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Clebsch–Gordan coefficients for the corepresentations of Shubnikov point groups: III. Groups of tetragonal, orthorhombic, monoclinic and triclinic crystal systems

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Abstract. The Clebsch–Gordan coefficients for single- and double-valued corepresentations for even and odd bases of 44 anti-unitary Shubnikov (magnetic) point groups of tetragonal, orthorhombic, monoclinic and triclinic (crystal) systems have been calculated. Basis functions, multiplication tables and compatibility tables are presented. A method based on the Racah lemma has been applied. The coefficients can be applied in crystal field theory and solid state spectroscopy (selection rules, Wigner–Eckart theorem, etc).

1. Introduction

The Clebsch–Gordan coefficients (CGC) for the corepresentations (coreps) of anti-unitary (AU) groups are introduced for the first time by Kotzev (1972, 1974). The CGC for coreps are also discussed in papers by Aviran and Litvin (1973), Rudra (1974), Sacata (1974), van den Broek (1979) and Dirl (1980), whose results are in a good agreement with those of Kotzev (1972). Some basic elements of Racah algebra for the coreps of the grey AU groups are discussed in the recent paper of Newmarch and Golding (1981). (A historical review can be found in Rudra and Sikdar (1976); see also Kotzev and Aroyo (1980), hereafter referred to as I.) A more effective method for the calculation of the CGC for coreps based on the generalised Racah lemma is suggested in Kotzev and Aroyo (1977, 1980). Using this method we have calculated the CGC for all 90 AU point groups (Kotzev and Aroyo 1978a, b, c); for cubic groups see Kotzev and Aroyo (1981), hereafter referred to as II. The reader is referred to I and II for notations and definitions.

In this paper the CGC for AU double point groups of the tetragonal, orthorhombic, monoclinic and triclinic systems are obtained using the method in I and II. The CGC are calculated both for even and odd basis functions for more convenient application. We should mention that in a number of papers (Balevičius *et al* 1963, Balevičius and Bolotin 1964, Lulek 1979, Butler and Reid 1979, Prasad and Bharathi 1980, Tang Au-chin *et al* 1979) properties of the CGC for some point groups of these systems are discussed. In these papers the time reversal symmetry of the basis functions for the representations is taken into account and the CGC which are obtained can be considered to a certain extent as CGC for the coreps of the grey Shubnikov point groups. In Rudra and Sikdar (1976, 1977) there are reports about the calculation of the CGC for AU point groups but only for even under space inversion basis functions and the tables are not contained in their papers.

2. Calculation of the CGC

The 44 AU double point groups of the tetragonal, orthorhombic, monoclinic and triclinic systems are arranged in 10 sets (each row of table 1, see also table 1 of II). Every set contains a proper rotation group ($G1'$ 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 are calculated using the Racah lemma method (see I) by a successive descent down the subgroup chain

$$O\otimes\Theta \supset D_4\otimes\Theta \supset D_2\otimes\Theta \supset C_2\otimes\Theta \supset C_1\otimes\Theta. \qquad (1)$$

So the starting coefficients are the CGC for the cubic groups (tabulated in II) while the 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 the CGC of the centrosymmetrical groups, related to each isomorphic set (third column of table 1) we get the following relations

Table 1. Shubnikov point groups of tetragonal, orthorhombic, monoclinic and triclinic systems and scheme of the calculation of the CGC for the coreps.

$O_h\otimes\Theta$	$D_4\otimes\Theta \longrightarrow$	$D_{4h}\otimes\Theta \longrightarrow$	$D_{4h}(D_4)$	$C_{4v}\otimes\Theta$, $D_{4h}(C_{4v})$, $D_{2d}\otimes\Theta$, $D_{4h}(D_{2d})$
	$C_4\otimes\Theta \longrightarrow$	$C_{4h}\otimes\Theta \longrightarrow$	$C_{4h}(C_4)$	$S_4\otimes\Theta$, $C_{4h}(S_4)$
$D_4\otimes\Theta \longrightarrow$	$D_4(C_4) \longrightarrow$	$D_{4h}(C_{4h}) \longrightarrow$	$C_{4v}(C_4)$	$D_{2d}(S_4)$
	$D_4(D_2) \longrightarrow$	$D_{4h}(D_{2h}) \longrightarrow$	$D_{2d}(D_2)$	$C_{4v}(C_{2v})$, $D_{2d}(C_{2v})$
	$C_4(C_2) \longrightarrow$	$C_{4h}(C_{2h}) \longrightarrow$		$S_4(C_2)$
	$D_2\otimes\Theta \longrightarrow$	$D_{2h}\otimes\Theta \longrightarrow$	$D_{2h}(D_2)$	$C_{2v}\otimes\Theta$, $D_{2h}(C_{2v})$
$D_2\otimes\Theta$	$D_2(C_2) \longrightarrow$	$D_{2h}(C_{2h}) \longrightarrow$	$C_{2v}(C_2)$	$C_{2v}(C_s)$
	$C_2\otimes\Theta \longrightarrow$	$C_{2h}\otimes\Theta \longrightarrow$	$C_{2h}(C_2)$	$C_s\otimes\Theta$, $C_{2h}(C_s)$
$C_2\otimes\Theta$	$C_2(C_1) \longrightarrow$	$C_{2h}(C_i) \longrightarrow$		$C_s(C_1)$
$C_1\otimes\Theta \longrightarrow$	$C_1\otimes\Theta \longrightarrow$	$C_i\otimes\Theta \longrightarrow$		$C_i(C_1)$

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

where $[\alpha_1 a_1 \alpha_2 a_2 | \alpha \rho_\alpha a]$ are the CGC of the corresponding proper rotation group.

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

$$[\alpha_1^{+} a_1 \alpha_2^{+} a_2 | \alpha^{+} \rho_{\alpha^+} a] = [\alpha_1^{e} a_1 \alpha_2^{e} a_2 | \alpha^{e} \rho_{\alpha^e} a] = [\alpha_1^{e} a_1 \alpha_2^{o} a_2 | \alpha^{o} \rho_{\alpha^o} a]$$
$$= [\alpha_1^{o} a_1 \alpha_2^{o} \alpha_2 | \alpha^{e} \rho_{\alpha^e} a] = [\alpha_1^{o} a_1 \alpha_2^{e} a_2 | \alpha^{o} \rho_{\alpha^o} a] \qquad (3)$$

where $[\alpha_1^{+} a_1 \alpha_2^{+} a_2 | \alpha^{+} \rho_{\alpha^+} a]$ are the CGC for the corresponding centrosymmetric group and the indices e and o stand for even and odd choice of basis functions, respectively, for the coreps of $G\bar{1}'$ (or $\bar{G}(H)$) type.

For the groups of $\bar{G}1'$ (or $\bar{G}\bar{1}'$, $\bar{G}(\bar{H})$) type the CGC for even bases coincide with those of the corresponding proper rotation group. However 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 enough to calculate the 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 non-zero CGC but the trivial ones. The coefficients which change a sign under the permutations $\alpha_1 a_1 \leftrightarrow \alpha_2 a_2$ are shown by an asterisk. For typographical reasons the square root signs are omitted. For example, in table 5, we have

$$5252\ 411 - i1/2, \text{ which means } [5252|411] = -i\surd(1/2).$$

In the case of odd bases it is sufficient to calculate the CGC for the groups of $\bar{G}1'$ (or $\bar{G}\bar{1}'$, $\bar{G}(\bar{H})$) only. For the other types of groups the relation between the CGC of even and odd bases is trivial (see equations (2) and (3)). The tables 'CGC for odd bases' $\alpha_1^{o} \times \alpha_2^{o}$; $\alpha_1^{o} \times \alpha_2^{e}$; $\alpha_1^{e} \times \alpha_2^{o}$ show not the CGC themselves but how the coefficient sign will change if one or both indices e (for even) are substituted by o (for odd) (all CGC for '$\alpha_1^{e} \times \alpha_2^{e}$ case' are given in an explicit form in the previous type of tables). We will explain the table by an example. On row '25' of table 16 is written

$$\begin{array}{cccc} \alpha_1\alpha_2 & \alpha_1^{o} \times \alpha_2^{o} & \alpha_1^{o} \times \alpha_2^{e} & \alpha_1^{e} \times \alpha_2^{o} \\ 2\,5 & \bar{5}_1^{*} + 5_2 & 5_1^{*} + 5_2 & \bar{5}_1^{*} + \bar{5}_2. \end{array} \qquad (4)$$

It means that $D_2 \times D_5 = D_5 \oplus D_5$. For even bases all CGC $[2^e a_1\, 5^e a_2 | 5^e 1 a]$ and $[2^e a_1\, 5^e a_2 | 5^e\, 2a]$ are given in table 15. These CGC change sign after the transition from $\alpha_1^{e} \times \alpha_2^{e}$ to $\alpha_1^{o} \times \alpha_2^{e}$ or $\alpha_1^{e} \times \alpha_2^{o}$ or $\alpha_1^{o} \times \alpha_2^{o}$ if there is a line above the corep number α and preserve the sign if the line is omitted. The asterisk indicates that the CGC change a sign after the transition $\alpha_1 a_1 \alpha_2 a_2 \to \alpha_2 a_2 \alpha_1 a_1$. (In the case of repeated coreps in $\alpha_1 \times \alpha_2$, the subindex is $\rho_\alpha = 1, 2, \ldots, (\alpha_1 \alpha_2 | \alpha)$.) For the above example we have from table 15

$$[2^e 1\ 5^e 1 | 5^e 22] = -1 \qquad [2^e 1\ 5^e 2 | 5^e 11] = 1$$

and with the help of (4), we find

$$\begin{aligned} [2^e 1\ 5^e 1 | 5^e 22] &= [2^o 1\ 5^o 1 | 5^e 22] = [5^o 1\ 2^o 1 | 5^e 22] \\ &= [2^o 1\ 5^e 1 | 5^o 22] = [5^e 1\ 2^o 1 | 5^o 22] \\ &= -[2^e 1\ 5^o 1 | 5^o 22] = -[5^o 1\ 2^e 1 | 5^o 22] = -1 \\ [2^e 1\ 5^e 2 | 5^e 11] &= -[2^o 1\ 5^o 2 | 5^e 11] = [5^o 2\ 2^o 1 | 5^e 11] \\ &= -[2^o 1\ 5^e 2 | 5^o 11] = [5^e 2\ 2^o 1 | 5^o 11] \\ &= -[2^e 1\ 5^o 2 | 5^o 11] = [5^o 2\ 2^e 1 | 5^o 11] = 1. \end{aligned}$$

In the basis function tables we give the even 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 include 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 coreps, the upper index specifies either the number of times $(\alpha_i\,|\,\beta_k)$ the corep 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 2. Basis functions.

$D_4\otimes\Theta$ $D_{4h}(D_4)$ $C_{4v}\otimes\Theta$ $D_{4h}(C_{4v})$ $D_{2d}\otimes\Theta$ $D_{4h}(D_{2d})$			$C_{4v}\otimes\Theta$ $D_{4h}(C_{4v})$		$D_{2d}\otimes\Theta$ $D_{4h}(D_{2d})$	
D_α	Γ_α	Φ_a^α	D_α	Ψ_a^α	D_α	Ψ_a^α
D_1	$\Gamma_1=A_1$	$\|00\rangle$	D_2	$-i\|\bar{0}0\rangle$	D_3	$\|\bar{0}0\rangle$
D_2	$\Gamma_2=A_2$	$\|10\rangle$	D_1	$i\|\bar{1}0\rangle$	D_4	$i\|\bar{1}0\rangle$
D_3	$\Gamma_3=B_1$	$\sqrt{(1/2)}(\|22\rangle+\|2\bar{2}\rangle)$	D_4	$\sqrt{(1/2)}(\|\bar{2}2\rangle+\|\bar{2}\bar{2}\rangle)$	D_1	$-\sqrt{(1/2)}(\|\bar{2}2\rangle+\bar{2}\bar{2}\rangle)$
D_4	$\Gamma_4=B_2$	$i\sqrt{(1/2)}(\|22\rangle-\|2\bar{2}\rangle)$	D_3	$i\sqrt{(1/2)}(\|\bar{2}2-\|2\bar{2}\rangle)$	D_2	$\sqrt{(1/2)}(\|\bar{2}2\rangle-\|\bar{2}\bar{2}\rangle)$
D_5	$\Gamma_5=E$	$\|11\rangle$ $\|1\bar{1}\rangle$	D_5	$-i\|\bar{1}1\rangle$ $i\|\bar{1}\bar{1}\rangle$	D_5	$\|\bar{1}\bar{1}\rangle$ $\|\bar{1}1\rangle$
D_6	$\Gamma_6=\bar{E}_1$	$\|1/2\ 1/2\rangle$ $\|1/2\ \overline{1/2}\rangle$	D_6	$i\|\overline{1/2}\ 1/2\rangle$ $-i\|\overline{1/2}\ \overline{1/2}\rangle$	D_7	$\|\overline{1/2}\ \overline{1/2}\rangle$ $-\|\overline{1/2}\ 1/2\rangle$
D_7	$\Gamma_7=\bar{E}_2$	$\|3/2\ 3/2\rangle$ $\|3/2\ 3/2\rangle$	D_7	$-i\|\overline{3/2}\ 3/2\rangle$ $i\|\overline{3/2}\ \overline{3/2}\rangle$	D_6	$\|\overline{3/2}\ \overline{3/2}\rangle$ $-\|\overline{3/2}\ \overline{3/2}\rangle$

Table 3. Compatibility table.

$O_h\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+
$D_{4h}\otimes\Theta$	1^+	3^+	1^++3^+	2^++5^+	4^++5^+	6^+	7^+	6^++7^+
$D_4\otimes\Theta$	1	3	1+3	2+5	4+5	6	7	6+7
$D_{4h}(D_4)$	1	3	1+3	2+5	4+5	6	7	6+7
$C_{4v}\otimes\Theta$	1	3	1+3	2+5	4+5	6	7	6+7
$D_{4h}(C_{4v})$	1	3	1+3	2+5	4+5	6	7	6+7
$D_{2d}\otimes\Theta$	1	3	1+3	2+5	4+5	6	7	6+7
$D_{4h}(D_{2d})$	1	3	1+3	2+5	4+5	6	7	6+7
$O_h\otimes\Theta$	1^-	2^-	3^-	4^-	5^-	6^-	7^-	8^-
$D_{4h}\otimes\Theta$	1^-	3^-	1^-+3^-	2^-+5^-	4^-+5^-	6^-	7^-	6^-+7^-
$D_4\otimes\Theta$	1	3	1+3	2+5	4+5	6	7	6+7
$D_{4h}(D_4)$	1	3	1+3	2+5	4+5	6	7	6+7
$C_{4v}\otimes\Theta$	2	4	2+4	1+5	3+5	6	7	6+7
$D_{4h}(C_{4v})$	2	4	2+4	1+5	3+5	6	7	6+7
$D_{2d}\otimes\Theta$	3	1	3+1	4+5	2+5	7	6	7+6
$D_{4h}(D_{2d})$	3	1	3+1	4+5	2+5	7	6	7+6

Table 4. Multiplication table.

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

Table 5. CGC for even bases for $D_4 \otimes \Theta$, etc.

2121	111	−1	3131	111	1	4141	111	1	5151	311	1/2
5151	411	i1/2	5152	111	1/2	5152	211	1/2*	5252	311	1/2
5252	411	−i1/2	6161	511	1	6162	111	1/2*	6162	211	1/2
6262	512	1	7171	512	−1	7172	111	1/2*	7172	211	1/2
7272	511	−1	2131	411	−i*	2141	311	i*	2151	511	−1*
2152	512	1*	2161	611	−1*	2162	612	1*	2171	711	−1*
2172	712	1*	3141	211	i*	3151	512	1	3152	511	1
3161	712	−1*	3162	711	1*	3171	612	−1*	3172	611	1*
4151	512	i	4152	511	−i	4161	712	−i*	4162	711	−i*
4171	612	−i*	4172	611	−i*	5161	711	1	5162	611	1*
5261	612	−1*	5262	712	1	5171	712	−1	5172	612	1*
5271	611	1*	5272	711	1	6171	311	1/2	6171	411	i1/2
6172	512	1*	6271	511	−1*	6272	311	1/2	6272	411	−i1/2

Table 6a. CGC for odd bases for $C_{4v} \otimes \Theta$ and $D_{4h}(C_{4v})$.

$\alpha_1\alpha_2$	$\alpha_1^{o} \times \alpha_2^{o}$	$\alpha_1^{o} \times \alpha_2^{e}$	$\alpha_1^{e} \times \alpha_2^{o}$
2 2	1	1	1
3 3	$\bar{1}$	1*	$\bar{1}$*
4 4	$\bar{1}$	1*	$\bar{1}$*
5 5	1+2*+$\bar{3}$+$\bar{4}$	$\bar{1}$*+2+$\bar{3}$+4	1*+$\bar{2}$+$\bar{3}$+4
6 6	1*+2+$\bar{5}$	1+$\bar{2}$*+$\bar{5}$	$\bar{1}$+2*+$\bar{5}$
7 7	1*+2+$\bar{5}$	$\bar{1}$+2*+$\bar{5}$	1+$\bar{2}$*+$\bar{5}$
2 3	$\bar{4}$	$\bar{4}$	$\bar{4}$*
2 4	3	3	$\bar{3}$*
2 5	5	$\bar{5}$	5
2 6	$\bar{6}$	6	6*
2 7	7	$\bar{7}$*	7
3 4	$\bar{2}$*	$\bar{2}$	$\bar{2}$
3 5	$\bar{5}$	$\bar{5}$	$\bar{5}$
3 6	7*	$\bar{7}$*	7*
3 7	$\bar{6}$*	6*	6*
4 5	5	5	$\bar{5}$
4 6	$\bar{7}$*	7*	7*
4 7	6*	$\bar{6}$*	6*
5 6	$\bar{6}$*+7	$\bar{6}$*+7	$\bar{6}$*+$\bar{7}$
5 7	6*+$\bar{7}$	6*+$\bar{7}$	$\bar{6}$*+$\bar{7}$
6 7	3+4+$\bar{5}$*	3+$\bar{4}$+5*	$\bar{3}$+4+5*

Table 6b. CGC for odd bases for $D_{2d}\otimes\Theta$ and $D_{4h}(D_{2d})$.

$\alpha_1\alpha_2$	$\alpha_1^{o}\times\alpha_2^{o}$	$\alpha_1^{o}\times\alpha_2^{e}$	$\alpha_1^{e}\times\alpha_2^{o}$
2 2	1	1^*	$\bar{1}^*$
3 3	1	$\bar{1}$	$\bar{1}$
4 4	1	$\bar{1}^*$	1^*
5 5	$1+\bar{2}^*+3+\bar{4}$	$\bar{1}+\bar{2}+3+\bar{4}^*$	$\bar{1}+2+3+4^*$
6 6	$1^*+\bar{2}+\bar{5}$	$\bar{1}+\bar{2}+\bar{5}^*$	$1+\bar{2}+5^*$
7 7	$1^*+\bar{2}+\bar{5}$	$1+\bar{2}+5^*$	$1+\bar{2}+\bar{5}^*$
2 3	$\bar{4}$	$\bar{4}^*$	$\bar{4}$
2 4	$\bar{3}^*$	3	3
2 5	$\bar{5}$	5	$\bar{5}^*$
2 6	$\bar{6}^*$	$\bar{6}^*$	$\bar{6}^*$
2 7	$\bar{7}^*$	$\bar{7}^*$	$\bar{7}^*$
3 4	$\bar{2}$	$\bar{2}$	$\bar{2}^*$
3 5	5	5	5
3 6	$\bar{7}$	7	7^*
3 7	$\bar{6}$	6	6^*
4 5	$\bar{5}^*$	5^*	5
4 6	7^*	7^*	$\bar{7}^*$
4 7	6^*	6^*	$\bar{6}^*$
5 6	$\bar{6}^*+7$	$6+\bar{7}^*$	$6+7^*$
5 7	$\bar{6}^*+\bar{7}$	$\bar{6}+7^*$	$6+7^*$
6 7	$3+\bar{4}+5^*$	$\bar{3}^*+4+\bar{5}$	$3+4+\bar{5}^*$

Table 7. Basic functions.

$C_4\otimes\Theta$ $C_{4h}(C_4)$ $S_4\otimes\Theta$ $C_{4h}(S_4)$			$S_4\otimes\Theta$ $C_{4h}(S_4)$	
D_α	Γ_α	Φ_a^α	D_α	Ψ_a^α
D_1	$\Gamma_1=A$	$\lvert 00\rangle$	D_2	$\lvert\bar{0}0\rangle$
D_2	$\Gamma_2=B$	$\surd(1/2)(\lvert 22\rangle+\lvert\bar{2}\bar{2}\rangle)$	D_1	$-\surd(1/2)(\lvert\bar{2}2\rangle+\lvert\bar{2}\bar{2}\rangle)$
D_3	$\Gamma_3={}^1E$	$\lvert 11\rangle$	D_3	$\lvert\bar{1}\bar{1}\rangle$
	$\Gamma_4={}^2E$	$\lvert 1\bar{1}\rangle$		$\lvert\bar{1}1\rangle$
D_5	$\Gamma_5={}^1E_1$	$\lvert 1/2\ 1/2\rangle$	D_8	$\lvert\overline{1/2}\ \overline{1/2}\rangle$
	$\Gamma_6={}^2E_1$	$\lvert 1/2\ \overline{1/2}\rangle$		$-\overline{1/2}\ 1/2\rangle$
D_8	$\Gamma_8={}^1E_2$	$\lvert 3/2\ 3/2\rangle$	D_5	$\lvert\overline{3/2}\ 3/2\rangle$
	$\Gamma_7={}^2E_2$	$\lvert 3/2\ \overline{3/2}\rangle$		$-\lvert\overline{3/2}\ \overline{3/2}\rangle$

Table 8. Compatibility table.

$D_{4h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	1^-	2^-	3^-	4^-	5^-	6^-	7^-
$C_{4h}\otimes\Theta$	1^+	1^+	2^+	2^+	3^+	5^+	8^+	1^-	1^-	2^-	2^-	3^-	5^-	8^-
$C_4\otimes\Theta$	1	1	2	2	3	5	8	1	1	2	2	3	5	8
$C_{4h}(C_4)$	1	1	2	2	3	5	8	1	1	2	2	3	5	8
$S_4\otimes\Theta$	1	1	2	2	3	5	8	2	2	1	1	3	8	5
$C_{4h}(S_4)$	1	1	2	2	3	5	8	2	2	1	1	3	8	5

Table 9. Multiplication table.

	1	2	3	5	8
1	[1]	2	3	5	8
2	2	[1]	3	5	8
3	3	3	$[1+2^2]+1$	$5+8$	$5+8$
5	5	8	$5+8$	$[1+3]+1$	2^2+3
8	8	5	$5+8$	2^2+3	$[1+3]+1$

Table 10. CGC for even bases for $C_4 \otimes \Theta$, etc.

2121	111	1	3131	211	1/2	3131	221	i1/2	3132	111	1/2
3132	121	i1/2*	3232	211	1/2	3232	221	−i1/2	5151	311	1
5152	111	1/2*	5152	121	i1/2	5252	312	1	8181	312	1
8182	111	1/2*	8182	121	i1/2	8282	311	1	2131	312	1
2132	311	1	2151	812	−1*	2152	811	1*	2181	512	−1*
2182	511	1*	3151	811	1	3152	511	1*	3251	512	−1*
3252	812	1	3181	812	−1*	3182	512	1	3281	511	1
3282	811	1*	5181	211	1/2	5181	221	i1/2	5182	312	1*
5281	311	−1*	5282	211	1/2	5282	221	−i1/2			

Table 11. CGC for odd bases for $S_4 \otimes \Theta$ and $C_{4h}(S_4)$.

$\alpha_1\alpha_2$	$\alpha_1^o \times \alpha_2^o$	$\alpha_1^o \times \alpha_2^e$	$\alpha_1^e \times \alpha_2^o$
2 2	1	$\bar{1}$	$\bar{1}$
3 3	$1_1+\bar{1}_2^*+2_1+\bar{2}_2$	$1_1+1_2+2_1+\bar{2}_2^*$	$\bar{1}_1+\bar{1}_2+2_1+2_2^*$
5 5	$1_1^*+\bar{1}_2+3$	$\bar{1}_1+1_2+\bar{3}^*$	$1_1+1_2+3^*$
8 8	$1_1^*+\bar{1}_2+3$	$\bar{1}_1+1_2+\bar{3}^*$	$1_1+1_2+3^*$
2 3	3	3	3
2 5	$\bar{8}$	8	8^*
2 8	$\bar{5}$	5	5^*
3 5	$\bar{5}+8^*$	$5+\bar{8}^*$	5^*+8
3 8	$5^*+\bar{8}$	$\bar{5}^*+8$	$5+8^*$
5 8	$2_1+\bar{2}_2+3^*$	$\bar{2}_1^*+2_2+3$	$2_1^*+2_2+\bar{3}$

Table 12. Basis functions.

	$D_4(D_2)$ $D_{2d}(D_2)$ $C_{4v}(C_{2v})$ $D_{2d}(C_{2v})$		$C_{4v}(C_{2v})$ $D_{2d}(C_{2v})$	
D_α	Γ_α	Φ_a^α	D_α	Ψ_a^α
D_1	$\Gamma_1=A$	$\lvert 00\rangle$	D_3	$-\lvert\bar{0}0\rangle$
D_3	$\Gamma_3=B_1$	$\lvert 10\rangle$	D_1	$i\lvert\bar{1}0\rangle$
D_2	$\Gamma_2=B_2$	$\lvert 11\rangle$	D_2	$-i\lvert\bar{1}1\rangle$
	$\Gamma_4=B_3$	$\lvert 1\bar{1}\rangle$		$i\lvert\bar{1}\bar{1}\rangle$
D_5	$\Gamma_5=\bar{E}$	$\lvert 1/2\ 1/2\rangle$	D_5	$i\lvert\overline{1/2}\ 1/2\rangle$
		$\lvert 1/2\ \overline{1/2}\rangle$		$-i\lvert\overline{1/2}\ \overline{1/2}\rangle$

Table 13. Compatibility table.

$D_{4h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	1^-	2^-	3^-	4^-	5^-	6^-	7^-
$D_{4h}(D_{2h})$	1^+	3^+	1^+	3^+	2^+	5^+	5^+	1^-	3^-	1^-	3^-	2^-	5^-	5^-
$D_4(D_2)$	1	3	1	3	2	5	5	1	3	1	3	2	5	5
$D_{2d}(D_2)$	1	3	1	3	2	5	5	1	3	1	3	2	5	5
$C_{4v}(C_{2v})$	1	3	1	3	2	5	5	3	1	3	1	2	5	5
$D_{2d}(C_{2v})$	1	3	1	3	2	5	5	3	1	3	1	2	5	5

Table 14. Multiplication table.

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

Table 15. CGC for even bases for $D_4(D_2)$, etc.

2121	121	1/2	2121	321	1/2	2122	111	1/2	2122	311	1/2*
2222	121	1/2	2222	321	−1/2	3131	111	−1	5151	211	1
5152	111	1/2*	5152	311	1/2	5252	212	1	2131	211	1*
2231	212	−1*	2151	522	−1	2152	511	1*	2251	512	−1*
2252	521	1	3151	511	−1*	3152	512	1*			

Table 16. CGC for odd bases for $C_{4v}(C_{2v})$ and $D_{2d}(C_{2v})$.

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

Table 17. Basis functions.

	$D_4(C_4)$ $C_{4v}(C_4)$ $D_{2d}(S_4)$		$D_{2d}(S_4)$	
D_α	Γ_α	Φ_a^α	D_α	Ψ_a^α
D_1	$\Gamma_1=A$	$\lvert 00\rangle$	D_2	$\lvert\bar{0}0\rangle$
D_2	$\Gamma_2=B$	$\sqrt{(1/2)}(\lvert 22\rangle+\lvert 2\bar{2}\rangle)$	D_1	$-\sqrt{(1/2)}(\lvert\bar{2}2\rangle+\lvert\bar{2}2\rangle)$
D_3	$\Gamma_3={}^1E$	$\lvert 11\rangle$	D_4	$\lvert\bar{1}1\rangle$
D_4	$\Gamma_4={}^2E$	$\lvert 1\bar{1}\rangle$	D_3	$\lvert\bar{1}\bar{1}\rangle$
D_5	$\Gamma_5={}^1E_1$	$\lvert 1/2\ 1/2\rangle$	D_8	$-\lvert\overline{1/2}\ 1/2\rangle$
D_6	$\Gamma_6={}^2E_1$	$\lvert 1/2\ \overline{1/2}\rangle$	D_7	$\lvert\overline{1/2}\ 1/2\rangle$
D_7	$\Gamma_8={}^1E_2$	$\lvert 3/2\ 3/2\rangle$	D_6	$-\lvert\overline{3/2}\ 3/2\rangle$
D_8	$\Gamma_7={}^2E_2$	$\lvert 3/2\ \overline{3/2}\rangle$	D_5	$\lvert\overline{3/2}\ \overline{3/2}\rangle$

Table 18. Compatibility table.

$D_{4h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+
$D_{4h}(C_{4h})$	1^+	1^+	2^+	2^+	$3^+ + 4^+$	$5^+ + 6^+$	$7^+ + 8^+$
$D_4(C_4)$	1	1	2	2	3+4	5+6	7+8
$C_{4v}(C_4)$	1	1	2	2	3+4	5+6	7+8
$D_{2d}(S_4)$	1	1	2	2	3+4	5+6	7+8
$D_{4h}\otimes\Theta$	1^-	2^-	3^-	4^-	5^-	6^-	7^-
$D_{4h}(C_{4h})$	1^-	1^-	2^-	2^-	$3^- + 4^-$	$5^- + 6^-$	$7^- + 8^-$
$D_4(C_4)$	1	1	2	2	3+4	5+6	7+8
$C_{4v}(C_4)$	1	1	2	2	3+4	5+6	7+8
$D_{2d}(S_4)$	2	2	1	1	4+3	8+7	6+5

Table 19. Multiplication table.

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

Table 20. CGC for even bases for $D_4(C_4)$, etc.

2121	111	1	3131	211	1	4141	211	1	5151	311	1
6161	411	1	7171	411	−1	8181	311	−1	2131	411	1
2141	311	1	2151	811	−1*	2161	711	1*	2171	611	−1*
2181	511	1*	3141	111	1	3151	711	1	3161	511	1*
3171	811	−1*	3181	611	1	4151	611	−1*	4161	811	1
4171	511	1	4181	711	1*	5161	111	1*	5171	211	1
5181	411	1*	6171	311	−1*	6181	211	1	7181	111	1*

Table 21. CGC for odd bases for $D_{2d}(S_4)$.

$\alpha_1\alpha_2$	$\alpha_1^o\alpha_2^o$	$\alpha_1^o\alpha_2^e$	$\alpha_1^e\alpha_2^o$	$\alpha_1\alpha_2$	$\alpha_1^o\alpha_2^o$	$\alpha_1^o\alpha_2^e$	$\alpha_1^e\alpha_2^o$	$\alpha_1\alpha_2$	$\alpha_1^o\alpha_2^o$	$\alpha_1^o\alpha_2^e$	$\alpha_1^e\alpha_2^o$	$\alpha_1\alpha_2$	$\alpha_1^o\alpha_2^o$	$\alpha_1^o\alpha_2^e$	$\alpha_1^e\alpha_2^o$
2 2	1	$\bar{1}$	$\bar{1}$	2 3	4	4	4	3 5	7*	$\bar{7}$*	7	4 8	$\bar{7}$	7	7*
3 3	2	2	2	2 4	3	3	3	3 6	$\bar{5}$	5	5*	5 6	1*	$\bar{1}$	1
4 4	2	2	2	2 5	$\bar{8}$	8	8*	3 7	$\bar{8}$	8	8*	5 7	2	$\bar{2}$*	2*
5 5	$\bar{3}$	$\bar{3}$*	3*	2 6	$\bar{7}$	7	7*	3 8	6*	$\bar{6}$*	6	5 8	4*	$\bar{4}$	$\bar{4}$
6 6	$\bar{4}$	$\bar{4}$*	4*	2 7	$\bar{6}$	6	6*	4 5	$\bar{6}$	6	6*	6 7	3*	$\bar{3}$	$\bar{3}$
7 7	$\bar{4}$	4*	$\bar{4}$*	2 8	$\bar{5}$	5	5*	4 6	8*	$\bar{8}$*	8	6 8	2*	$\bar{2}$	2
8 8	$\bar{3}$	3*	$\bar{3}$*	3 4	1	$\bar{1}$	$\bar{1}$	4 7	5*	$\bar{5}$*	5	7 8	1	$\bar{1}$*	1*

Table 22. Basis functions.

$C_4(C_2)$ $S_4(C_2)$		
D_α	Γ_α	Φ^α_a
D_1	Γ_1	$\|00\rangle$
D_2	Γ_2	$\|11\rangle$
	Γ_2	$\|1\bar{1}\rangle$
D_3	Γ_3	$\|1/2\ 1/2\rangle$
	Γ_4	$\|1/2\ \overline{1/2}\rangle$

Table 23. Compatibility table.

$C_{4h}\otimes\Theta$	1^+	2^+	3^+	5^+	8^+	1^-	2^-	3^-	5^-	8^-
$C_{4h}(C_{2h})$	1^+	1^+	2^+	3^+	5^+	1^-	1^-	2^-	3^-	5^-
$C_4(C_2)$	1	1	2	3	5	1	1	2	3	5
$S_4(C_2)$	1	1	2	3	5	1	1	2	3	5

Table 24. Multiplication table.

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

Table 25. CGC for $C_4(C_2)$, etc.

2121	131	1/2	2121	141	i1/2	2122	111	1/2	2122	121	i1/2*
2222	131	1/2	2222	141	−i1/2*	3131	211	1	3132	111	1/2*
3132	121	i1/2	3232	212	1	2131	322	−1	2132	311	1*
2231	312	−1*	2232	321	1						

Table 26. Basis functions.

$D_2\otimes\Theta$ $D_{2h}(D_2)$ $C_{2v}\otimes\Theta$ $D_{2h}(C_{2v})$			$C_{2v}\otimes\Theta$ $D_{2h}(C_{2v})$		$D_2(C_2)$ $C_{2v}(C_2)$ $C_{2v}(C_s)$			$C_{2v}(C_s)$	
D_α	Γ_α	Φ^α_a	D_α	Ψ^α_a	D_α	Γ_α	Φ^α_a	D_α	Ψ^α_a
D_1	$\Gamma_1=A$	$\|00\rangle$	D_3	$-i\|\bar{0}0\rangle$	D_1	$\Gamma_1=A$	$\|00\rangle$	D_2	$\|\bar{0}0\rangle$
D_2	$\Gamma_2=B_2$	$\sqrt{(1/2)}(\|11\rangle+\|11\rangle)$	D_4	$\sqrt{(1/2)}(\|\bar{1}1\rangle+\|\bar{1}\bar{1}\rangle)$	D_2	$\Gamma_2=B$	$\|11\rangle$	D_1	$\|\bar{1}1\rangle$
D_3	$\Gamma_3=B_1$	$\|10\rangle$	D_1	$i\|\bar{1}0\rangle$	D_1	—	—	D_2	—
D_4	$\Gamma_4=B_3$	$i\sqrt{(1/2)}(\|11\rangle-\|1\bar{1}\rangle)$	D_2	$i\sqrt{(1/2)}(\|\bar{1}\bar{1}\rangle-\|\bar{1}1\rangle)$	D_2	—	—	D_1	—
D_5	$\Gamma_5=\bar{E}$	$\|1/2\ 1/2\rangle$	D_5	$i\|\overline{1/2}\ 1/2\rangle$	D_3	$\Gamma_3={}^1\bar{E}$	$\|1/2\ 1/2\rangle$	D_4	$\|\overline{1/2}\ 1/2\rangle$
		$\|1/2\ \overline{1/2}\rangle$		$-i\|\overline{1/2}\ \overline{1/2}\rangle$	D_4	$\Gamma_4={}^2\bar{E}$	$\|1/2\ \overline{1/2}\rangle$	D_3	$\|\overline{1/2}\ \overline{1/2}\rangle$

Table 27a. Compatibility table.

$D_{4h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	6^+	7^+	1^-	2^-	3^-	4^-	5^-	6^-	7^-
$D_{2h}\otimes\Theta$	1^+	3^+	1^+	3^+	2^++4^+	5^+	5^+	1^-	3^-	1^-	3^-	2^-+4^-	5^-	5^-
$D_2\otimes\Theta$	1	3	1	3	2+4	5	5	1	3	1	3	2+4	5	5
$D_{2h}(D_2)$	1	3	1	3	2+4	5	5	1	3	1	3	2+4	5	5
$C_{2v}\otimes\Theta$	1	3	1	3	2+4	5	5	3	1	3	1	4+2	5	5
$D_{2h}(C_{2v})$	1	3	1	3	2+4	5	5	3	1	3	1	4+2	5	5

Table 27b. Compatibility table.

$D_{2h}\otimes\Theta$	1^+	2^+	3^+	4^+	5^+	1^-	2^-	3^-	4^-	5^-
$D_{2h}(C_{2h})$	1^+	2^+	1^+	2^+	3^++4^+	1^-	2^-	1^-	2^-	3^-+4^-
$D_2(C_2)$	1	2	1	2	3+4	1	2	1	2	3+4
$C_{2v}(C_2)$	1	2	1	2	3+4	1	2	1	2	3+4
$C_{2v}(C_s)$	1	2	1	2	3+4	2	1	2	1	4+3

Table 28. (*a*) Multiplication table for $D_2\otimes\Theta$, etc. (*b*) Multiplication table for $D_2(C_2)$, etc.

(*a*)	1	2	3	4	5	(*b*)	1	2	3	4
1	[1]	2	3	4	5	1	[1]	2	3	4
2	2	[1]	4	3	5	2	2	[1]	4	3
3	3	4	[1]	2	5	3	3	4	[2]	1
4	4	3	2	[1]	5	4	4	3	1	[2]
5	5	5	5	5	[2+3+4]+1					

Table 29a. CGC for even bases for $D_2\otimes\Theta$, etc.

2121	111	1	3131	111	1	4141	111	1	5151	211	1/2
5151	411	i1/2	5152	111	1/2*	5152	311	1/2	5252	211	1/2
5252	411	−i1/2	2131	411	i*	2141	311	i*	2151	512	−1*
2152	511	1*	3141	211	i*	3151	511	−1*	3152	512	1*
4151	512	−i*	4152	511	−i*						

Table 29b. CGC for even bases for $D_2(C_2)$, etc.

2121	111	1	3131	211	1	4141	211	1	2131	411	−1*
2141	311	1*	3141	111	1*						

Table 30a. CGC for odd bases for $C_{2v} \otimes \Theta$ and $D_{2h}(C_{2v})$.

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

Table 30b. CGC for odd bases for $C_{2v}(C_s)$.

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

Table 31. Basis functions.

$C_2 \otimes \Theta$ $C_{2h}(C_2)$ $C_s \otimes \Theta$ $C_{2h}(C_s)$			$C_s \otimes \Theta$ $C_{2h}(C_s)$		$C_2(C_1)$ $C_s(C_1)$		
D_α	Γ_α	Φ_a^α	D_α	Ψ_a^α	D_α	Γ_α	Φ_a^α
D_1	$\Gamma_1 = A$	$\|00\rangle$	D_2	$\|\bar{0}0\rangle$	D_1	$\Gamma_1 = A$	$\|00\rangle$
D_2	$\Gamma_2 = B$	$\sqrt{(1/2)}(\|11\rangle + \|1\bar{1}\rangle)$	D_1	$\sqrt{(1/2)}(\|\bar{1}1\rangle + \|\bar{1}\bar{1}\rangle)$	D_1	—	
D_3	$\Gamma_3 = {}^1E$	$\|1/2\ 1/2\rangle$	D_3	$\|\overline{1/2}\ \overline{1/2}\rangle$	D_2	$\Gamma_2 = \bar{A}$	$\sqrt{(1/2)}(\|1/2\ 1/2\rangle + \|1/2\ \overline{1/2}\rangle)$
	$\Gamma_4 = {}^2E$	$\|1/2\ \overline{1/2}\rangle$		$-\|\overline{1/2}\ 1/2\rangle$	D_2	—	

Table 32a. Compatibility table.

$D_{2h} \otimes \Theta$	1^+	2^+	3^+	4^+	5^+	1^-	2^-	3^-	4^-	5^-
$C_{2h} \otimes \Theta$	1^+	2^+	1^+	2^+	3^+	1^-	2^-	1^-	2^-	3^-
$C_2 \otimes \Theta$	1	2	1	2	3	1	2	1	2	3
$C_{2h}(C_2)$	1	2	1	2	3	1	2	1	2	3
$C_s \otimes \Theta$	1	2	1	2	3	2	1	2	1	3
$C_{2h}(C_s)$	1	2	1	2	3	2	1	2	1	3

Table 32b. Compatibility table.

$C_{2h}\otimes\Theta$	1^+	2^+	3^+	1^-	2^-	3^-
$C_{2h}(C_i)$	1^+	1^+	2^{2+}	1^-	1^-	2^{2-}
$C_2(C_1)$	1	1	2^2	1	1	2^2
$C_s(C_1)$	1	1	2^2	1	1	2^2

Table 33. (*a*) Multiplication table for $C_2\otimes\Theta$, etc. (*b*) Multiplication table for $C_2(C_1)$, etc.

(*a*)	1	2	3	(*b*)	1	2
1	[1]	2	3	1	[1]	2
2	2	[1]	3	2	2	[1]
3	3	3	$[1+2^2]+1$			

Table 34a. CGC for even bases for $C_2\otimes\Theta$, etc.

2121	111	1	3131	211	1/2	3131	221	i1/2	3132	111	1/2*
3132	121	i1/2	3232	211	1/2	3232	221	−i1/2	2131	312	−1*
2132	311	1*									

Table 34b. CGC for even bases for $C_2(C_1)$, etc.

2121	111	i

Table 35. CGC for odd bases for $C_s\otimes\Theta$ and $C_{2h}(C_s)$.

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

Table 36. Basis functions.

	$C_1\otimes\Theta$ $C_i(C_1)$	
D_α	Γ_α	Φ_a^α
D_1	$\Gamma_1=A$	$\|00\rangle$
D_2	$\Gamma_2=\bar{A}$	$\|1/2\ 1/2\rangle$
	$\Gamma_2=\bar{A}$	$\|1/2\ \overline{1/2}\rangle$

Table 37. Compatibility table.

$C_{2h}\otimes\Theta$	1^+	2^+	3^+	1^-	2^-	3^-
$C_i\otimes\Theta$	1^+	1^+	2^+	1^-	1^-	2^-
$C_1\otimes\Theta$	1	1	2	1	1	2
$C_i(C_1)$	1	1	2	1	1	2

Table 38. Multiplication table.

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

Table 39. CGC for $C_1\otimes\Theta$.

2121	131	1/2	2121	141	i1/2	2122	111	1/2*	2122	121	i1/2
2222	131	1/2	2222	141	−i1/2						

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