Table 1.5.4.2
Additional symmetry operations due to a centring vector **t** and their locations

Symmetry operation at the origin		Additional symmetry operations									Representative space groups (numbers)
		$C, t(\frac{1}{2},\frac{1}{2},0)$		$A, t(0,\frac{1}{2},\frac{1}{2})$		$B, t(\frac{1}{2},0,\frac{1}{2})$		$I, t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		F	
Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	
m	$0, y, z$	b	$\frac{1}{4}, y, z$	n	$0, y, z$	c	$\frac{1}{4}, y, z$	n	$\frac{1}{4}, y, z$	b, n, c	*Cmmm*, *Ammm*, *Bmmm* (65)
c		n		b		m		b			*Immm* (71), *Fmmm* (69)
b		m		c		n		c			*Cccm*, *Amaa*, *Bbmb* (66), *Ibca* (73)
$d(0,\frac{1}{4},\frac{1}{4})$		$d(0,\frac{3}{4},\frac{1}{4})$		$d(0,\frac{3}{4},\frac{3}{4})$		$d(0,\frac{1}{4},\frac{3}{4})$				d, d, d	*Fddd* (70)
m	$x, 0, z$	a	$x, \frac{1}{4}, z$	c	$x, \frac{1}{4}, z$	n	$x, 0, z$	n	$x, \frac{1}{4}, z$	a, c, n	As above
a		m		n		c		c			
c		n		m		a		a			
$d(\frac{1}{4},0,\frac{1}{4})$		$d(\frac{3}{4},0,\frac{1}{4})$		$d(\frac{1}{4},0,\frac{3}{4})$		$d(\frac{3}{4},0,\frac{3}{4})$				d, d, d	
m	$x, y, 0$	n	$x, y, 0$	b	$x, y, \frac{1}{4}$	a	$x, y, \frac{1}{4}$	n	$x, y, \frac{1}{4}$	n, b, a	As above
b		a		m		n		a			
a		b		n		m		b			
$d(\frac{1}{4},\frac{1}{4},0)$		$d(\frac{3}{4},\frac{3}{4},0)$		$d(\frac{1}{4},\frac{3}{4},0)$		$d(\frac{3}{4},\frac{1}{4},0)$				d, d, d	
m	x, x, z	$g(\frac{1}{2},\frac{1}{2},0)$	x, x, z	$g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$	$x, x+\frac{1}{4}, z$	$g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$	$x, x-\frac{1}{4}, z$	$n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	x, x, z	g, g, g	*I*4*mm* (107), *F*$\bar{4}$3*m* (216)
c		$n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$g(\frac{1}{4},\frac{1}{4},0)$		$g(\frac{1}{4},\frac{1}{4},0)$		$g(\frac{1}{2},\frac{1}{2},0)$		n, g, g	*F*$\bar{4}$3*c* (219)
$d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$								$d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$			*I*$\bar{4}$3*d* (220)
2	$x, 0, 0$	2_1	$x, \frac{1}{4}, 0$	2	$x, \frac{1}{4}, \frac{1}{4}$	2_1	$x, 0, \frac{1}{4}$	2_1	$x, \frac{1}{4}, \frac{1}{4}$	$2_1, 2, 2_1$	*C*222, *A*222, *B*222 (21)
2	$0, y, 0$	2_1	$\frac{1}{4}, y, 0$	2_1	$0, y, \frac{1}{4}$	2	$\frac{1}{4}, y, \frac{1}{4}$	2_1	$\frac{1}{4}, y, \frac{1}{4}$	$2_1, 2_1, 2$	*I*222 (23)
2	$0, 0, z$	2	$\frac{1}{4}, \frac{1}{4}, z$	2_1	$0, \frac{1}{4}, z$	2_1	$\frac{1}{4}, 0, z$	2_1	$\frac{1}{4}, \frac{1}{4}, z$	$2, 2_1, 2_1$	*F*222 (22)
2	$x, \bar{x}, 0$	2	$x, \bar{x}+\frac{1}{2}, 0$	$2_1(-\frac{1}{4},\frac{1}{4},0)$	$x, \bar{x}+\frac{1}{4}, \frac{1}{4}$	$2_1(\frac{1}{4},-\frac{1}{4},0)$	$x, \bar{x}+\frac{1}{4}, \frac{1}{4}$	2	$x, \bar{x}, \frac{1}{4}$	$2, 2_1, 2_1$	*C*422 (*P*422) (89), *I*422 (97)
4	$0, 0, z$	4	$0, \frac{1}{2}, z$	4_2	$-\frac{1}{4}, \frac{1}{4}, z$	4_2	$\frac{1}{4}, \frac{1}{4}, z$	4_2	$0, \frac{1}{2}, z$	$4, 4_2, 4_2$	*F*432 (209)
4_1	$0, 0, z$	4_1	$0, \frac{1}{2}, z$	4_3	$-\frac{1}{4}, \frac{1}{4}, z$	4_3	$\frac{1}{4}, \frac{1}{4}, z$	4_3	$0, \frac{1}{2}, z$	$4_1, 4_3, 4_3$	*F*$4_1$32 (210)
$\bar{1}$	$0, 0, 0$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\bar{1}, \bar{1}, \bar{1}$	*Immm* (71), *Fmmm* (69)

This example illustrates in particular the occurrence of symmetry elements of screw or glide type even in the case of symmorphic space groups where all coset representatives $W = (\boldsymbol{W}, \boldsymbol{w})$ with respect to the translation subgroup can be chosen with $\boldsymbol{w} = \boldsymbol{o}$.

Note that, mainly for historical reasons, the screw rotations resulting from the threefold rotation along the [111] direction are not included in the extended Hermann–Mauguin symbol of cubic space groups, *cf.* Table 1.5.4.4. However, these screw rotations are represented in the cubic symmetry-element diagrams by the symbols

 and 

(*cf.* Table 2.1.2.7), as can be observed in the symmetry-element diagram for a group of type *P*23 (195) in Fig. 1.5.4.1.

Example 4

A twofold rotation $W = y, x, \bar{z}$ with the line $x, x, 0$ as geometric element has linear part

$$\boldsymbol{W} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}.$$

The composition W' of W with the translation $t(0, 1, 0)$ has intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and location part $\boldsymbol{w}'_l = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$. Since $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$, the symmetry operation $W' = y, x+\frac{1}{2}, \bar{z}$ is a screw rotation $2\,(\frac{1}{2},\frac{1}{2},0)\; x, x+\frac{1}{2}, 0$ with the line $x, x+\frac{1}{2}, 0$ as geometric element and is thus of a different type to W (*cf.* Table 1.5.4.1).

In an *I*-centred lattice, the composition of W with the centring translation $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ has intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and location part $\boldsymbol{w}'_l = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$. One has $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$, hence the symmetry operation $W' = y+\frac{1}{2}, x+\frac{1}{2}, \bar{z}+\frac{1}{2}$ is a screw rotation $2\,(\frac{1}{2},\frac{1}{2},0)\; x, x, \frac{1}{4}$ with the line $x, x, \frac{1}{4}$ as geometric element and is thus of a different type to W.

On the other hand, the translation subgroup $\mathcal{T}$ also contains the translation $t(\frac{1}{2},-\frac{1}{2},\frac{1}{2})$. In this case, the intrinsic translation part of $W' = y+\frac{1}{2}, x-\frac{1}{2}, \bar{z}+\frac{1}{2}$ is $\boldsymbol{w}'_g = \boldsymbol{o}$, hence W' is of the same type as W, *i.e.* a twofold rotation. The location part is $\boldsymbol{w}'_l = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$ and since $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{4} \end{pmatrix}$, the geometric element of W' is the line $x+\frac{1}{2}, x, \frac{1}{4}$.