

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	$m_{01\bar{1}}$