \overline{1/2}$		$\vert \overline{1/2}\ 1/2\rangle$		$i\vert \overline{1/2}\ \overline{1/2}$
D_8	$\Gamma_8 \bar{E}_2 \bar{E}_2 \bar{E}_2$	$\vert 5/2\ 5/2\rangle$	D_7	$-\vert \overline{5/2}\ \overline{5/2}$	D_8	$-i\vert \overline{5/2}\ 5/2\rangle$
		$\vert 5/2\ \overline{5/2}\rangle$		$\vert \overline{5/2}\ 5/2\rangle$		$i\vert \overline{5/2}\ \overline{5/2}\rangle$
D_9	$\Gamma_9 \bar{E}_3 \bar{E}_3 \bar{E}_3$	$\vert 3/2\ 3/2\rangle$	D_9	$\vert \overline{3/2}\ \overline{3/2}\rangle$	D_9	$-i\vert \overline{3/2}\ 3/2\rangle$
		$\vert 3/2\ \overline{3/2}\rangle$		$\vert \overline{3/2}\ 3/2\rangle$		$i\vert \overline{3/2}\ \overline{3/2}\rangle$

Table 3. Compatibility table.

$O_3\otimes\Theta$	0^+	1^+	2^+	3^+	$1/2^+$	$3/2^+$	$5/2^+$
$D_{6h}\otimes\Theta$	1^+	2^++5^+	$1^++5^++6^+$	$2^++3^++4^++5^++6^+$	7^+	7^++9^+	$7^++8^++9^+$
$D_6\otimes\Theta$	1	2+5	1+5+6	2+3+4+5+6	7	7+9	7+8+9
$D_{6h}(D_6)$	1	2+5	1+5+6	2+3+4+5+6	7	7+9	7+8+9
$D_{3h}\otimes\Theta$	1	2+5	1+5+6	2+3+4+5+6	7	7+9	7+8+9
$D_{6h}(D_{3h})$	1	2+5	1+5+6	2+3+4+5+6	7	7+9	7+8+9
$C_{6v}\otimes\Theta$	1	2+5	1+5+6	2+3+4+5+6	7	7+9	7+8+9
$D_{6h}(C_{6v})$	1	2+5	1+5+6	2+3+4+5+6	7	7+9	7+8+9
$O_3\otimes\Theta$	0^-	1^-	2^-	3^-	$1/2^-$	$3/2^-$	$5/2^-$
$D_{6h}\otimes\Theta$	1^-	2^-+5^-	$1^-+5^-+6^-$	$2^-+3^-+4^-+5^-+6^-$	7^-	7^-+9^-	$7^-+8^-+9^-$
$D_6\otimes\Theta$	1	2+5	1+5+6	2+3+4+5+6	7	7+9	7+8+9
$D_{6h}(D_6)$	1	2+5	1+5+6	2+3+4+5+6	7	7+9	7+8+9
$D_{3h}\otimes\Theta$	4	3+6	4+6+5	3+2+1+6+5	8	8+9	8+7+9
$D_{6h}(D_{3h})$	4	3+6	4+5+6	3+2+1+6+5	8	8+9	8+7+9
$C_{6v}\otimes\Theta$	2	1+5	2+5+6	1+4+3+5+6	7	7+9	7+8+9
$D_{6h}(C_{6v})$	2	1+5	2+5+6	1+4+3+5+6	7	7+9	7+8+9

Table 4. Multiplication table for $D_6 \otimes \Theta$, etc.

	1	2	3	4	5	6	7	8	9
1	[1]	2	3	4	5	6	7	8	9
2	2	[1]	4	3	5	6	7	8	9
3	3	4	[1]	2	6	5	8	7	9
4	4	3	2	[1]	6	5	8	7	9
5	5	5	6	6	[1+6]+2	3+4+5	7+9	8+9	7+8
6	6	6	5	5	3+4+5	[1+6]+2	8+9	7+9	7+8
7	7	7	8	8	7+9	8+9	[2+5]+1	3+4+6	5+6
8	8	8	7	7	8+9	7+9	3+4+6	[2+5]+1	5+6
9	9	9	9	9	7+8	7+8	5+6	5+6	[2+3+4]+1

Table 5. CGC for even bases for $D_6 \otimes \Theta$, etc.

2121	111	−1	3131	111	1	4141	111	1	5151	611	1
5152	111	1/2	5152	211	1/2*	5252	612	1	6161	612	1
6162	111	1/2	6162	211	1/2*	6262	611	1	7171	511	1
7172	111	1/2*	7172	211	1/2	7272	512	1	8181	512	1
8182	111	1/2*	8182	211	1/2	8282	511	1	9191	311	i1/2
9191	411	1/2	9192	111	1/2*	9192	211	1/2	9292	311	−i1/2
9292	411	1/2	2131	411	i*	2141	311	−i*	2151	511	−1*
2152	512	1*	2161	611	−1*	2162	612	1*	2171	711	−1*
2172	712	1*	2181	811	−1*	2182	812	1*	2191	911	−1*
2192	912	1*	3141	211	−i*	3151	612	i	3152	611	−i
3161	512	i	3162	511	−i	3171	812	−i*	3172	811	−i*
3181	712	−i*	3182	711	−i*	3191	912	−i*	3192	911	−i*
4151	612	1	4152	611	1	4161	512	1	4162	511	1
4171	812	−1*	4172	811	1*	4181	712	−1*	4182	711	1*
4191	912	−1*	4192	911	1*	5161	311	i1/2	5161	411	1/2
5162	512	1	5261	511	1	5262	311	−i1/2	5262	411	1/2
5171	911	1	5172	711	1*	5271	712	−1*	5272	912	1
5181	812	−1*	5182	912	1	5281	911	1	5282	811	1*
5191	811	1	5192	712	1	5291	711	1	5292	812	1
6171	811	1	6172	911	1*	6271	912	−1*	6272	812	1
6181	912	−1*	6182	712	1	6281	711	1	6282	911	1*
6191	812	−1*	6192	711	1*	6291	712	−1*	6292	811	1*
7181	311	i1/2	7181	411	1/2	7182	612	1*	7281	611	−1*
7282	311	−i1/2	7282	411	1/2	7191	611	1	7192	512	1*
7291	511	−1*	7292	612	1	8191	612	1	8192	511	1*
8291	512	−1*	8292	611	1						

Table 6. (*a*) CGC for odd bases for $D_{6h}(D_{3h})$ and $D_{3h}\otimes\Theta$. (*b*) CGC for odd bases for $C_{6v}\otimes\Theta$ and $D_{6h}(C_{6v})$.

(*a*) $\alpha_1\alpha_2$	$\alpha_1^o\times\alpha_2^o$	$\alpha_1^o\times\alpha_2^e$	$\alpha_1^e\times\alpha_2^o$	(*b*) $\alpha_1\alpha_2$	$\alpha_1^o\times\alpha_2^o$	$\alpha_1^o\times\alpha_2^e$	$\alpha_1^e\times\alpha_2^o$
2 2	1	$\bar{1}^*$	1^*	2 2	1	1	1
3 3	1	1^*	$\bar{1}^*$	3 3	1	$\bar{1}^*$	1^*
4 4	1	1	1	4 4	1	1^*	$\bar{1}^*$
5 5	$1+\bar{2}^*+6$	$1+\bar{2}+6$	$1+2+6$	5 5	$1+2^*+\bar{6}$	$\bar{1}^*+2+6$	$1^*+\bar{2}+6$
6 6	$1+\bar{2}^*+6$	$1+\bar{2}+6$	$1+2+6$	6 6	$1+2^*+\bar{6}$	$\bar{1}^*+2+\bar{6}$	$1^*+\bar{2}+\bar{6}$
7 7	$1^*+\bar{2}+5$	$\bar{1}+2+5^*$	$1+2+\bar{5}^*$	7 7	$1^*+2+\bar{5}$	$\bar{1}+2^*+5$	$1+\bar{2}^*+5$
8 8	$1^*+\bar{2}+5$	$\bar{1}+2+5^*$	$1+2+\bar{5}^*$	8 8	$1^*+2+\bar{5}$	$\bar{1}+2^*+\bar{5}$	$1+\bar{2}^*+\bar{5}$
9 9	$1^*+\bar{2}+\bar{3}+4$	$1+\bar{2}+3+\bar{4}^*$	$\bar{1}+\bar{2}+3+4^*$	9 9	$1^*+2+\bar{3}+\bar{4}$	$\bar{1}+2^*+3+\bar{4}$	$1+\bar{2}^*+3+\bar{4}$
2 3	$\bar{4}^*$	4	4	2 3	4	4	$\bar{4}^*$
2 4	$\bar{3}$	$\bar{3}^*$	$\bar{3}$	2 4	$\bar{3}$	$\bar{3}$	$\bar{3}^*$
2 5	$\bar{5}$	5	$\bar{5}^*$	2 5	5	$\bar{5}$	5^*
2 6	$\bar{6}$	6	$\bar{6}^*$	2 6	6	$\bar{6}$	6^*
2 7	7^*	$\bar{7}^*$	7^*	2 7	7	$\bar{7}$	7^*
2 8	8^*	8^*	$\bar{8}^*$	2 8	8	$\bar{8}$	8^*
2 9	$\bar{9}^*$	$\bar{9}^*$	$\bar{9}^*$	2 9	9	$\bar{9}$	9^*
3 4	2	$\bar{2}^*$	2	3 4	$\bar{2}^*$	2	2
3 5	$\bar{6}^*$	6^*	$\bar{6}$	3 5	6	6	$\bar{6}$
3 6	$\bar{5}^*$	5^*	$\bar{5}$	3 6	5	5	$\bar{5}$
3 7	$\bar{8}^*$	$\bar{8}^*$	$\bar{8}^*$	3 7	8^*	8^*	$\bar{8}^*$
3 8	$\bar{7}^*$	7^*	7^*	3 8	7^*	7^*	$\bar{7}^*$
3 9	9^*	9^*	$\bar{9}^*$	3 9	9^*	9^*	$\bar{9}^*$
4 5	6	6	6	4 5	$\bar{6}$	$\bar{6}$	$\bar{6}$
4 6	5	5	5	4 6	$\bar{5}$	$\bar{5}$	$\bar{5}$
4 7	8	$\bar{8}$	8^*	4 7	$\bar{8}^*$	$\bar{8}^*$	$\bar{8}^*$
4 8	7	$\bar{7}$	7^*	4 8	$\bar{7}^*$	$\bar{7}^*$	$\bar{7}^*$
4 9	$\bar{9}$	9	9^*	4 9	$\bar{9}^*$	$\bar{9}^*$	$\bar{9}^*$
5 6	$\bar{3}+4+5$	$\bar{3}^*+4+5$	3^*+4+5	5 6	$\bar{3}+\bar{4}+5$	$3+\bar{4}+\bar{5}$	$3+\bar{4}+5$
5 7	$7+\bar{9}^*$	$\bar{7}+\bar{9}^*$	$7^*+\bar{9}$	5 7	$7^*+\bar{9}$	7^*+9	$\bar{7}^*+9$
5 8	$8+\bar{9}^*$	$8+\bar{9}^*$	$\bar{8}^*+\bar{9}$	5 8	$\bar{8}^*+9$	$\bar{8}^*+\bar{9}$	$\bar{8}^*+9$
5 9	7^*+8^*	$\bar{7}^*+\bar{8}^*$	$7+8$	5 9	$7+\bar{8}$	$\bar{7}+8$	$7+8$
6 7	$\bar{8}^*+9$	$\bar{8}^*+\bar{9}$	$\bar{8}+9^*$	6 7	$\bar{8}+9^*$	$8+9^*$	$8+\bar{9}^*$
6 8	$\bar{7}^*+9$	7^*+9	$7+\bar{9}^*$	6 8	$7+\bar{9}^*$	$\bar{7}+\bar{9}^*$	$7+\bar{9}^*$
6 9	$\bar{7}+\bar{8}$	$\bar{7}+\bar{8}$	$\bar{7}^*+\bar{8}^*$	6 9	$7^*+\bar{8}^*$	$7^*+\bar{8}^*$	$\bar{7}^*+\bar{8}^*$
7 8	$\bar{3}+4+6^*$	$3+4^*+\bar{6}$	$\bar{3}+4^*+6$	7 8	$\bar{3}+\bar{4}+6^*$	$3+\bar{4}+\bar{6}^*$	$3+\bar{4}+6^*$
7 9	$5+\bar{6}$	$\bar{5}+\bar{6}$	$\bar{5}+6^*$	7 9	$5^*+\bar{6}$	$\bar{5}^*+6$	5^*+6
8 9	$5^*+\bar{6}$	$5+6^*$	$5+\bar{6}^*$	8 9	$5^*+\bar{6}$	$5^*+\bar{6}$	$\bar{5}^*+\bar{6}$

Using table 5 for the above example, we have

$$[5^e1\ 7^e1\,|\,9^e11]=1 \qquad [5^e2\ 7^e1\,|\,7^e12]=-1$$

and with the help of (4), we find

$$
\begin{aligned}
&[5^e1\ 7^e11\,|\,9^e11]\\
&\quad=-[5^o1\ 7^o1\,|\,9^e11]=[7^o1\ 5^o1\,|\,9^e11]\\
&\quad=-[5^o1\ 7^e1\,|\,9^o11]=[7^e1\ 5^o1\,|\,9^o11]\\
&\quad=-[5^e1\ 7^o1\,|\,9^o11]=-[7^o1\ 5^e1\,|\,9^o11]=1\\
&[5^e2\ 7^e1\,|\,7^e12]\\
&\quad=[5^o2\ 7^o1\,|\,7^e12]=[7^o2\ 5^o1\,|\,7^e12]\\
&\quad=-[5^o2\ 7^e1\,|\,7^o12]=-[7^e2\ 5^o1\,|\,7^o12]\\
&\quad=[5^e2\ 7^o1\,|\,7^o12]=-[7^o1\ 5^e2\,|\,7^o12]=-1.
\end{aligned}
$$

In the 'basis function tables' we give the even (under space inversion) bases for the groups in question while the odd bases are given for the groups which include inversion axes and planes of symmetry as unitary and AU elements. We also indicate the corresponding reps of the unitary subgroups (see II for details).

In the 'compatibility tables' and 'multiplication tables' the numbers correspond to the indices of the correps, the upper index specifies either the number of times $(\alpha_i\,|\,\beta_k)$ the coreps β_k is contained in the decomposition of the supergroup corep α_i (compatibility tables) or the multiplicity index $(\alpha_1\alpha_2\,|\,\alpha)$ (multiplication tables). The indices of the coreps, contained in the symmetry corep square are given in square brackets.

Table 7. Basis functions.

		$C_6\otimes\Theta$ $C_{6h}(C_6)$	$C_{3h}\otimes\Theta$ $C_{6h}(C_{3h})$		$C_{3h}\otimes\Theta$ $C_{6h}(C_{3h})$	
D_α	Γ_α			Φ_a^α	D_α	Ψ_a^α
D_1	Γ_1	A	A′	$\|00\rangle$	D_2	$\|\bar{0}0\rangle$
D_2	Γ_4	B	A″	$\sqrt{(1/2)}(\|33\rangle+\|3\bar{3}\rangle)$	D_1	$\sqrt{(1/2)}(\|\bar{3}3\rangle+\|\bar{3}\bar{3}\rangle)$
D_3	Γ_3 Γ_2	${}^1E_1$ ${}^2E_1$	${}^1E'$ ${}^2E'$	$\|22\rangle$ $\|2\bar{2}\rangle$	D_5	$\|\bar{2}\bar{2}\rangle$ $\|\bar{2}2\rangle$
D_5	Γ_5 Γ_6	${}^1E_2$ ${}^2E_2$	${}^1E''$ ${}^2E''$	$\|11\rangle$ $\|1\bar{1}\rangle$	D_3	$\|\bar{1}\bar{1}\rangle$ $\|\bar{1}1\rangle$
D_7	Γ_7 Γ_8	${}^1\bar{E}_3$ ${}^2\bar{E}_3$	${}^1\bar{E}_3$ ${}^2\bar{E}_3$	$\|1/2\ 1/2\rangle$ $\|1/2\ \overline{1/2}\rangle$	D_{11}	$-\|\overline{1/2}\ \overline{1/2}\rangle$ $\|\overline{1/2}\ 1/2\rangle$
D_9	Γ_{12} Γ_{11}	${}^2\bar{E}_1$ ${}^1\bar{E}_1$	${}^2\bar{E}_1$ ${}^1\bar{E}_1$	$\|3/2\ 3/2\rangle$ $\|3/2\ \overline{3/2}\rangle$	D_9	$\|\overline{3/2}\ \overline{3/2}\rangle$ $-\|\overline{3/2}\ 3/2\rangle$
D_{11}	Γ_{10} Γ_9	${}^1\bar{E}_2$ ${}^2\bar{E}_2$	${}^1\bar{E}_2$ ${}^2\bar{E}_2$	$\|5/2\ 5/2\rangle$ $\|5/2\ \overline{5/2}\rangle$	D_7	$-\|\overline{5/2}\ \overline{5/2}\rangle$ $\|\overline{5/2}\ 5/2\rangle$

Table 8. Compatibility table.

$D_{6h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+	9^+	1^-	2^-	3^-	4^-	5^-	6^-	7^-	8^-	9^-
$C_{6h}\otimes\Theta$	1^+	1^+	2^+	2^+	5^+	3^+	7^+	11^+	9^+	1^-	1^-	2^-	2^-	5^-	3^-	7^-	11^-	9^-
$C_6\otimes\Theta$	1	1	2	2	5	3	7	11	9	1	1	2	2	5	3	7	11	9
$C_{6h}(C_6)$	1	1	2	2	5	3	7	11	9	1	1	2	2	5	3	7	11	9
$C_{3h}\otimes\Theta$	1	1	2	2	5	3	7	11	9	2	2	1	1	3	5	11	7	9
$C_{6h}(C_{3h})$	1	1	2	2	5	3	7	11	9	2	2	1	1	3	5	11	7	9

Table 9. Multiplication table for $C_6\otimes\Theta$, etc.

	1	2	3	5	7	9	11
1	[1]	2	3	5	7	9	11
2	2	[1]	5	3	11	9	7
3	3	5	[1]+1+3	2^2+5	9+11	7+11	7+9
5	5	3	2^2+5	[1+3]+1	7+9	7+11	9+11
7	7	11	9+11	7+9	[1+5]+1	3+5	2^2+3
9	9	9	7+11	7+11	3+5	[1+2]+1+2	3+5
11	11	7	7+9	9+11	2^2+3	3+5	[1+5]+1

Table 10. CGC for even bases for $C_6\otimes\Theta$, etc.

2 121	111	1	3 131	312	1	3 132	111	1/2	3 132	121	i1/2*
3 232	311	1	5 151	311	1	5 152	111	1/2	5 152	121	i1/2*
5 252	312	1	7 171	511	1	7 172	111	1/2*	7 172	121	i1/2
7 272	512	1	9 191	211	1/2	9 191	221	i1/2	9 192	111	1/2*
9 192	121	i1/2	9 292	211	1/2	9 292	221	−i1/2	111 111	512	1
111 112	111	1/2*	111 112	121	i1/2	112 112	511	1	2 131	512	1
2 132	511	1	2 151	312	1	2 152	311	1	2 171	1112	−1*
2 172	1111	1*	2 191	912	−1	2 192	911	1	21 111	712	−1*
21 112	711	1*	3 151	211	1/2	3 151	221	i1/2	3 152	511	1
3 251	512	1	3 252	211	1/2	3 252	221	−i1/2	3 171	1111	1
3 172	911	1*	3 271	912	−1*	3 272	1112	1	3 191	1112	−1*
3 192	711	1*	3 291	712	−1*	3 292	1111	1*	31 111	912	−1*
31 112	712	1	32 111	711	1	32 112	911	1*	5 171	911	1
5 172	711	1*	5 271	712	−1*	5 272	912	1	5 191	1111	1
5 192	712	1	5 291	711	1	5 292	1112	1	51 111	1112	−1*
51 112	912	1	52 111	911	1	52 112	1111	1*	7 191	311	1
7 192	512	1*	7 291	511	−1*	7 292	312	1	71 111	211	1/2
71 111	221	i1/2	71 112	312	1*	72 111	311	−1*	72 112	211	1/2
72 112	221	−i1/2	91 111	312	1	91 112	512	1*	92 111	511	−1*
92 112	311	1									

Table 11. CGC for odd bases for $C_{3h}\otimes\Theta$ and $C_{6h}(C_{3h})$.

$\alpha_1\alpha_2$	$\alpha_1^o\times\alpha_2^o$	$\alpha_1^o\times\alpha_2^e$	$\alpha_1^e\times\alpha_2^o$
2 2	1	1	1
3 3	$1_1+\bar{1}_2^*+3$	$1_1+\bar{1}_2+3$	1_1+1_2+3
5 5	$1_1+\bar{1}_2^*+3$	$1_1+\bar{1}_2+3$	1_1+1_2+3
7 7	$1_1^*+\bar{1}_2+5$	$\bar{1}_1+1_2+5^*$	$1_1+1_2+\bar{5}^*$
9 9	$1_1^*+\bar{1}_2+2_1+\bar{2}_2$	$1_1+\bar{1}_2+\bar{2}_1^*+2_2$	$\bar{1}_1+\bar{1}_2+2_1^*+2_2$
11 11	$1_1^*+1_2+5$	$\bar{1}_1+1_2+5^*$	$1_1+1_2+\bar{5}^*$
2 3	5	5	5
2 5	3	3	3
2 7	11	$\overline{11}$	11^*
2 9	$\bar{9}$	9	9
2 11	7	$\bar{7}$	7^*
3 5	$2_1+\bar{2}_2+5$	$2_1+2_2^*+5$	$2_1+2_2^*+5$
3 7	$9+\overline{11}^*$	$9+11^*$	$\bar{9}^*+11$
3 9	$\bar{7}+\overline{11}$	$\bar{7}+\overline{11}$	$\bar{7}^*+\overline{11}^*$
3 11	$\bar{7}^*+9$	7^*+9	$7+\bar{9}^*$
5 7	$7+\bar{9}^*$	$\bar{7}+\bar{9}^*$	$7^*+\bar{9}$
5 9	7^*+11^*	$\bar{7}^*+11^*$	$7+\overline{11}$
5 11	$\bar{9}^*+11$	$\bar{9}^*+\overline{11}$	$\bar{9}+11^*$
7 9	$\bar{3}+\bar{5}^*$	$3^*+\bar{5}$	$3^*+\bar{5}$
7 11	$2_1+\bar{2}_2+3^*$	$2_1^*+\bar{2}_2+\bar{3}$	$\bar{2}_1^*+\bar{2}_2+3$
9 11	$\bar{3}+\bar{5}^*$	$\bar{3}^*+5$	$\bar{3}^*+5$

Table 12. Basis functions.

		$D_6(C_6)$ $C_{6v}(C_6)$	$D_{3h}(C_{3h})$		$D_{3h}(C_{3h})$	
D_α	Γ_α			Φ_a^α	D_α	Ψ_a^α
D_1	Γ_1	A	A′	$\|00\rangle$	D_2	$\|\bar{0}0\rangle$
D_2	Γ_4	B	A″	$\sqrt{(1/2)}(\|33\rangle+\|3\bar{3}\rangle)$	D_1	$\sqrt{(1/2)}(\|\bar{3}3\rangle+\|\bar{3}\bar{3}\rangle)$
D_3	Γ_3	$^1E_1$	$^1E'$	$\|22\rangle$	D_6	$\|\bar{2}2\rangle$
D_4	Γ_2	$^2E_1$	$^2E'$	$\|2\bar{2}\rangle$	D_5	$\|\bar{2}\bar{2}\rangle$
D_5	Γ_5	$^1E_2$	$^1E''$	$\|11\rangle$	D_4	$\|\bar{1}1\rangle$
D_6	Γ_6	$^2E_2$	$^2E''$	$\|1\bar{1}\rangle$	D_3	$\|\bar{1}\bar{1}\rangle$
D_7	Γ_7	$^1\bar{E}_3$	$^1\bar{E}_3$	$\|1/2\ 1/2\rangle$	D_{12}	$\|\overline{1/2}\ 1/2\rangle$
D_8	Γ_8	$^2\bar{E}_3$	$^2\bar{E}_3$	$\|1/2\ \overline{1/2}\rangle$	D_{11}	$-\|\overline{1/2}\ \overline{1/2}\rangle$
D_9	Γ_{12}	$^2\bar{E}_1$	$^2\bar{E}_1$	$\|3/2\ 3/2\rangle$	D_{10}	$-\|\overline{3/2}\ 3/2\rangle$
D_{10}	Γ_{11}	$^1\bar{E}_1$	$^1\bar{E}_1$	$\|3/2\ \overline{3/2}\rangle$	D_9	$\|\overline{3/2}\ \overline{3/2}\rangle$
D_{11}	Γ_{10}	$^1\bar{E}_2$	$^1\bar{E}_2$	$\|5/2\ 5/2\rangle$	D_8	$\|\overline{5/2}\ 5/2\rangle$
D_{12}	Γ_9	$^2\bar{E}_2$	$^2\bar{E}_2$	$\|5/2\ \overline{5/2}\rangle$	D_7	$-\|\overline{5/2}\ \overline{5/2}\rangle$

Table 13. Compatibility table.

$D_{6h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+	9^+
$D_{6h}(C_{6h})$	1^+	1^+	2^+	2^+	$5^+ + 6^+$	$3^+ + 4^+$	$7^+ + 8^+$	$11^+ + 12^+$	$9^+ + 10^+$
$D_6(C_6)$	1	1	2	2	5+6	3+4	7+8	11+12	9+10
$C_{6v}(C_6)$	1	1	2	2	5+6	3+4	7+8	11+12	9+10
$D_{3h}(C_{3h})$	1	1	2	2	5+6	3+4	7+8	11+12	9+10
$D_{6h}\otimes\Theta$	1^-	2^-	3^-	4^-	5^-	6^-	7^-	8^-	9^-
$D_{6h}(C_{6h})$	1^-	1^-	2^-	2^-	$5^- + 6^-$	$3^- + 4^-$	$7^- + 8^-$	$11^- + 12^-$	$9^- + 10^-$
$D_6(C_6)$	1	1	2	2	5+6	3+4	7+8	11+12	9+10
$C_{6v}(C_6)$	1	1	2	2	5+6	3+4	7+8	11+12	9+10
$D_{3h}(C_{3h})$	2	2	1	1	4+3	6+5	12+11	8+7	10+9

Table 14. Multiplication table for $D_6(C_6)$, etc.

	1	2	3	4	5	6	7	8	9	10	11	12
1	1	2	3	4	5	6	7	8	9	10	11	12
2	2	1	6	5	4	3	12	11	10	9	8	7
3	3	6	4	1	2	5	11	9	12	7	10	8
4	4	5	1	3	6	2	10	12	8	11	7	9
5	5	4	2	6	3	1	9	7	11	8	12	10
6	6	3	5	2	1	4	8	10	7	12	9	11
7	7	12	11	10	9	8	5	1	3	6	2	4
8	8	11	9	12	7	10	1	6	5	4	3	2
9	9	10	12	8	11	7	3	5	2	1	4	6
10	10	9	7	11	8	12	6	4	1	2	5	3
11	11	8	10	7	12	9	2	3	4	5	6	1
12	12	7	8	9	10	11	4	2	6	3	1	5

Table 15. CGC for even bases for $D_6(C_6)$, etc.

2 121	111	1	3 131	411	1	4 141	311	1	5 151	311	1
6 161	411	1	7 171	511	1	8 181	611	1	9 191	211	1
101 101	211	1	111 111	611	1	121 121	511	1	2 131	611	−1
2 141	511	1	2 151	411	1	2 161	311	1	2 171	1211	−1*
2 181	1111	1*	2 191	1011	−1*	21 101	911	1*	21 111	811	−1*
21 121	711	1*	3 141	111	1	3 151	211	1	3 161	511	1
3 171	1111	1	3 181	911	1*	3 191	1211	−1*	31 101	711	1*
31 111	1011	−1*	31 121	811	1	4 151	611	1	4 161	211	1
4 171	1011	−1*	4 181	1211	1	4 191	811	−1*	41 101	1111	1*
41 111	711	1	41 121	911	1*	5 161	111	1	5 171	911	1
5 181	711	1*	5 191	1111	1	51 101	811	1	51 111	1211	−1*
51 121	1011	1	6 171	811	−1*	6 181	1011	1	6 191	711	1
61 101	1211	1	61 111	911	1	61 121	1111	1*	7 181	111	1
7 191	311	1	71 101	611	1*	71 111	211	1	71 121	411	1*
8 191	511	−1*	81 101	411	1	81 111	311	−1*	81 121	211	1
91 101	111	1*	91 111	411	1	91 121	611	−1*	101 111	511	1*
101 121	311	1	111 121	111	1*						

Table 16. CGC for odd bases for $D_{3h}(C_{3h})$.

α_1	α_2	$\alpha_1^o \times \alpha_2^o$	$\alpha_1^o \times \alpha_2^e$	$\alpha_1^e \times \alpha_2^o$	α_1	α_2	$\alpha_1^o \times \alpha_2^o$	$\alpha_1^o \times \alpha_2^e$	$\alpha_1^e \times \alpha_2^o$	α_1	α_2	$\alpha_1^o \times \alpha_2^o$	$\alpha_1^o \times \alpha_2^e$	$\alpha_1^e \times \alpha_2^o$	α_1	α_2	$\alpha_1^o \times \alpha_2^o$	$\alpha_1^o \times \alpha_2^e$	$\alpha_1^e \times \alpha_2^o$
2	2	1	1	1	2	9	$\overline{10}$	10	10*	4	8	$\overline{12}$*	12*	12	6	12	11	$\overline{11}$	11*
3	3	4	4	4	2	10	$\bar{9}$	9	9*	4	9	$\bar{8}$	$\bar{8}$	$\bar{8}$*	7	8	$\bar{1}$	$\bar{1}$	1
4	4	3	3	3	2	11	8	$\bar{8}$	8*	4	10	$\overline{11}$	$\overline{11}$	$\overline{11}$*	7	9	$\bar{3}$	$\bar{3}$*	3*
5	5	3	3	3	2	12	7	$\bar{7}$	7*	4	11	$\bar{7}$*	7*	7	7	10	6*	$\bar{6}$	$\bar{6}$
6	6	4	4	4	3	4	1	1	1	4	12	9	9	$\bar{9}$*	7	11	2	2*	$\bar{2}$
7	7	5	$\bar{5}$*	5*	3	5	2	2	2	5	6	1	1	1	7	12	4*	$\bar{4}$	4*
8	8	6	$\bar{6}$*	6*	3	6	5	5	5	5	7	$\bar{9}$*	$\bar{9}$*	$\bar{9}$	8	9	5*	$\bar{5}$	$\bar{5}$
9	9	2	$\bar{2}$*	2*	3	7	$\overline{11}$*	11*	11	5	8	7	$\bar{7}$	7*	8	10	$\bar{4}$	$\bar{4}$*	4*
10	10	2	$\bar{2}$*	2*	3	8	9	9	$\bar{9}$*	5	9	11*	11*	$\overline{11}$	8	11	3*	$\bar{3}$	3
11	11	6	6*	$\bar{6}$*	3	9	$\overline{12}$	$\overline{12}$	$\overline{12}$*	5	10	8*	8*	$\bar{8}$	8	12	2	2*	$\bar{2}$*
12	12	5	5*	$\bar{5}$*	3	10	$\bar{7}$	$\bar{7}$	$\bar{7}$*	5	11	12	$\overline{12}$	12*	9	10	1*	1	$\bar{1}$
2	3	$\bar{6}$	$\bar{6}$	$\bar{6}$	3	11	10	10	$\overline{10}$*	5	12	$\overline{10}$*	$\overline{10}$*	$\overline{10}$	9	11	$\bar{4}$	4*	$\bar{4}$*
2	4	5	5	5	3	12	$\bar{8}$*	8*	8	6	7	8	$\bar{8}$	8*	9	12	$\bar{6}$*	6	6
2	5	4	4	4	4	5	6	6	6	6	8	$\overline{10}$*	$\overline{10}$*	$\overline{10}$	10	11	5*	$\bar{5}$	$\bar{5}$
2	6	3	3	$\bar{3}$	4	6	2	2	2	6	9	7*	7*	$\bar{7}$	10	12	$\bar{3}$	3*	$\bar{3}$*
2	7	12	$\overline{12}$	12*	4	7	10	10	$\overline{10}$*	6	10	12*	12*	$\overline{12}$	11	12	1*	$\bar{1}$	1
2	8	11	$\overline{11}$	11*						6	11	$\bar{9}$*	$\bar{9}$*	$\bar{9}$					

Table 17. Basis functions.

	$D_6(D_3)$ $D_{3h}(D_3)$ $C_{6v}(C_{3v})$ $D_{3h}(C_{3v})$		$C_{6v}(C_{3v})$ $D_{3h}(C_{3v})$	
D_α	Γ_α	Φ_a^α	D_α	Ψ_a^α
D_1	$\Gamma_1 = A_1$	$\|00\rangle$	D_2	$-i\|\bar{0}0\rangle$
D_2	$\Gamma_2 = A_2$	$\|10\rangle$	D_1	$i\|\bar{1}0\rangle$
D_3	$\Gamma_3 = E$	$\|11\rangle$	D_3	$-i\|\bar{1}1\rangle$
		$\|1\bar{1}\rangle$		$i\|\bar{1}\bar{1}\rangle$
D_4	$\Gamma_4 = \bar{E}_1$	$\|1/2\ 1/2\rangle$	D_4	$-i\|\overline{1/2}\ 1/2\rangle$
		$\|1/2\ \overline{1/2}\rangle$		$i\|\overline{1/2}\ \overline{1/2}\rangle$·
D_5	Γ_5	$\sqrt{(1/2)}(i\|3/2\ 3/2\rangle + \|3/2\ \overline{3/2}\rangle)$	D_6	$\sqrt{(1/2)}(i\|\overline{3/2}\ 3/2\rangle - \|\overline{3/2}\ \overline{3/2}\rangle)$
D_6	Γ_6	$\sqrt{(1/2)}(-\|3/2\ 3/2\rangle + i\|3/2\ \overline{3/2}\rangle)$	D_5	$-\sqrt{(1/2)}(\|\overline{3/2}\ 3/2\rangle - i\|\overline{3/2}\ \overline{3/2}\rangle)$

Table 18. Compatibility table.

$D_{6h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+	9^+	1^-	2^-	3^-	4^-	5^-	6^-	7^-	8^-	9^-
$D_{6h}(D_{3d})$	1^+	2^+	1^+	2^+	3^+	3^+	4^+	4^+	$5^+ + 6^+$	1^-	2^-	1^-	2^-	3^-	3^-	4^-	4^-	$5^- + 6^-$
$D_6(D_3)$	1	2	1	2	3	3	4	4	5+6	1	2	1	2	3	3	4	4	5+6
$D_{3h}(D_3)$	1	2	1	2	3	3	4	4	5+6	1	2	1	2	3	3	4	4	5+6
$C_{6v}(C_{3v})$	1	2	1	2	3	3	4	4	5+6	2	1	2	1	3	3	4	4	6+5
$D_{3h}(C_{3v})$	1	2	1	2	3	3	4	4	5+6	2	1	2	1	3	3	4	4	6+5

Table 19. Multiplication table for $D_6(D_3)$, etc.

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

Table 20. CGC for even bases for $D_6(D_3)$, etc.

2121	111	−1	3131	312	1*	3132	111	1/2	3132	211	1/2*
3232	311	−1*	4141	311	1	4142	111	1/2*	4142	211	1/2
4242	312	1	5151	211	i	6161	211	i	2131	311	−1*
2132	312	1*	2141	411	−1*	2142	412	1*	2151	611	i*
2161	511	−i*	3141	511	−i1/2	3141	611	−1/2	3142	411	1*
3241	412	−1*	3242	511	1/2	3242	611	i1/2	3151	412	1
3251	411	i	3161	412	−i	3261	411	−1	4151	312	1*
4251	311	−i*	4161	312	−i*	4261	311	1*	5161	111	1*

Table 21. CGC for odd bases for $C_{6v}(C_{3v})$ and $D_{3h}(C_{3v})$.

$\alpha_1\alpha_2$	$\alpha_1^o\times\alpha_2^o$	$\alpha_1^o\times\alpha_2^e$	$\alpha_1^e\times\alpha_2^o$	$\alpha_1\alpha_2$	$\alpha_1^o\times\alpha_2^o$	$\alpha_1^o\times\alpha_2^e$	$\alpha_1^e\times\alpha_2^o$
2 2	1	1	1	2 6	5	$\bar{5}$	5^*
3 3	$1+2^*+\bar{3}^*$	$\bar{1}^*+2+\bar{3}^*$	$1^*+\bar{2}+\bar{3}^*$	3 4	$4^*+\bar{5}+\bar{6}$	4^*+5+6	$\bar{4}^*+5+6$
4 4	$1^*+2+\bar{3}$	$\bar{1}+2^*+3$	$1+\bar{2}^*+3$	3 5	4	$\bar{4}$	4
5 5	2	2^*	$\bar{2}^*$	3 6	4	$\bar{4}$	4
6 6	2	2^*	$\bar{2}^*$	4 5	3^*	$\bar{3}^*$	3^*
2 3	3	$\bar{3}$	3^*	4 6	3^*	$\bar{3}^*$	3^*
2 4	4	$\bar{4}$	4^*	5 6	1^*	$\bar{1}$	1
2 5	6	$\bar{6}$	6^*				

Table 22. Basis functions.

	$C_6(C_3)$ $C_{3h}(C_3)$	
D_α	Γ_α	Φ_a^α
D_1	$\Gamma_1=A$	$\|00\rangle$
D_2	$\Gamma_2={}^1E$	$\|11\rangle$
	$\Gamma_3={}^2E$	$\|1\bar{1}\rangle$
D_4	$\Gamma_4={}^1\bar{E}$	$\|1/2\ 1/2\rangle$
	$\Gamma_5={}^2\bar{E}$	$\|1/2\ \overline{1/2}\rangle$
D_6	$\Gamma_6=\bar{A}$	$\sqrt{(1/2)}(\|3/2\ 3/2\rangle+\|3/2\ \overline{3/2}\rangle)$

Table 23. Compatibility table.

$D_{6h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+	9^+	1^-	2^-	3^-	4^-	5^-	6^-	7^-	8^-	9^-
$C_{6h}(C_{3i})$	1^+	1^+	1^+	1^+	2^+	2^+	4^+	4^+	6^{2+}	1^-	1^-	1^-	1^-	2^-	2^-	4^-	4^-	6^{2-}
$C_6(C_3)$	1	1	1	1	2	2	4	4	6^2	1	1	1	1	2	2	4	4	6^2
$C_{3h}(C_3)$	1	1	1	1	2	2	4	4	6^2	1	1	1	1	2	2	4	4	6^2

Table 24. Multiplication table for $C_6(C_3)$, etc.

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

Table 25. CGC for even bases for $C_6(C_3)$, etc.

2121	212	1*	2122	111	1/2	2122	121	1/2*	2222	211	−1*
4141	211	1	4142	111	1/2*	4142	121	1/2	4242	212	1
6161	111	1	2141	611	1/2	2141	621	i1/2	2142	411	1*
2241	412	−1*	2242	611	1/2	2242	621	−i1/2	2161	412	1
2261	411	1	4161	212	1*	4261	211	−1*			

Table 26. Basis functions.

	$D_3\otimes\Theta$ $D_{3d}(D_3)$ $C_{3v}\otimes\Theta$ $D_{3d}(C_{3v})$		$C_{3v}\otimes\Theta$ $D_{3d}(C_{3v})$	
D_α	Γ_α	Φ_a^α	D_α	Ψ_a^α
D_1	$\Gamma_1=A_1$	$\lvert 00\rangle$	D_2	$-i\lvert\bar{0}0\rangle$
D_2	$\Gamma_2=A_2$	$\lvert 10\rangle$	D_1	$i\lvert\bar{1}0\rangle$
D_3	$\Gamma_3=E$	$\lvert 11\rangle$ $\lvert 1\bar{1}\rangle$	D_3	$-i\lvert\bar{1}1\rangle$ $i\lvert\bar{1}\bar{1}\rangle$
D_4	$\Gamma_4=\bar{E}_1$	$\lvert 1/2\ 1/2\rangle$ $\lvert 1/2\ \overline{1/2}\rangle$	D_4	$-i\lvert\overline{1/2}\ 1/2\rangle$ $i\lvert\overline{1/2}\ \overline{1/2}\rangle$
D_5	$\begin{cases}\Gamma_5={}^1\bar{E}\\ \Gamma_6={}^2\bar{E}\end{cases}$	$\lvert 3/2\ 3/2\rangle$ $\lvert 3/2\ \overline{3/2}\rangle$	D_5	$-i\lvert\overline{3/2}\ 3/2\rangle$ $i\lvert\overline{3/2}\ \overline{3/2}\rangle$

Table 27. Compatibility table.

$D_{6h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+	9^+	1^-	2^-	3^-	4^-	5^-	6^-	7^-	8^-	9^-
$D_{3d}\otimes\Theta$	1^+	2^+	2^+	1^+	3^+	3^+	4^+	4^+	5^+	1^-	2^-	2^-	1^-	3^-	3^-	4^-	4^-	5^-
$D_3\otimes\Theta$	1	2	2	1	3	3	4	4	5	1	2	2	1	3	3	4	4	5
$D_{3d}(D_3)$	1	2	2	1	3	3	4	4	5	1	2	2	1	3	3	4	4	5
$C_{3v}\otimes\Theta$	1	2	2	1	3	3	4	4	5	2	1	1	2	3	3	4	4	5
$D_{3d}(C_{3v})$	1	2	2	1	3	3	4	4	5	2	1	1	2	3	3	4	4	5

Table 28. Multiplication table for $D_3\otimes\Theta$, etc.

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

Table 29. CGC for even bases for $D_3 \otimes \Theta$, etc.

2121	111	−1	3131	312	1	3132	111	1/2	3132	211	1/2*
3232	311	1	4141	311	1	4142	111	1/2*	4142	211	1/2
4242	312	1	5151	121	1/2	5151	221	−1/2	5152	111	1/2*
5152	211	1/2	5252	121	1/2	5252	221	1/2	2131	311	−1*
2132	312	1*	2141	411	−1*	2142	412	1*	2151	511	−1*
2152	512	1*	3141	511	1	3142	411	1*	3241	412	−1*
3242	512	1	3151	422	−1	3152	412	1	3251	411	1
3252	421	1	4151	322	1	4152	312	1*	4251	311	−1*
4252	321	1									

Table 30. CGC for odd bases for $C_{3v} \otimes \Theta$ and $D_{3d}(C_{3v})$.

$\alpha_1\alpha_2$	$\alpha_1^o \times \alpha_2^o$	$\alpha_1^o \times \alpha_2^e$	$\alpha_1^e \times \alpha_2^o$	$\alpha_1\alpha_2$	$\alpha_1^o \times \alpha_2^o$	$\alpha_1^o \times \alpha_2^e$	$\alpha_1^e \times \alpha_2^o$
2 2	1	1	1	2 4	4	$\bar{4}$	4^*
3 3	$1+2^*+\bar{3}$	$\bar{1}^*+2+\bar{3}$	$1^*+\bar{2}+\bar{3}$	2 5	5	$\bar{5}$	5^*
4 4	$1^*+2+\bar{3}$	$\bar{1}+2^*+3$	$1+\bar{2}^*+3$	3 4	$4^*+\bar{5}$	4^*+5	$\bar{4}^*+5$
5 5	$1_1^*+\bar{1}_2$ $+2_1+\bar{2}_2$	$\bar{1}_1+1_2$ $+2_1^*+\bar{2}_2$	1_1+1_2 $+\bar{2}_1^*+\bar{2}_2$	3 5	$4_1+\bar{4}_2$	$\bar{4}_1+4_2$	4_1+4_2
2 3	3	$\bar{3}$	3^*	4 5	$3_1^*+\bar{3}_2$	$\bar{3}_1+\bar{3}_2$	$3_1^*+\bar{3}_2$

Table 31. Basis functions.

	$C_3 \otimes \Theta$ $C_{3i}(C_3)$	
D_1	$\Gamma_1 = A_1$	$\|00\rangle$
D_2	$\Gamma_2 = {}^2E$	$\|11\rangle$
	$\Gamma_3 = {}^1E$	$\|1\bar{1}\rangle$
D_4	$\Gamma_4 = {}^1\bar{E}$	$\|1/2\ 1/2\rangle$
	$\Gamma_5 = {}^2\bar{E}$	$\|1/2\ \overline{1/2}\rangle$
D_6	$\Gamma_6 = \bar{A}$	$\|3/2\ 3/2\rangle$
	$\Gamma_6 = \bar{A}$	$\|3/2\ \overline{3/2}\rangle$

Table 32. Compatibility table.

$D_{6h} \otimes \Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+	9^+	1^-	2^-	3^-	4^-	5^-	6^-	7^-	8^-	9^-
$C_{3i} \otimes \Theta$	1^+	1^+	1^+	1^+	2^+	2^+	4^+	4^+	6^+	1^-	1^-	1^-	1^-	2^-	2^-	4^-	4^-	6^-
$C_3 \otimes \Theta$	1	1	1	1	2	2	4	4	6	1	1	1	1	2	2	4	4	6
$C_{3i}(C_3)$	1	1	1	1	2	2	4	4	6	1	1	1	1	2	2	4	4	6

Table 33. Multiplication table for $C_3 \otimes \Theta$, etc.

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

Table 34. CGC for even bases for $C_3 \otimes \Theta$, etc.

2121	212	1	2122	111	1/2	2122	121	i1/2*	2222	211	1
4141	211	1	4142	111	1/2	4142	121	i1/2*	4242	212	1
6161	131	−i1/2	6161	141	1/2	6162	111	1/2*	6162	121	i1/2
6262	131	i1/2	6262	141	1/2	2141	611	1	2142	411	1*
2241	412	−1*	2242	612	1	2161	422	−1	2162	412	1
2261	411	1	2262	421	1	4161	222	1	4162	212	1*
4261	211	−1*	4262	221	1						

Table 35. Basis functions.

	$C_{3v}(C_3)$ $D_3(C_3)$	
D_α	Γ_α	Φ_α
D_1	$\Gamma_1 = A_1$	$\|00\rangle$
D_2	$\Gamma_2 = {}^2E$	$\|11\rangle$
D_3	$\Gamma_3 = {}^1E$	$\|1\bar{1}\rangle$
D_4	$\Gamma_4 = {}^1\bar{E}$	$\|1/2\ 1/2\rangle$
D_5	$\Gamma_5 = {}^2\bar{E}$	$\|1/2\ \overline{1/2}\rangle$
D_6	$\Gamma_6 = \bar{A}$	$\|3/2\ 3/2\rangle$

Table 36. Compatibility table.

$D_{6h} \otimes \Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+	9^+
$D_{3d}(C_{3i})$	1^+	1^+	1^+	1^+	$2^+ + 3^+$	$2^+ + 3^+$	$4^+ + 5^+$	$4^+ + 5^+$	6^{2+}
$D_3(C_3)$	1	1	1	1	2+3	2+3	4+5	4+5	6^2
$C_{3v}(C_3)$	1	1	1	1	2+3	2+3	4+5	4+5	6^2
$D_{6h} \otimes \Theta$	1^-	2^-	3^-	4^-	5^-	6^-	7^-	8^-	9^-
$D_{3d}(C_{3i})$	1^-	1^-	1^-	1^-	$2^- + 3^-$	$2^- + 3^-$	$4^- + 5^-$	$4^- + 5^-$	6^{2-}
$D_3(C_3)$	1	1	1	1	2+3	2+3	4+5	4+5	6^2
$C_{3v}(C_3)$	1	1	1	1	2+3	2+3	4+5	4+5	6^2

Table 37. Multiplication table for $C_{3v}(C_3)$, etc.

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

Table 38. CGC for even bases for $C_{3v}(C_3)$, etc.

2121	311	1	3131	211	1	4141	211	1	5151	311	1
6161	111	1	2131	111	1	2141	611	1	2151	411	1*
2161	511	−1	3141	511	−1*	3151	611	1	3161	411	1
4151	111	1*	4161	311	1*	5161	211	−1*			

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