

MPG No. 27.9.157  $6'/m'mm'$  ( $6'/m'm'm$  setting) [ Type III, hexagonal ]

Table 1: Wyckoff site:  $1\circ$ , site symmetry:  $6'/m'm'm$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 2: Wyckoff site:  $2a$ , site symmetry:  $6'm'm$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 10, 11, 12, 13, 14, 15, 22, 23, 24]$
2	$[0, 0, -z]$	$[4, 5, 6, 7, 8, 9, 16, 17, 18, 19, 20, 21]$

Table 3: Wyckoff site:  $6b$ , site symmetry:  $m'2'm$

No.	position	mapping
1	$[x, 0, 0]$	$[1, 4, 20, 23]$
2	$[0, x, 0]$	$[2, 5, 21, 24]$
3	$[-x, -x, 0]$	$[3, 6, 19, 22]$
4	$[-x, 0, 0]$	$[7, 10, 14, 17]$
5	$[0, -x, 0]$	$[8, 11, 15, 18]$
6	$[x, x, 0]$	$[9, 12, 13, 16]$

Table 4: Wyckoff site:  $6c$ , site symmetry:  $m'm'2$

No.	position	mapping
1	$[x, 2x, 0]$	$[1, 10, 17, 20]$
2	$[-2x, -x, 0]$	$[2, 11, 18, 21]$
3	$[x, -x, 0]$	$[3, 12, 16, 19]$
4	$[-x, -2x, 0]$	$[4, 7, 14, 23]$
5	$[2x, x, 0]$	$[5, 8, 15, 24]$
6	$[-x, x, 0]$	$[6, 9, 13, 22]$

Table 5: Wyckoff site:  $12d$ , site symmetry:  $\dots m$

No.	position	mapping
1	$[x, 0, z]$	$[1, 23]$
2	$[0, x, z]$	$[2, 24]$
3	$[-x, -x, z]$	$[3, 22]$

*continued ...*

Table 5

No.	position	mapping
4	$[-x, 0, z]$	[10,14]
5	$[0, -x, z]$	[11,15]
6	$[x, x, z]$	[12,13]
7	$[0, x, -z]$	[5,21]
8	$[x, 0, -z]$	[4,20]
9	$[-x, -x, -z]$	[6,19]
10	$[0, -x, -z]$	[8,18]
11	$[-x, 0, -z]$	[7,17]
12	$[x, x, -z]$	[9,16]

Table 6: Wyckoff site: 12e, site symmetry: .m'.

No.	position	mapping
1	$[x, 2x, z]$	[1,10]
2	$[-2x, -x, z]$	[2,11]
3	$[x, -x, z]$	[3,12]
4	$[-x, -2x, z]$	[14,23]
5	$[2x, x, z]$	[15,24]
6	$[-x, x, z]$	[13,22]
7	$[2x, x, -z]$	[5,8]
8	$[-x, -2x, -z]$	[4,7]
9	$[-x, x, -z]$	[6,9]
10	$[-2x, -x, -z]$	[18,21]
11	$[x, 2x, -z]$	[17,20]
12	$[x, -x, -z]$	[16,19]

Table 7: Wyckoff site: 12f, site symmetry: m'..

No.	position	mapping
1	$[x, y, 0]$	[1,20]
2	$[-y, x - y, 0]$	[2,21]
3	$[-x + y, -x, 0]$	[3,19]
4	$[-x, -y, 0]$	[7,14]
5	$[y, -x + y, 0]$	[8,15]
6	$[x - y, x, 0]$	[9,13]
7	$[y, x, 0]$	[5,24]
8	$[x - y, -y, 0]$	[4,23]
9	$[-x, -x + y, 0]$	[6,22]
10	$[-y, -x, 0]$	[11,18]
11	$[-x + y, y, 0]$	[10,17]
12	$[x, x - y, 0]$	[12,16]

Table 8: Wyckoff site: 24g, site symmetry: 1

No.	position	mapping
1	[ $x, y, z$ ]	[1]
2	[ $-y, x - y, z$ ]	[2]
3	[ $-x + y, -x, z$ ]	[3]
4	[ $-x, -y, z$ ]	[14]
5	[ $y, -x + y, z$ ]	[15]
6	[ $x - y, x, z$ ]	[13]
7	[ $y, x, -z$ ]	[5]
8	[ $x - y, -y, -z$ ]	[4]
9	[ $-x, -x + y, -z$ ]	[6]
10	[ $-y, -x, -z$ ]	[18]
11	[ $-x + y, y, -z$ ]	[17]
12	[ $x, x - y, -z$ ]	[16]
13	[ $-x, -y, -z$ ]	[7]
14	[ $y, -x + y, -z$ ]	[8]
15	[ $x - y, x, -z$ ]	[9]
16	[ $x, y, -z$ ]	[20]
17	[ $-y, x - y, -z$ ]	[21]
18	[ $-x + y, -x, -z$ ]	[19]
19	[ $-y, -x, z$ ]	[11]
20	[ $-x + y, y, z$ ]	[10]
21	[ $x, x - y, z$ ]	[12]
22	[ $y, x, z$ ]	[24]
23	[ $x - y, -y, z$ ]	[23]
24	[ $-x, -x + y, z$ ]	[22]