



## 1.2. REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

Table 1.2.6.5 (cont.)

(g)  $D_3$

$D_3$	$\varepsilon$	$\alpha$	$\beta$
$n$	1	2	3
Order	1	3	2
$\Gamma_1$	1	1	1
$\Gamma_2$	1	1	-1
$\Gamma_3$	2	-1	0

Matrices of the two-dimensional representation:

	$\varepsilon$	$\alpha$	$\beta$
$\Gamma_3$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}$

32	$\alpha = C_{3z}$	$\Gamma_1 : A_1 = \chi_1$	$x^2 + y^2, z^2$
$D_3$	$\beta = C_{2x}$	$\Gamma_2 : A_2 = \chi_2$ $\Gamma_3 : E = \chi_1$	$z$ $x, y$ $xz, yz, xy, x^2 - y^2$
3m	$\alpha = C_{3z}$	$\Gamma_1 : A_1 = \chi_1$	$x^2 + y^2, z^2$
$C_{3v}$	$\beta = \sigma_v$	$\Gamma_2 : A_2 = \chi_2$ $\Gamma_3 : E = \chi_1$	$z$ $x, y$ $xz, yz, xy, x^2 - y^2$

(h)  $D_4$

$D_4$	$\varepsilon$	$\alpha$	$\alpha^2$	$\beta$	$\alpha\beta$
$n$	1	2	1	2	2
Order	1	4	2	2	2
$\Gamma_1$	1	1	1	1	1
$\Gamma_2$	1	1	1	-1	-1
$\Gamma_3$	1	-1	1	1	-1
$\Gamma_4$	1	-1	1	-1	1
$\Gamma_5$	2	0	-2	0	0

Matrices of the two-dimensional representation:

	$\Gamma_5$
$\varepsilon$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
$\alpha$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
$\alpha^2$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
$\beta$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
$\alpha\beta$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$

422	$\alpha = C_{4z}$	$\Gamma_1 : A_1 = \chi_1$	$x^2 + y^2, z^2$
$D_4$	$\beta = C_{2x}$	$\Gamma_2 : A_2 = \chi_2$ $\Gamma_3 : B_1 = \chi_3$ $\Gamma_4 : B_2 = \chi_4$ $\Gamma_5 : E = \chi_1$	$z$ $x^2 - y^2$ $xy$ $x, y$ $xz, yz$
4mm	$\alpha = C_{4z}$	$\Gamma_1 : A_1 = \chi_1$	$x^2 + y^2, z^2$
$C_{4v}$	$\beta = \sigma_v$	$\Gamma_2 : A_2 = \chi_2$ $\Gamma_3 : B_1 = \chi_3$ $\Gamma_4 : B_2 = \chi_4$ $\Gamma_5 : E = \chi_1$	$z$ $x^2 - y^2$ $xy$ $x, y$ $xz, yz$
$\bar{4}2m$	$\alpha = S_{4z}$	$\Gamma_1 : A_1 = \chi_1$	$x^2 + y^2, z^2$
$D_{2d}$	$\beta = C_{2v}$ $\alpha\beta = \sigma_d$	$\Gamma_2 : A_2 = \chi_2$ $\Gamma_3 : B_1 = \chi_3$ $\Gamma_4 : B_2 = \chi_4$ $\Gamma_5 : E = \chi_1$	$z$ $x^2 - y^2$ $xy$ $x, y$ $xz, yz$

(i)  $D_6$

$D_6$	$\varepsilon$	$\alpha$	$\alpha^2$	$\alpha^3$	$\beta$	$\alpha\beta$
$n$	1	2	2	1	3	3
Order	1	6	3	2	2	2
$\Gamma_1$	1	1	1	1	1	1
$\Gamma_2$	1	1	1	1	-1	-1
$\Gamma_3$	1	-1	1	-1	1	-1
$\Gamma_4$	1	-1	1	-1	-1	1
$\Gamma_5$	2	1	-1	-2	0	0
$\Gamma_6$	2	-1	-1	2	0	0

Matrices of the two-dimensional representations:

	$\Gamma_5$	$\Gamma_6$
$\varepsilon$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
$\alpha$	$\begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$
$\alpha^2$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$
$\alpha^3$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
$\beta$	$\begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}$
$\alpha\beta$	$\begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$

622	$\alpha = C_{6z}$	$\Gamma_1 : A_1 = \chi_1$	$x^2 + y^2, z^2$
$D_6$	$\beta = C_{2x}$	$\Gamma_2 : A_2 = \chi_2$ $\Gamma_3 : B_1 = \chi_3$ $\Gamma_4 : B_2 = \chi_4$ $\Gamma_5 : E_1 = \chi_1$ $\Gamma_6 : E_2 = \chi_2$	$z$ $x^2 - y^2$ $xy$ $x, y$ $xz, yz$

6mm	$\alpha = C_{6z}$	$\Gamma_1 : A_1 = \chi_1$	$x^2 + y^2, z^2$
$C_{6v}$	$\beta = \sigma_v$	$\Gamma_2 : A_2 = \chi_2$ $\Gamma_3 : B_1 = \chi_3$ $\Gamma_4 : B_2 = \chi_4$ $\Gamma_5 : E_1 = \chi_1$ $\Gamma_6 : E_2 = \chi_2$	$z$ $x^2 - y^2$ $xy$ $x, y$ $xz, yz$

$\bar{6}2m$	$\alpha = S_{6z}$	$\Gamma_1 : A'_1 = \chi_1$	$x^2 + y^2, z^2$
$D_{3h}$	$\beta = C_{2v}$ $\alpha\beta = \sigma_d$	$\Gamma_2 : A'_2 = \chi_2$ $\Gamma_3 : A''_1 = \chi_3$ $\Gamma_4 : A'_2 = \chi_4$ $\Gamma_5 : E' = \chi_2$ $\Gamma_6 : E'' = \chi_1$	$z$ $x^2 - y^2$ $xy$ $x, y$ $xz, yz$

$\bar{3}m$	$\alpha = S_{3z}$	$\Gamma_1 : A_{1g} = \chi_1^+$	$x^2 + y^2, z^2$
$D_{3d}$	$\beta = \sigma_d$	$\Gamma_2 : A_{2g} = \chi_2^+$ $\Gamma_3 : A_{1u} = \chi_1^-$ $\Gamma_4 : A_{2u} = \chi_2^-$ $\Gamma_5 : E_u = \chi_1^-$ $\Gamma_6 : E_g = \chi_1^+$	$z$ $x, y$ $xz, yz, xy, x^2 - y^2$

(j)  $T$  [ $\omega = \exp(2\pi i/3)$ ].

$T$	$\varepsilon$	$\alpha$	$\alpha^2$	$\beta$
$n$	1	4	4	3
Order	1	3	3	2
$\Gamma_1$	1	1	1	1
$\Gamma_2$	1	$\omega$	$\omega^2$	1
$\Gamma_3$	1	$\omega^2$	$\omega$	1
$\Gamma_4$	3	0	0	-1

# 1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

Table 1.2.6.5 (cont.)

Real representations of dimension  $d > 1$ :

	$\Gamma_2 \oplus \Gamma_3$	$\Gamma_4$
$\varepsilon$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\alpha$	$\begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$
$\alpha^2$	$\begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
$\beta$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

23  $\alpha = C_{3d}$   $\Gamma_1 : A = \chi_1$   $x^2 + y^2 + z^2$   
 $T$   $\beta = C_{2z}$   $\Gamma_2 \oplus \Gamma_3 : E = \chi_{3c} + \chi_{3c}^*$   $x^2 - y^2, x^2 - z^2$   
 $\Gamma_4 : T = \chi_1$   $x, y, z$   $xy, xz, yz$

(k)  $O$

$O$	$\varepsilon$	$\beta$	$\alpha^2$	$\alpha$	$\alpha\beta$
$n$	1	8	3	6	6
Order	1	3	2	4	2
$\Gamma_1$	1	1	1	1	1
$\Gamma_2$	1	1	1	-1	-1
$\Gamma_3$	2	-1	2	0	0
$\Gamma_4$	3	0	-1	1	-1
$\Gamma_5$	3	0	-1	-1	1

Higher-dimensional representations:

	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$
$\varepsilon$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\beta$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
$\alpha^2$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\alpha$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$\alpha\beta$	$\begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$

432  $\alpha = C_{4z}$   $\Gamma_1 : A_1 = \chi_1$   $x^2 + y^2 + z^2$   
 $O$   $\beta = C_{3d}$   $\Gamma_2 : A_2 = \chi_2$   
 $\alpha\beta = C_2$   $\Gamma_3 : E = \chi_3$   $x^2 - y^2, y^2 - z^2$   
 $\Gamma_4 : T_1 = \chi_1$   $x, y, z$   
 $\Gamma_5 : T_2 = \chi_2$   $xy, xz, yz$

$\bar{4}3m$   $\alpha = S_{4z}$   $\Gamma_1 : A_1 = \chi_1$   $x^2 + y^2 + z^2$   
 $T_d$   $\beta = C_{3d}$   $\Gamma_2 : A_2 = \chi_2$   
 $\alpha\beta = \sigma_d$   $\Gamma_3 : E = \chi_3$   $x^2 - y^2, y^2 - z^2$   
 $\Gamma_4 : T_1 = \chi_1$   $x, y, z$   
 $\Gamma_5 : T_2 = \chi_2$   $xy, yz, xz$

Other point groups which are of second class and contain  $-E$ . See Table 1.2.6.6(a).

Group	Isomorphism class	Rotation subgroup
$4/m$	$C_4 \times \mathbb{Z}_2$	4
$6/m$	$C_6 \times \mathbb{Z}_2$	6
$mmm$	$D_2 \times \mathbb{Z}_2$	222
$4/mmm$	$D_4 \times \mathbb{Z}_2$	422
$6/mmm$	$D_6 \times \mathbb{Z}_2$	622
$m\bar{3}$	$T \times \mathbb{Z}_2$	23
$m\bar{3}m$	$O \times \mathbb{Z}_2$	432

Table 1.2.6.6. Direct products with  $\{E, \bar{1}\}$  and  $\{E, 1'\}$

(a) With  $\{E, \bar{1}\}$ .

$K \times \mathbb{Z}_2$	$R \in K$	$\bar{R}$
$\Gamma_g$	$\chi(R)$	$\chi(R)$
$\Gamma_u$	$\chi(R)$	$-\chi(R)$

$4/m$   $C_4 \times \mathbb{Z}_2$  cf. 4  
 $6/m$   $C_6 \times \mathbb{Z}_2$  cf. 6  
 $mmm$   $D_2 \times \mathbb{Z}_2$  cf. 222  
 $4/mmm$   $D_4 \times \mathbb{Z}_2$  cf. 422  
 $6/mmm$   $D_6 \times \mathbb{Z}_2$  cf. 622  
 $m\bar{3}$   $T \times \mathbb{Z}_2$  cf. 23  
 $m\bar{3}m$   $O \times \mathbb{Z}_2$  cf. 432

(b) With  $\{E, 1'\}$ .

$K \times \mathbb{Z}_2$	$R \in K$	$R'$
$\Gamma_+$	$\chi(R)$	$\chi(R)$
$\Gamma_-$	$\chi(R)$	$-\chi(R)$

$1'$   $C_1 \times \mathbb{Z}_2$  cf. 1  
 $21'$   $C_2 \times \mathbb{Z}_2$  cf. 2  
 $m1'$   $C_2 \times \mathbb{Z}_2$  cf.  $m$   
 $2221'$   $D_2 \times \mathbb{Z}_2$  cf. 222  
 $2mm1'$   $D_2 \times \mathbb{Z}_2$  cf.  $2mm$   
 $41'$   $C_4 \times \mathbb{Z}_2$  cf. 4  
 $\bar{4}1'$   $C_4 \times \mathbb{Z}_2$  cf.  $\bar{4}$   
 $4mm1'$   $D_4 \times \mathbb{Z}_2$  cf.  $4mm$   
 $4221'$   $D_4 \times \mathbb{Z}_2$  cf. 422  
 $\bar{4}2m1'$   $D_4 \times \mathbb{Z}_2$  cf.  $\bar{4}2m$   
 $31'$   $C_3 \times \mathbb{Z}_2$  cf. 3  
 $321'$   $D_3 \times \mathbb{Z}_2$  cf. 32  
 $31'$   $C_6 \times \mathbb{Z}_2$  cf. 3  
 $3m1'$   $D_3 \times \mathbb{Z}_2$  cf.  $3m$   
 $6mm1'$   $D_6 \times \mathbb{Z}_2$  cf.  $6mm$   
 $61'$   $C_6 \times \mathbb{Z}_2$  cf. 6  
 $\bar{6}1'$   $C_6 \times \mathbb{Z}_2$  cf.  $\bar{6}$   
 $6221'$   $D_6 \times \mathbb{Z}_2$  cf. 622  
 $\bar{6}2m1'$   $D_6 \times \mathbb{Z}_2$  cf.  $\bar{6}2m$   
 $231'$   $T \times \mathbb{Z}_2$  cf. 23  
 $4321'$   $O \times \mathbb{Z}_2$  cf. 432  
 $43m1'$   $O \times \mathbb{Z}_2$  cf.  $43m$

(c) With  $\{E, \bar{1}\}$  and  $\{E, 1'\}$ .

$K \times \mathbb{Z}_2 \times \mathbb{Z}_2$	$R \in K$	$\bar{R}$	$R'$	$\bar{R}'$
$\Gamma_{g+}$	$\chi(R)$	$\chi(R)$	$\chi(R)$	$\chi(R)$
$\Gamma_{u+}$	$\chi(R)$	$-\chi(R)$	$\chi(R)$	$-\chi(R)$
$\Gamma_{g-}$	$\chi(R)$	$\chi(R)$	$-\chi(R)$	$-\chi(R)$
$\Gamma_{u-}$	$\chi(R)$	$-\chi(R)$	$-\chi(R)$	$\chi(R)$

$\bar{1}'$   $C_1 \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf. 1  
 $21'/m$   $C_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf. 2  
 $4/m1'$   $C_4 \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf. 4  
 $6/m1'$   $C_6 \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf. 6  
 $mmm1'$   $D_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf. 222  
 $4/mmm1'$   $D_4 \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf. 422  
 $\bar{3}m1'$   $D_6 \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf.  $3m$   
 $6/mmm1'$   $D_6 \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf. 622  
 $m31'$   $T \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf. 23  
 $m(\bar{3})m1'$   $O \times \mathbb{Z}_2 \times \mathbb{Z}_2$  cf. 432