

1.2. REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

groups generated by  $\bar{1}, 1'$  and  $\{\bar{1}, 1'\}$  are given in Tables 1.2.6.6(a), (b) and (c), respectively.

Table 1.2.6.7. The representations of a point group are also representations of their double groups. In addition, there are extra representations which give projective representations of the point groups. For several cases, these are associated with an ordinary representation. As extra representations, those irreducible representations of the double point groups that give rise to projective representations of the point groups with a factor system that is not associated with the trivial one are given. These do not correspond to ordinary representations of the single group.

Table 1.2.6.8. If one chooses for each element of a point group one of the two corresponding  $SU(2)$  elements, the latter form a projective representation of the point group. If one selects for the rotation  $R \in K \subset SO(3)$  the element

$$u(R) = E \cos(\varphi/2) + i(\boldsymbol{\sigma} \cdot \mathbf{n}) \sin(\varphi/2),$$

where  $\varphi$  is the rotation angle and  $\mathbf{n}$  the rotation axis, and for  $R \in K \subset O(3) \setminus SO(3)$  the element

$$u(R) = E \cos(\psi/2) + i(\boldsymbol{\sigma} \cdot \mathbf{n}) \sin(\psi/2),$$

where  $\psi$  and  $\mathbf{n}$  are the rotation angle and axis of the rotation  $-R$ , the matrices  $u(R)$  form a projective representation:

$$u(R)u(R') = \omega_s(R, R')u(RR').$$

The factor system  $\omega_s$  is the spin factor system. It is determined via the generators and defining relations

$$W_i(A_1, \dots, A_p) = E$$

of the point group  $K$ . Then

$$W_i(u(A_1), \dots, u(A_p)) = \lambda_i E,$$

and the factors  $\lambda_i$  fix uniquely the class of the factor system  $\omega_s$ . These factors are given in the table.

Because  $\bar{1}$  is represented by the unit matrix in spin space, the double groups of two isomorphic point groups obtained from each other by replacing the elements  $R \in O(3) \setminus SO(3)$  by  $-R$  are the same.

The projective representations with factor system  $\omega_s$  may sometimes be associated with one with a trivial factor system. If this is the case, there are actually no extra representations of the

Table 1.2.6.7. Extra representations of double groups

$222^d$ $\Gamma_5'$	$E$	$-E$	$\pm A$	$\pm B$	$\pm AB$				
	2	-2	0	0	0				
$422^d$ $\Gamma_6'$ $\Gamma_7'$	$E$	$-E$	$\pm A^2$	$A$	$-A$	$\pm B$	$\pm AB$		
	2	-2	0	$\sqrt{2}$	$-\sqrt{2}$	0	0		
	2	-2	0	$-\sqrt{2}$	$\sqrt{2}$	0	0		
$622^d$ $\Gamma_8'$ $\Gamma_9'$ $\Gamma_7'$	$E$	$-E$	$A^2$	$-A^2$	$\pm B$	$\pm A^3$	$A^5$	$-A^5$	$\pm A^3 B$
	2	-2	1	-1	0	0	$\sqrt{3}$	$-\sqrt{3}$	0
	2	-2	1	-1	0	0	$-\sqrt{3}$	$\sqrt{3}$	0
	2	-2	-2	2	0	0	0	0	0
$23^d$ $\Gamma_5'$ $\Gamma_6'$ $\Gamma_7'$	$E$	$-E$	$A$	$-A$	$A^2$	$-A^2$	$\pm B$		
	2	-2	1	-1	1	-1	0		
	2	-2	$\omega$	$\omega^4$	$\omega^2$	$\omega^5$	0		
	2	-2	$\omega^5$	$\omega^2$	$\omega^4$	$\omega$	0		
$432^d$ $\Gamma_6'$ $\Gamma_7'$ $\Gamma_8'$	$E$	$-E$	$B$	$-B$	$\pm A^2$	$A$	$-A$	$\pm AB$	
	2	-2	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	
	2	-2	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	
	4	-4	-1	1	0	0	0	0	

Table 1.2.6.8. Projective spin representations of the 32 crystallographic point groups

Point group	Relations giving $\lambda_i$	Double group	Extra representations
$\bar{1}$ $\bar{1}$	$A = E$ $A^2 = E$	$1^d$	No No
$2, m$ $2/m$	$A^2 = -E$ $A^2 = B^2 = -E, (AB)^2 = E$	$2^d$	No
$222, 2mm$ $mmm$	$A^2 = B^2 = (AB)^2 = -E$ $A^2 = B^2 = (AB)^2 = -E$ $C^2 = E, AC = CA, BC = CB$	$222^d$	Yes
$4, \bar{4}$ $4/m$	$A^4 = -E$ $A^4 = B^2 = -E, AB = BA$	$4^d$	No
$422, 4mm, \bar{4}2m$ $4/mmm$	$A^4 = B^2 = (AB)^2 = -E$ As above, plus $C^2 = E, AC = CA, BC = CB$	$422^d$	Yes
$\bar{3}$ $\bar{3}$	$A^3 = -E$ $A^6 = E$	$3^d$	No
$\bar{3}2, 3m$ $\bar{3}m$	$A^3 = B^2 = (AB)^2 = -E$ $A^6 = E, B^2 = (AB)^2 = -E$	$32^d$	No
$6, \bar{6}$ $6/m$	$A^6 = -E$ $A^6 = B^2 = -E, AB = BA$	$6^d$	No
$622, 6mm, \bar{6}2m$ $6/mmm$	$A^6 = B^2 = (AB)^2 = -E$ As above, plus $C^2 = E, AC = CA, BC = CB$	$622^d$	Yes
$23$ $m\bar{3}$	$A^3 = B^2 = (AB)^3 = -E$ As above, plus $C^2 = E, AC = CA, BC = CB$	$23^d$	Yes
$432, \bar{4}3m$ $m\bar{3}m$	$A^4 = B^3 = (AB)^2 = -E$ As above, plus $C^2 = E, AC = CA, BC = CB$	$432^d$	Yes