

MPG No. 27.5.104  $6'/m'mm'$  ( $6'/m'mm'$  setting) [ Type III, hexagonal ]

 Table 1: Wyckoff site: 1o, site symmetry:  $6'/m'mm'$ 

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:  $6'mm'$ 

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:  $m'2m$ 

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:  $m'm2$ 

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]