

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

**Table 1.4.2.1**

Linear parts **R** of the Seitz symbols  $\{R|v\}$  for space-group symmetry operations of cubic, tetragonal, orthorhombic, monoclinic and triclinic crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix-column presentation, the type of symmetry operation and its characteristic direction.

IT A description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	$x, y, z$	1		1
2	$\bar{x}, \bar{y}, z$	2	0, 0, z	$2_{001}$
3	$\bar{x}, y, \bar{z}$	2	0, y, 0	$2_{010}$
4	$x, \bar{y}, \bar{z}$	2	x, 0, 0	$2_{100}$
5	$z, x, y$	$3^+$	x, x, x	$3_{111}^+$
6	$z, \bar{x}, \bar{y}$	$3^+$	$\bar{x}, x, \bar{x}$	$3_{1\bar{1}\bar{1}}^+$
7	$\bar{z}, \bar{x}, y$	$3^+$	x, $\bar{x}, \bar{x}$	$3_{\bar{1}\bar{1}1}^+$
8	$\bar{z}, x, \bar{y}$	$3^+$	$\bar{x}, \bar{x}, x$	$3_{\bar{1}1\bar{1}}^+$
9	$y, z, x$	$3^-$	x, x, x	$3_{111}^-$
10	$\bar{y}, z, \bar{x}$	$3^-$	x, $\bar{x}, \bar{x}$	$3_{1\bar{1}\bar{1}}^-$
11	$y, \bar{z}, \bar{x}$	$3^-$	$\bar{x}, \bar{x}, x$	$3_{\bar{1}\bar{1}1}^-$
12	$\bar{y}, \bar{z}, x$	$3^-$	$\bar{x}, x, \bar{x}$	$3_{\bar{1}1\bar{1}}^-$
13	$y, x, \bar{z}$	2	x, x, 0	$2_{110}$
14	$\bar{y}, \bar{x}, \bar{z}$	2	x, $\bar{x}, 0$	$2_{\bar{1}\bar{1}0}$
15	$y, \bar{x}, z$	$4^-$	0, 0, z	$4_{001}^-$
16	$\bar{y}, x, z$	$4^+$	0, 0, z	$4_{001}^+$
17	$x, z, \bar{y}$	$4^-$	x, 0, 0	$4_{100}^-$
18	$\bar{x}, z, y$	2	0, y, y	$2_{011}$
19	$\bar{x}, \bar{z}, \bar{y}$	2	0, y, $\bar{y}$	$2_{01\bar{1}}$
20	$x, \bar{z}, y$	$4^+$	x, 0, 0	$4_{100}^+$
21	$z, y, \bar{x}$	$4^+$	0, y, 0	$4_{010}^+$
22	$z, \bar{y}, x$	2	x, 0, x	$2_{101}$
23	$\bar{z}, y, x$	$4^-$	0, y, 0	$4_{010}^-$
24	$\bar{z}, \bar{y}, \bar{x}$	2	$\bar{x}, 0, x$	$2_{\bar{1}01}$
25	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
26	$x, y, \bar{z}$	<i>m</i>	x, y, 0	$m_{001}$
27	$x, \bar{y}, z$	<i>m</i>	x, 0, z	$m_{010}$
28	$\bar{x}, y, z$	<i>m</i>	0, y, z	$m_{100}$
29	$\bar{z}, \bar{x}, \bar{y}$	$\bar{3}^+$	x, x, x	$\bar{3}_{111}^+$
30	$\bar{z}, x, y$	$\bar{3}^+$	$\bar{x}, x, \bar{x}$	$\bar{3}_{1\bar{1}\bar{1}}^+$
31	$z, x, \bar{y}$	$\bar{3}^+$	x, $\bar{x}, \bar{x}$	$\bar{3}_{\bar{1}\bar{1}1}^+$
32	$z, \bar{x}, y$	$\bar{3}^+$	$\bar{x}, \bar{x}, x$	$\bar{3}_{\bar{1}1\bar{1}}^+$
33	$\bar{y}, \bar{z}, \bar{x}$	$\bar{3}^-$	x, x, x	$\bar{3}_{111}^-$
34	$y, \bar{z}, x$	$\bar{3}^-$	x, $\bar{x}, \bar{x}$	$\bar{3}_{1\bar{1}\bar{1}}^-$
35	$\bar{y}, z, x$	$\bar{3}^-$	$\bar{x}, \bar{x}, x$	$\bar{3}_{\bar{1}\bar{1}1}^-$
36	$y, z, \bar{x}$	$\bar{3}^-$	$\bar{x}, x, \bar{x}$	$\bar{3}_{\bar{1}1\bar{1}}^-$
37	$\bar{y}, \bar{x}, z$	<i>m</i>	x, $\bar{x}, z$	$m_{110}$
38	$y, x, z$	<i>m</i>	x, x, z	$m_{\bar{1}\bar{1}0}$
39	$\bar{y}, x, \bar{z}$	$\bar{4}^-$	0, 0, z	$\bar{4}_{001}^-$
40	$y, \bar{x}, \bar{z}$	$\bar{4}^+$	0, 0, z	$\bar{4}_{001}^+$
41	$\bar{x}, \bar{z}, y$	$\bar{4}^-$	x, 0, 0	$\bar{4}_{100}^-$
42	$x, \bar{z}, \bar{y}$	<i>m</i>	x, y, $\bar{y}$	$m_{011}$
43	$x, z, y$	<i>m</i>	x, y, y	$m_{01\bar{1}}$
44	$\bar{x}, z, \bar{y}$	$\bar{4}^+$	x, 0, 0	$\bar{4}_{100}^+$
45	$\bar{z}, \bar{y}, x$	$\bar{4}^+$	0, y, 0	$\bar{4}_{010}^+$
46	$\bar{z}, y, \bar{x}$	<i>m</i>	$\bar{x}, y, x$	$m_{101}$
47	$z, \bar{y}, \bar{x}$	$\bar{4}^-$	0, y, 0	$\bar{4}_{010}^-$
48	$z, y, x$	<i>m</i>	x, y, x	$m_{\bar{1}01}$

**Table 1.4.2.2**

Linear parts **R** of the Seitz symbols  $\{R|v\}$  for space-group symmetry operations of hexagonal and trigonal crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix-column presentation, the type of symmetry operation and its characteristic direction.

IT A description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	$x, y, z$	1		1
2	$\bar{y}, x - y, z$	$3^+$	0, 0, z	$3_{001}^+$
3	$\bar{x} + y, \bar{x}, z$	$3^-$	0, 0, z	$3_{001}^-$
4	$\bar{x}, \bar{y}, z$	2	0, 0, z	$2_{001}$
5	$y, \bar{x} + y, z$	$6^-$	0, 0, z	$6_{001}^-$
6	$x - y, x, z$	$6^+$	0, 0, z	$6_{001}^+$
7	$y, x, \bar{z}$	2	x, x, 0	$2_{110}$
8	$x - y, \bar{y}, \bar{z}$	2	x, 0, 0	$2_{100}$
9	$\bar{x}, \bar{x} + y, \bar{z}$	2	0, y, 0	$2_{010}$
10	$\bar{y}, \bar{x}, \bar{z}$	2	x, $\bar{x}, 0$	$2_{\bar{1}\bar{1}0}$
11	$\bar{x} + y, y, \bar{z}$	2	x, 2x, 0	$2_{120}$
12	$x, x - y, \bar{z}$	2	2x, x, 0	$2_{210}$
13	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
14	$y, \bar{x} + y, \bar{z}$	$\bar{3}^+$	0, 0, z	$\bar{3}_{001}^+$
15	$x - y, x, \bar{z}$	$\bar{3}^-$	0, 0, z	$\bar{3}_{001}^-$
16	$x, y, \bar{z}$	<i>m</i>	x, y, 0	$m_{001}$
17	$\bar{y}, x - y, \bar{z}$	$\bar{6}^-$	0, 0, z	$\bar{6}_{001}^-$
18	$\bar{x} + y, \bar{x}, \bar{z}$	$\bar{6}^+$	0, 0, z	$\bar{6}_{001}^+$
19	$\bar{y}, \bar{x}, z$	<i>m</i>	x, $\bar{x}, z$	$m_{110}$
20	$\bar{x} + y, y, z$	<i>m</i>	x, 2x, z	$m_{100}$
21	$x, x - y, z$	<i>m</i>	2x, x, z	$m_{010}$
22	$y, x, z$	<i>m</i>	x, x, z	$m_{1\bar{1}0}$
23	$x - y, \bar{y}, z$	<i>m</i>	x, 0, z	$m_{120}$
24	$\bar{x}, \bar{x} + y, z$	<i>m</i>	0, y, z	$m_{210}$

**Table 1.4.2.3**

Linear parts **R** of the Seitz symbols  $\{R|v\}$  for symmetry operations of rhombohedral space groups (rhombohedral-axes setting)

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix-column presentation, the type of symmetry operation and its characteristic direction.

IT A description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	$x, y, z$	1		1
2	$z, x, y$	$3^+$	x, x, x	$3_{111}^+$
3	$y, z, x$	$3^-$	x, x, x	$3_{111}^-$
4	$\bar{z}, \bar{y}, \bar{x}$	2	$\bar{x}, 0, x$	$2_{\bar{1}01}$
5	$\bar{y}, \bar{x}, \bar{z}$	2	x, $\bar{x}, 0$	$2_{\bar{1}\bar{1}0}$
6	$\bar{x}, \bar{z}, \bar{y}$	2	0, y, $\bar{y}$	$2_{01\bar{1}}$
7	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
8	$\bar{z}, \bar{x}, \bar{y}$	$\bar{3}^+$	x, x, x	$\bar{3}_{111}^+$
9	$\bar{y}, \bar{z}, \bar{x}$	$\bar{3}^-$	x, x, x	$\bar{3}_{111}^-$
10	$z, y, x$	<i>m</i>	x, y, x	$m_{\bar{1}01}$
11	$y, x, z$	<i>m</i>	x, x, z	$m_{1\bar{1}0}$
12	$x, z, y$	<i>m</i>	x, y, y	$m_{01\bar{1}}$