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Table 4.1.2.3. *Additional symmetry elements due to a centring vector* **t** *and their locations*

Symmetry element at the origin		Additional symmetry elements									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, e	*Cmmm*, *Ammm*, *Bmmm* (65)
c		n		b		m		b			*Immm* (71), *Fmmm* (69)
b		m		c		n		c			*Cccm*, *Amaa*, *Bbmb* (66) *Ibca* (73)
e				e							*Aem*2 (39)
$d(0, \frac{1}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{3}{4})$		$d(0, \frac{1}{4}, \frac{3}{4})$				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, e	As above
a		m		n		c		c			
c		n		m		a		a			
e						e					*Fmm*2 (42)
$d(\frac{1}{4}, 0, \frac{1}{4})$		$d(\frac{3}{4}, 0, \frac{1}{4})$		$d(\frac{1}{4}, 0, \frac{3}{4})$		$d(\frac{3}{4}, 0, \frac{3}{4})$				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, e	As above
b		a		m		n		a			
a		b		n		m		b			
e		e									*Cmme* (67)
$d(\frac{1}{4}, \frac{1}{4}, 0)$		$d(\frac{3}{4}, \frac{3}{4}, 0)$		$d(\frac{1}{4}, \frac{3}{4}, 0)$		$d(\frac{3}{4}, \frac{1}{4}, 0)$				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), $F\bar{4}3m$ (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	$F\bar{4}3c$ (219)
e								e			*I*4*cm* (108)
$d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$								$d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$			$I\bar{4}3d$ (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	$0, \frac{1}{2}, z$	$4_1, 4_3, 4_3$	$F4_132$ (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)

Inversions. The 'midpoint rule' given under (i) for integral translations remains valid. When *M* occupies successively the eight positions of inversion centres in the primitive cell (*cf.* Table 4.1.2.1), each of the centrings *C, A, B* and *I* creates eight supplementary centres, whereas the *F* centring produces $3 \times 8 = 24$ supplementary centres, leading to a total of 32 inversion centres.

Example

For *C* centring, add $\frac{1}{4}, \frac{1}{4}, 0$ (*cf.* Table 4.1.2.3) to the eight locations of symmetry centres, given in Table 4.1.2.1, in order to obtain the eight additional symmetry centres $\frac{1}{4}, \frac{1}{4}, 0$; $\frac{3}{4}, \frac{1}{4}, 0$; $\frac{1}{4}, \frac{3}{4}, 0$; $\frac{3}{4}, \frac{3}{4}, 0$; $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$; $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$; $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$; $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$.

Table 4.1.2.3 contains only representative cases. For 4 and 4_1 axes, only the standard orientation [001] is given. For diagonal twofold axes, only the orientation $[\bar{1}10]$ is considered. When the locations of *all* additional symmetry elements of a chosen species are desired, it is sufficient to insert the location of one of the elements into the coordinate triplets of the general position and to remove redundancies.

Example

Insert the location $x, x+\frac{2}{3}, x+\frac{1}{3}$ of a 3_1 axis (see Table 4.1.2.2) into the general position of a cubic space group to obtain four distinct locations of 3_1 axes in *P* groups and sixteen in *F* groups.

4.1.2.3. *The priority rule*

When more than one kind of symmetry element occurs for a given symmetry direction, the question of choice arises for defining the appropriate Hermann–Mauguin symbol. This choice is made in order of descending priority:

m, *e*, *a*, *b*, *c*, *n*, *d*; and rotation axes before screw axes.

This *priority rule* is explicitly stated in *IT* (1952), pages 55 and 543. It is applied to the space-group symbols in *IT* (1952) and the present edition. There are a few exceptions, however:

(i) For glide planes in *centred monoclinic* space groups, the priority rule is purposely not followed in this volume, in order to bring out the relations between the three 'cell choices' given for each setting (*cf.* Sections 2.2.16 and 4.3.2).

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(ii) For *orthorhombic* space groups, the priority rule is applied only to the 'standard symbol'. The symbols for the other five settings are obtained from the standard symbol by the appropriate transformations, without invoking the priority rule again (*cf.* Table 4.3.2.1).

(iii) Space groups $I222$ (23) and $I2_12_12_1$ (24) are two distinct groups. Both contain parallel twofold rotation and screw axes and thus would receive the same symbol according to the priority rule. In $I222$, the three rotation axes and the three screw axes intersect, whereas in $I2_12_12_1$ neither the three rotation axes nor the three screw axes intersect (*cf.* Section 4.3.3).

(iv) For space group No. 73, the standard symbol *Ibca* was adopted, instead of *Ibaa* according to the rule, because *Ibca* displays the equivalence of the three symmetry directions clearly.

(v) The full symbols of space groups *Ibca* (73) and *Imma* (74) were written $I2/b\ 2/c\ 2/a$ and $I2/m\ 2/m\ 2/a$ in *IT* (1952), in application of the priority rule. In the present edition, these symbols are changed to $I2_1/b\,2_1/c\,2_1/a$ and $I2_1/m\,2_1/m\,2_1/a$, because both space groups contain $I2_12_12_1$ (and not $I222$) as subgroup.

(vi) In *tetragonal* space groups with both *a* and *b* glide planes parallel to [001], the preference was given to *b*, as in *P*4*bm* (100).

(vii) In *cubic* space groups where tertiary symmetry planes with glide components $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$ and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ coexist, the tertiary symmetry element was called *n* in *P* groups (instead of *a*, *b* or *c*) but *c* in *F* groups, because these symmetry elements intersect the origin.

(viii) Space groups $I23$ (197) and $I2_13$ (199) are two distinct space groups. For this pair, the same arguments apply as given above for $I222$ and $I2_12_12_1$.