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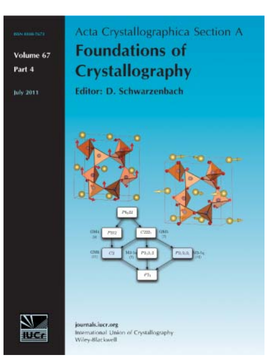

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Seitz notation for symmetry operations of space groups

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Space-group symmetry operations are given a geometric description and a shorthand matrix notation in *International Tables for Crystallography*, Volume A, *Space-Group Symmetry*. We give here the space-group symmetry operations subtables with the corresponding Seitz (R|**t**) notation for each included symmetry operation.

International Tables for Crystallography, Volume A, *Space-Group Symmetry* (2005) (abbreviated here as *ITC-A*) and its forerunner *International Tables for X-ray Crystallography*, Volume I, *Symmetry Groups* (1976) (abbreviated here as *ITC52*) have provided the scientific community with its main source of information on crystallographic symmetry in direct or physical space. These volumes have been widely used, designed, as stated on the home page of the online version of *International Tables for Crystallography*, Volume A, 'not only for professional crystallographers, but also for chemists, physicists, mineralogists, biologists and material scientists who employ crystallographic methods and who are concerned with the structure and the properties of crystalline materials.'

One of the central properties of the space groups given in these volumes is the set of symmetry operations of each of the space groups. Let **G** denote a space group and **T** its translational subgroup. The space group **G** can be written as a left *coset decomposition* with respect to its translational subgroup **T** as

$$\mathbf{G} = \mathbf{T} + g_2\mathbf{T} + \ldots + g_n\mathbf{T}, \tag{1}$$

i.e. decomposed into *n cosets* $g_i\mathbf{T}$, $i = 1, 2, \ldots, n$. The elements g_i, $i = 1, 2, \ldots, n$ are referred to as *coset representatives*. To specify the symmetry operations of a space group **G**, one can specify the translational subgroup **T**, and the symmetry operations g_i, $i = 1, 2, \ldots, n$, *i.e.* the symmetry operations corresponding to the set of coset representatives g_i, $i = 1, 2, \ldots, n$.

In *ITC52* the symmetry operations of the space groups were provided only indirectly by symbols representing translational groups **T** and by the general positions representing the symmetry operations g_i, $i = 1, 2, \ldots, n$ of equation (1): the general positions are interpreted as a shorthand description of the symmetry operations in matrix notation. For example, a general position '$\bar{x}$, $y + \frac{1}{2}$, $\bar{z}$' is a shorthand description of the matrix notation describing the symmetry operation of a rotation of 180° about the *y* axis followed by a translation of one-half the shortest lattice translation along the *y* axis. For centered space groups, the translational subgroup **T** is decomposed as

$$\mathbf{T} = \mathbf{T}_P + t_2\mathbf{T}_P + \ldots + t_m\mathbf{T}_P, \tag{2}$$

where the t_i, $i = 1, 2, \ldots, m$ are the *centering translations*, and the notation

$$(t_1)+ \quad (t_2)+ \quad \ldots \quad (t_m)+ \tag{3}$$

with each centering translation given as a trio of numbers is placed above the general positions. For example, above the general positions of the face-centered space group *F*23 one finds:

$$(0, 0, 0)+ \quad \left(0, \tfrac{1}{2}, \tfrac{1}{2}\right)+ \quad \left(\tfrac{1}{2}, 0, \tfrac{1}{2}\right)+ \quad \left(\tfrac{1}{2}, \tfrac{1}{2}, 0\right)+ \tag{4}$$

In *ITC-A*, in addition to representing the symmetry operations indirectly by symbols representing translational groups **T** and by general positions representing the symmetry operations g_i, $i = 1, 2, \ldots, n$ of equation (1), a second *geometric description* of the symmetry operations g_i, $i = 1, 2, \ldots, n$ was introduced under the heading 'Symmetry operations'. In this geometric description the previous symmetry operation is given as '2 $(0, \frac{1}{2}, 0)$ $0, y, 0$', where the '2' denotes a rotation of 360°/2 = 180°, '$0, y, 0$' the orientation and position of the axis of rotation, *i.e.* along the *y* direction passing through $x = z = 0$, and '$(0, \frac{1}{2}, 0)$' a translation of one-half the shortest lattice translation along the *y* axis. For space groups without centering translations, the format of a 'Symmetry operations' subtable is

$$\begin{array}{l}\textbf{Symmetry operations}\\ g_i, i = 1, 2, \ldots, n\end{array} \tag{5}$$

with the g_i, $i = 1, 2, \ldots, n$ given in this geometric description notation. For space groups with centering translations, the format is:

$$\begin{array}{l}\textbf{Symmetry operations}\\ (0, 0, 0)+ \ \text{set}\\ g_i, i = 1, 2, \ldots, n\\ \\ (t_2)+ \ \text{set}\\ t_2 g_i, i = 1, 2, \ldots, n\\ \quad\vdots\\ (t_m)+ \ \text{set}\\ t_m g_i, i = 1, 2, \ldots, n.\end{array} \tag{6}$$

In addition to this general-position shorthand description of the matrix notation of symmetry operations and the geometric description of symmetry operations, there is a third notation which has been adopted and is used by solid-state physicists (Burns & Glazer, 2007). This is the so-called *Seitz notation* (R|**t**) introduced by Seitz (1934, 1935*a*,*b*, 1936) in a series of papers on the matrix–algebraic development of the crystallographic groups. In this notation 'R' denotes a

1	2a	2b	2c	3	4	5	6	7	8	9	10	11	12
1)	1		x,y,z	1	e	E	E	1	1	h_1	E	ε	1
2)	2	0,0,z	$\bar{x},\bar{y},z$	2_z	2_z	C_{2z}	C_{2z}	2_z	4_3^2	h_4	U^z	δ_{2z}	4
3)	2	0,y,0	$\bar{x},y,\bar{z}$	2_y	2_y	C_{2y}	C_{2y}	2_y	4_2^2	h_3	U^y	δ_{2y}	3
4)	2	x,0,0	$x,\bar{y},\bar{z}$	2_x	2_x	C_{2x}	C_{2x}	2_x	4_1^2	h_2	U^x	δ_{2x}	2
5)	3^+	x,x,x	z,x,y	3_{xyz}	3_p	C_{31}^+	C_{31}^+	3_δ	3_1	h_9	C_3^{xyz}	δ_{3xyz}	9
6)	3^+	$\bar{x},x,\bar{x}$	$z,\bar{x},\bar{y}$	$3_{x\bar{y}z}^{-1}$	3_s	C_{34}^+	C_{34}^+	3_β	3_3	h_{10}	$C_3^{2x\bar{y}z}$	$\delta_{3\bar{x}y\bar{z}}$	10
7)	3^+	$x,\bar{x},\bar{x}$	$\bar{z},\bar{x},y$	$3_{\bar{x}yz}^{-1}$	3_r	C_{33}^+	C_{33}^+	3_α	3_4	h_{12}	$C_3^{2\bar{x}yz}$	$\delta_{3x\bar{y}\bar{z}}$	12
8)	3^+	$\bar{x},\bar{x},x$	$\bar{z},x,\bar{y}$	$3_{xy\bar{z}}^{-1}$	3_q	C_{32}^+	C_{32}^+	3_γ	3_2	h_{11}	$C_3^{2xy\bar{z}}$	$\delta_{3\bar{x}\bar{y}z}$	11
9)	3^-	x,x,x	y,z,x	3_{xyz}^{-1}	3_p^2	C_{31}^-	C_{31}^-	3_δ^2	3_1^2	h_5	C_3^{2xyz}	δ_{3xyz}^{-1}	5
10)	3^-	$x,\bar{x},\bar{x}$	$\bar{y},z,\bar{x}$	$3_{\bar{x}yz}$	3_r^2	C_{33}^-	C_{33}^-	3_α^2	3_4^2	h_7	$C_3^{\bar{x}yz}$	$\delta_{3x\bar{y}\bar{z}}^{-1}$	7
11)	3^-	$\bar{x},\bar{x},x$	$y,\bar{z},\bar{x}$	$3_{xy\bar{z}}$	3_q^2	C_{32}^-	C_{32}^-	3_γ^2	3_2^2	h_6	$C_3^{xy\bar{z}}$	$\delta_{3\bar{x}\bar{y}z}^{-1}$	6
12)	3^-	$\bar{x},x,\bar{x}$	$\bar{y},\bar{z},x$	$3_{x\bar{y}z}$	3_s^2	C_{34}^-	C_{34}^-	3_β^2	3_3^2	h_8	$C_3^{x\bar{y}z}$	$\delta_{3\bar{x}y\bar{z}}^{-1}$	8
13)	2	x,x,0	$y,x,\bar{z}$	2_{xy}	2_{xy}	C_{2a}	C'_{2a}	2_e	2_1	h_{16}	U^{xy}	δ_{xy}	16
14)	2	$x,\bar{x},0$	$\bar{y},\bar{x},\bar{z}$	$2_{\bar{x}y}$	$2_{x\bar{y}}$	C_{2b}	C'_{2b}	2_f	2_2	h_{13}	$U^{\bar{x}y}$	$\delta_{\bar{x}y}$	13
15)	4^-	0,0,z	$y,\bar{x},z$	4_z^{-1}	4_z^3	C_{4z}^-	C_{4z}^-	4_z^3	4_3^3	h_{15}	C_4^{3z}	δ_{4z}^{-1}	15
16)	4^+	0,0,z	$\bar{y},x,z$	4_z	4_z	C_{4z}^+	C_{4z}^+	4_z	4_3	h_{14}	C_4^z	δ_{4z}	14
17)	4^-	x,0,0	$x,z,\bar{y}$	4_x^{-1}	4_x^3	C_{4x}^-	C_{4x}^-	4_x^3	4_1^3	h_{20}	C_4^{3x}	δ_{4x}^{-1}	20
18)	2	0,y,y	$\bar{x},z,y$	2_{yz}	2_{yz}	C_{2d}	C'_{2d}	2_a	2_5	h_{18}	U^{yz}	δ_{yz}	18
19)	2	$0,y,\bar{y}$	$\bar{x},\bar{z},\bar{y}$	$2_{\bar{y}z}$	$2_{y\bar{z}}$	C_{2f}	C'_{2f}	2_b	2_6	h_{17}	$U^{\bar{y}z}$	$\delta_{\bar{y}z}$	17
20)	4^+	x,0,0	$x,\bar{z},y$	4_x	4_x	C_{4x}^+	C_{4x}^+	4_x	4_1	h_{19}	C_4^x	δ_{4x}	19
21)	4^+	0,y,0	$z,y,\bar{x}$	4_y	4_y	C_{4y}^+	C_{4y}^+	4_y	4_2	h_{24}	C_4^y	δ_{4y}	24
22)	2	x,0,x	$z,\bar{y},x$	2_{xz}	2_{zx}	C_{2c}	C'_{2c}	2_c	2_3	h_{23}	U^{xz}	δ_{xz}	23
23)	4^-	0,y,0	$\bar{z},y,x$	4_y^{-1}	4_y^3	C_{4y}^-	C_{4y}^-	4_y^3	4_2^3	h_{22}	C_4^{3y}	δ_{4y}^{-1}	22
24)	2	$\bar{x},0,x$	$\bar{z},\bar{y},\bar{x}$	$2_{\bar{x}z}$	$2_{z\bar{x}}$	C_{2e}	C'_{2e}	2_d	2_4	h_{21}	$U^{\bar{x}z}$	$\delta_{\bar{x}z}$	21
25)	$\bar{1}$	0,0,0	$\bar{x},\bar{y},\bar{z}$	$\bar{1}$	i	I	i	$\bar{1}$	$\tilde{2}$	h_{25}	I	i	25
26)	m	x,y,0	$x,y,\bar{z}$	m_z	m_z	σ_z	σ_z	m_z	m_3	h_{28}	σ^z	ρ_z	28
27)	m	x,0,z	$x,\bar{y},z$	m_y	m_y	σ_y	σ_y	m_y	m_2	h_{27}	σ^y	ρ_y	27
28)	m	0,y,z	$\bar{x},y,z$	m_x	m_x	σ_x	σ_x	m_x	m_1	h_{26}	σ^x	ρ_x	26
29)	$\bar{3}^+$	x,x,x	$\bar{z},\bar{x},\bar{y}$	$\bar{3}_{xyz}$	$\bar{3}_p$	S_{61}^-	S_{61}^-	$\bar{3}_\delta$	$\tilde{6}_1^5$	h_{33}	S_6^{5xyz}	σ_{6xyz}	33
30)	$\bar{3}^+$	$\bar{x},x,\bar{x}$	$\bar{z},x,y$	$\bar{3}_{x\bar{y}z}^{-1}$	$\bar{3}_s$	S_{64}^-	S_{64}^-	$\bar{3}_\beta$	$\tilde{6}_3^5$	h_{34}	$S_6^{x\bar{y}z}$	$\sigma_{6\bar{x}y\bar{z}}$	34
31)	$\bar{3}^+$	$x,\bar{x},\bar{x}$	$z,x,\bar{y}$	$\bar{3}_{\bar{x}yz}^{-1}$	$\bar{3}_r$	S_{63}^-	S_{63}^-	$\bar{3}_\alpha$	$\tilde{6}_4^5$	h_{36}	$S_6^{\bar{x}yz}$	$\sigma_{6x\bar{y}\bar{z}}$	36
32)	$\bar{3}^+$	$\bar{x},\bar{x},x$	$z,\bar{x},y$	$\bar{3}_{xy\bar{z}}^{-1}$	$\bar{3}_q$	S_{62}^-	S_{62}^-	$\bar{3}_\gamma$	$\tilde{6}_2^5$	h_{35}	$S_6^{xy\bar{z}}$	$\sigma_{6\bar{x}\bar{y}z}$	35
33)	$\bar{3}^-$	x,x,x	$\bar{y},\bar{z},\bar{x}$	$\bar{3}_{xyz}^{-1}$	$\bar{3}_p^5$	S_{61}^+	S_{61}^+	$\bar{3}_\delta^2$	$\tilde{6}_1$	h_{29}	S_6^{xyz}	σ_{6xyz}^{-1}	29
34)	$\bar{3}^-$	$x,\bar{x},\bar{x}$	$y,\bar{z},x$	$\bar{3}_{\bar{x}yz}$	$\bar{3}_r^5$	S_{63}^+	S_{63}^+	$\bar{3}_\alpha^2$	$\tilde{6}_4$	h_{31}	$S_6^{5\bar{x}yz}$	$\sigma_{6x\bar{y}\bar{z}}^{-1}$	31
35)	$\bar{3}^-$	$\bar{x},\bar{x},x$	$\bar{y},z,x$	$\bar{3}_{xy\bar{z}}$	$\bar{3}_q^5$	S_{62}^+	S_{62}^+	$\bar{3}_\gamma^2$	$\tilde{6}_2$	h_{30}	$S_6^{5xy\bar{z}}$	$\sigma_{6\bar{x}\bar{y}z}^{-1}$	30
36)	$\bar{3}^-$	$\bar{x},x,\bar{x}$	$y,z,\bar{x}$	$\bar{3}_{x\bar{y}z}$	$\bar{3}_s^5$	S_{64}^+	S_{64}^+	$\bar{3}_\beta^2$	$\tilde{6}_3$	h_{32}	$S_6^{5x\bar{y}z}$	$\sigma_{6\bar{x}y\bar{z}}^{-1}$	32
37)	m	$x,\bar{x},z$	$\bar{y},\bar{x},z$	m_{xy}	m_{xy}	σ_{da}	σ_{d1}	m_e	m_5	h_{40}	σ^{xy}	ρ_{xy}	40
38)	m	x,x,z	y,x,z	$m_{\bar{x}y}$	$m_{x\bar{y}}$	σ_{db}	σ_{d2}	m_f	m_4	h_{37}	$\sigma^{\bar{x}y}$	$\rho_{\bar{x}y}$	37
39)	$\bar{4}^-$	0,0,z	$\bar{y},x,\bar{z}$	$\bar{4}_z^{-1}$	$\bar{4}_z^3$	S_{4z}^+	S_{4z}^+	$\bar{4}_z^3$	$\tilde{4}_3$	h_{39}	S_4^z	σ_{4z}^{-1}	39
40)	$\bar{4}^+$	0,0,z	$y,\bar{x},\bar{z}$	$\bar{4}_z$	$\bar{4}_z$	S_{4z}^-	S_{4z}^-	$\bar{4}_z$	$\tilde{4}_3^3$	h_{38}	S_4^{3z}	σ_{4z}	38
41)	$\bar{4}^-$	x,0,0	$\bar{x},\bar{z},y$	$\bar{4}_x^{-1}$	$\bar{4}_x^3$	S_{4x}^+	S_{4x}^+	$\bar{4}_x^3$	$\tilde{4}_1$	h_{44}	S_4^x	σ_{4x}^{-1}	44
42)	m	$x,y,\bar{y}$	$x,\bar{z},\bar{y}$	m_{yz}	m_{yz}	σ_{dd}	σ_{d4}	m_a	m_9	h_{42}	σ^{yz}	ρ_{yz}	42
43)	m	x,y,y	x,z,y	$m_{\bar{y}z}$	$m_{y\bar{z}}$	σ_{df}	σ_{d6}	m_b	m_8	h_{41}	$\sigma^{\bar{y}z}$	$\rho_{\bar{y}z}$	41
44)	$\bar{4}^+$	x,0,0	$\bar{x},z,\bar{y}$	$\bar{4}_x$	$\bar{4}_x$	S_{4x}^-	S_{4x}^-	$\bar{4}_x$	$\tilde{4}_1^3$	h_{43}	S_4^{3x}	σ_{4x}	43
45)	$\bar{4}^+$	0,y,0	$\bar{z},\bar{y},x$	$\bar{4}_y$	$\bar{4}_y$	S_{4y}^-	S_{4y}^-	$\bar{4}_y$	$\tilde{4}_2^3$	h_{48}	S_4^{3y}	σ_{4x}	48
46)	m	$\bar{x},y,x$	$\bar{z},y,\bar{x}$	m_{xz}	m_{zx}	σ_{dc}	σ_{d3}	m_c	m_7	h_{47}	σ^{xz}	ρ_{xz}	47
47)	$\bar{4}^-$	0,y,0	$z,\bar{y},\bar{x}$	$\bar{4}_y^{-1}$	$\bar{4}_y^3$	S_{4y}^+	S_{4y}^+	$\bar{4}_y^3$	$\tilde{4}_2$	h_{46}	S_4^y	σ_{4x}^{-1}	46
48)	m	x,y,x	z,y,x	$m_{\bar{x}z}$	$m_{z\bar{x}}$	σ_{de}	σ_{d5}	m_d	m_6	h_{45}	$\sigma^{\bar{x}z}$	$\rho_{\bar{z}x}$	45

Figure 1
Comparison table of notation used for the point-group R operation of Seitz notation and the corresponding symbols used in *ITC-A*: cubic point-group operations.

rotation or rotation–inversion through the origin of the coordinate system used, and '**t**' is a translation. The identity, product and inverse of symmetry operations are written, in Seitz notation, as

$$\begin{aligned}
&(1|0,0,0)\\
&(\mathrm{R}_1|\mathbf{t}_1)(\mathrm{R}_2|\mathbf{t}_2) = (\mathrm{R}_1\mathrm{R}_2|\mathrm{R}_1\mathbf{t}_2 + \mathbf{t}_1)\\
&(\mathrm{R}|\mathbf{t})^{-1} = (\mathrm{R}^{-1}|-\mathrm{R}^{-1}\mathbf{t}).
\end{aligned} \tag{7}$$

For each symmetry operation $\mathbf{t}_i g_j$, $i = 1, 2, \ldots, m$; $j = 1, 2, \ldots, n$ which appears in the 'Symmetry operation' subtable of each space group we have added, below the geometric notation, its corresponding Seitz notation.[1] For example, for the space group $P4_2mc$ we have:

Symmetry operations

(1) 1	(2) 2 0, 0, z	(3) 4^+ $(0, 0, \frac{1}{2})$ 0, 0, z	(4) 4^- $(0, 0, \frac{1}{2})$ 0, 0, z
$(1\|0, 0, 0)$	$(2_z\|0, 0, 0)$	$(4_z\|0, 0, \frac{1}{2})$	$(4z^{-1}\|0, 0, \frac{1}{2})$
(5) m x, 0, z	(6) m 0, y, z	(7) c $x, \bar{x}, z$	(8) c x, x, z
$(m_y\|0, 0, 0)$	$(m_x\|0, 0, 0)$	$(m_{xy}\|0, 0, \frac{1}{2})$	$(m_{\bar{x}y}\|0, 0, \frac{1}{2})$

The R-symbol notation of the Seitz notation (R|**t**) used in these tables is that used for the Seitz notation in the symmetry-operations tables in *International Tables for Crystallography*, Volume E, *Subperiodic Groups* (2010) and in the international-like tables of properties of both magnetic subperiodic groups (Litvin, 2005) and magnetic space groups (Litvin, 2008). However, there is a wide variety of notation used for the symbol R in Seitz notation and consequently we have included in Appendix *A* a conversion table for ten varieties of notations used for the symbol R.

APPENDIX *A*

We compare here the notation used for the point-group operation R of Seitz symbols (R| **t**) in the supplementary material 'Seitz nota-

[1] Supplementary tables 'Seitz notation for symmetry operations of one-, two- and three-dimensional space groups' are available from the IUCr electronic archives (Reference: PZ5089). Services for accessing these archives are described at the back of the journal. These tables may also be downloaded from http://www.bk.psu.edu/faculty/Litvin/download.html.

1	2a	2b	2c	3	4	5	6	7	8	9	10	11	12
1)	1		x,y,z	1	e	E	E	1	1	h_1	E	ε	1
2)	3^+	0,0,z	$\bar{y},x-y,z$	3_z	3_z	C_3^+	C_3^+	3	6^2	h_3	C_6^{2z}	δ_{3z}	3
3)	3^-	0,0,z	$\bar{x}+y,\bar{x},z$	3_z^{-1}	3_z^2	C_3^-	C_3^-	3^2	6^4	h_5	C_6^{4z}	δ_{3z}^{-1}	5
4)	2	0,0,z	$\bar{x},\bar{y},z$	2_z	2_z	C_2	C_2	2	6^3	h_4	C_2	δ_{2z}	4
5)	6^-	0,0,z	$y,\bar{x}+y,z$	6_z^{-1}	6_z^5	C_6^-	C_6^-	6^5	6^5	h_6	C_6^{5z}	δ_{6z}^{-1}	6
6)	6^+	0,0,z	x-y,x,z	6_z	6_z	C_6^+	C_6^+	6	6	h_2	C_6^z	δ_{6z}	2
7)	2	x,x,0	$y,x,\bar{z}$	2_{xy}	$2_{x''}$	C''_{23}	C''_{23}	2_5	2_5	h_{11}	U^{xy}	δ'_{22}	9
8)	2	x,0,0	$x-y,\bar{y},\bar{z}$	2_x	2_x	C''_{21}	C''_{21}	2_1	2_1	h_9	U^x	δ'_{24}	7
9)	2	0,y,0	$\bar{x},\bar{x}+y,\bar{z}$	2_y	$2_{x'}$	C''_{22}	C''_{22}	2_3	2_3	h_7	U^y	δ'_{23}	11
10)	2	$x,\bar{x},0$	$\bar{y},\bar{x},\bar{z}$	2_3	$2_{y''}$	C'_{23}	C'_{23}	2_6	2_2	h_8	U^3	δ''_{22}	12
11)	2	x,2x,0	$\bar{x}+y,y,\bar{z}$	2_2	2_y	C'_{21}	C'_{21}	2_2	2_4	h_{12}	U^2	δ''_{24}	10
12)	2	2x,x,0	$x,x-y,\bar{z}$	2_1	$2_{y'}$	C'_{22}	C'_{22}	2_4	2_6	h_{10}	U^1	δ''_{23}	8
13)	$\bar{1}$	0,0,0	$\bar{x},\bar{y},\bar{z}$	$\bar{1}$	i	I	i	$\bar{1}$	$\tilde{2}$	h_{13}	I	i	13
14)	$\bar{3}^+$	0,0,z	$y,\bar{x}+y,\bar{z}$	$\bar{3}_z$	$\bar{3}_z$	S_6^-	S_6^-	$\bar{3}$	$\tilde{6}^5$	h_{15}	S_6^{5z}	σ_6	15
15)	$\bar{3}^-$	0,0,z	$x-y,x,\bar{z}$	$\bar{3}_z^{-1}$	$\bar{3}_z^5$	S_6^+	S_6^+	$\bar{3}^2$	$\tilde{6}$	h_{17}	S_6^z	σ_6^{-1}	17
16)	m	x,y,0	$x,y,\bar{z}$	m_z	m_z	σ_h	m	m	m	h_{16}	σ^z	σ	16
17)	$\bar{6}^-$	0,0,z	$\bar{y},x-y,\bar{z}$	$\bar{6}_z^{-1}$	$\bar{6}^5$	S_3^+	S_3^+	$\bar{6}^5$	$\tilde{3}$	h_{18}	S_3^z	σ_3^{-1}	18
18)	$\bar{6}^+$	0,0,z	$\bar{x}+y,\bar{x},\bar{z}$	$\bar{6}_z$	$\bar{6}_z$	S_3^-	S_3^-	$\bar{6}$	$\tilde{3}^5$	h_{14}	S_3^{2z}	σ_3	14
19)	m	$x,\bar{x},z$	$\bar{y},\bar{x},z$	m_{xy}	$m_{x''}$	σ_{v3}	σ_{v3}	m_5	m_2	h_{23}	σ^{xy}	σ'_{22}	21
20)	m	x,2x,z	$\bar{x}+y,y,z$	m_x	m_x	σ_{v1}	σ_{v1}	m_1	m_6	h_{21}	σ^x	σ'_{24}	19
21)	m	2x,x,z	x,x-y,z	m_y	$m_{x'}$	σ_{v2}	σ_{v2}	m_3	m_4	h_{19}	σ^y	σ'_{23}	23
22)	m	x,x,z	y,x,z	m_3	$m_{y''}$	σ_{d3}	σ_{d3}	m_6	m_5	h_{20}	σ^3	σ''_{22}	24
23)	m	x,0,z	$x-y,\bar{y},z$	m_2	m_y	σ_{d1}	σ_{d1}	m_2	m_3	h_{24}	σ^2	σ''_{24}	22
24)	m	0,y,z	$\bar{x},\bar{x}+y,z$	m_1	$m_{y'}$	σ_{d2}	σ_{d2}	m_4	m_1	h_{22}	σ^1	σ''_{23}	20

Figure 2
Comparison table of notation used for the point-group R operation of Seitz notation and the corresponding symbols used in *ITC-A*: hexagonal point-group operations.

1	2a	2b	2c	3
1)	1		x,y,z	1
2)	3^+	x,x,x	z,x,y	3_{xyz}
3)	3^-	x,x,x	y,z,x	3_{xyz}^{-1}
4)	2	$x,\bar{x},0$	$\bar{y},\bar{x},\bar{z}$	$2_{\bar{x}y}$
5)	2	$0,y,\bar{y}$	$\bar{x},\bar{z},\bar{y}$	$2_{\bar{y}z}$
6)	2	$\bar{x},0,x$	$\bar{z},\bar{y},\bar{x}$	$2_{\bar{x}z}$
7)	$\bar{1}$	0,0,0	$\bar{x},\bar{y},\bar{z}$	$\bar{1}$
8)	$\bar{3}^+$	x,x,x	$\bar{z},\bar{x},\bar{y}$	$\bar{3}_{xyz}$
9)	$\bar{3}^-$	x,x,x	$\bar{y},\bar{z},\bar{x}$	$\bar{3}_{xyz}^{-1}$
10)	m	x,x,z	y,x,z	$m_{\bar{x}y}$
11)	m	x,y,y	x,z,y	$m_{\bar{y}z}$
12)	m	x,y,x	z,y,x	$m_{\bar{x}z}$

Figure 3
Comparison table of notation used for the point-group R operation of Seitz notation and the corresponding symbols used in *ITC-A*: trigonal space groups with rhombohedral coordinate axes.

tion for symmetry operations of one-, two- and three-dimensional space groups' with the corresponding symbols used in *ITC-A* and in other sets of symbols of point-group operations. The comparison table is divided into three parts, the first for cubic point-group operations (Fig. 1), the second for hexagonal point-group operations (Fig. 2), and the third for the point-group-operation notation used in *ITC-A* for trigonal space groups described with rhombohedral coordinate axes (Fig. 3). Each subtable is divided into 12 columns, except for the third which contains only three and compares the point-group operations used in the Seitz symbols only to the corresponding symbols used in *ITC-A*:

Column (1). Sequential numbering of the point-group operations in each figure: this numbering also specifies the point-group operation as the point-group operation associated with the *symmetry operation* of the same number listed in *ITC-A* for, respectively, the cubic space group No. 221, $Pm\bar{3}m$, the hexagonal space group No. 191, $P6/mmm$, and the trigonal space group No. 166, $R\bar{3}m$, described in rhombohedral coordinate axes.

Columns (2*a*) and (2*b*). Point-group operation description taken from the geometric description of the symmetry operation given in *ITC-A*.

Column (2*c*). Corresponding coordinate triplets found in the *General positions* in *ITC-A*. These may be interpreted as a shorthand description of the point-group operation in matrix notation. This notation is also known as Jones faithful representation.

Column (3). Point-group notation used for R in the tabulations of 'Seitz notation for symmetry operations of one-, two- and three-dimensional space groups' in the supplementary material. This notation has been used in the Seitz notation given in Vol. E, *Subperiodic Groups* of *International Tables for Crystallography* (2010), and in the international-like tables of the properties of both magnetic subperiodic groups (Litvin, 2005) and magnetic space groups (Litvin, 2008).

Column (4). Point-group notation used in Chapter 3.4 of Vol. D of *International Tables of Crystallography*, *Physical Properties of Crystals* (Janovec & Privratska, 2003) and Kopský & Bocek (2003) in accompanying software.

Column (5). Point-group notation used by Bradley & Cracknell (1972).

Column (6). Point-group notation used by Altmann & Herzig (1994).

Column (7). Point-group notation used by Ascher (1966).

Column (8). Point-group notation used by Koptsik (1966, 1971).

Column (9). Point-group notation used by Kovalev (1965).

Column (10). Point-group notation used by Zak *et al.* (1969).

Column (11). Point-group notation used by Herring (1942, 1974).

Column (12). Point-group notation used by Miller & Love (1967).

References

Altmann, S. L. & Herzig, P. (1994). *Point Group Theory Tables*. Oxford: Clarendon Press.

Ascher, E. (1966). *Properties of Shubnikov Point Groups*, Part 1. Battelle Report, Geneva.

Bradley, C. J. & Cracknell, A. P. (1972). *The Mathematical Theory of Symmetry in Solids*. Oxford University Press.

Burns, G. & Glazer, A. M. (2007). *Space Groups for Solid State Physicists*, 2nd ed. New York: Academic Press.

Herring, C. (1942). *J. Franklin Inst.* **233**, 525–543.

Herring, C. (1974). *Character Tables for Two Space Groups*, Table 9.1.1 in *Symmetry Principles in Solid State and Molecular Physics*, edited by M. Lax. New York: Wiley-Interscience.

International Tables for Crystallography (2005). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn. Heidelberg: Springer. (Previous editions: 1983, 1987, 1995 and 2002.)

International Tables for Crystallography (2010). Vol. E, *Subperiodic Groups*, edited by V. Kopský & D. B. Litvin. Chichester: Wiley. (Previous edition: 2002.)

International Tables for X-ray Crystallography (1976). Vol. I, *Symmetry Groups*, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press. (Previous editions: 1952, 1965, 1969.)

Janovec, V. & Privratska, J. (2003). *International Tables for Crystallography*, Vol. D, *Physical Properties of Crystals*, edited by A. Authier, ch. 3.4, *Domain structures*. Dordrecht: Kluwer Academic Publishers.

Kopský, V. & Bocek, P. (2003). Supplementary software *GI*KoBo-1* to *International Tables for Crystallography*, Vol. D, *Physical Properties of Crystals*, edited by A. Authier. Dordrecht: Kluwer Academic Publishers.

Koptsik, V. A. (1966). *Shubnikov Groups. Handbook on the Symmetry and Physical Properties of Crystal Structures*. Moscow: Izd MGU.

Koptsik, V. A. (1971). *Shubnikov Groups. Handbook on the Symmetry and Physical Properties of Crystal Structures*, translated by J. Kopecky & B. O. Loopstra. Fysica Memo 175, Stichting, Reactor Centrum Nederlands.

Kovalev, O. V. (1965). *Irreducible Representations of the Space Groups*. New York: Gordon and Breach.

Litvin, D. B. (2005). *Acta Cryst.* A**61**, 382–385.

Litvin, D. B. (2008). *Acta Cryst.* A**64**, 419–424.

Miller, S. C. & Love, W. F. (1967). *Tables of Irreducible Representations of Space Groups and Co-Representations of Magnetic Space Groups*. Boulder: Pruett Press.

Seitz, F. (1934). *Z. Kristallogr.* **88**, 433–459.

Seitz, F. (1935*a*). *Z. Kristallogr.* **90**, 289–313.

Seitz, F. (1935*b*). *Z. Kristallogr.* **91**, 336–366.

Seitz, F. (1936). *Z. Kristallogr.* **94**, 100–130.

Zak, J., Casher, A., Gluck, M. & Gur, Y. (1969). *The Irreducible Representations of Space Groups*. New York: W. A. Benjamin, Inc.