

MSG No. 194.263 $P6_3/mmc$ [Type I, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: -3m.

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

Table 2: Wyckoff site: 2b, site symmetry: -6m2

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

Table 3: Wyckoff site: 2c, site symmetry: -6m2

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

Table 4: Wyckoff site: 2d, site symmetry: -6m2

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

Table 5: Wyckoff site: 4e, site symmetry: 3m.

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

Table 6: Wyckoff site: 4f, site symmetry: 3m.

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

Table 7: Wyckoff site: 6g, site symmetry: .2/m.

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

Table 8: Wyckoff site: 6h, site symmetry: mm2

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

Table 9: Wyckoff site: 12i, site symmetry: .2.

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

continued ...

Table 9

No.	position	mapping
12	$[0, x, \frac{1}{2}]$	[18,24]

Table 10: Wyckoff site: 12j, site symmetry: $\mathbf{m}..$

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

Table 11: Wyckoff site: 12k, site symmetry: $.\mathbf{m}.$

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

Table 12: Wyckoff site: 24l, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x - y, x, z + \frac{1}{2}]$	[2]

continued ...

Table 12

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