MSG No. 191.235 $P6/m'mm$ [Type III, hexagonal]

Table 1: Wyckoff site: `1a`, 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: `1b`, site symmetry: `6/m'mm`

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	[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 3: Wyckoff site: `2c`, site symmetry: `-6'm2'`

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

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

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

Table 5: Wyckoff site: `2e`, site symmetry: `6mm`

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

Table 6: Wyckoff site: `3f`, site symmetry: `m'mm`

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

Table 7: Wyckoff site: `3g`, site symmetry: `m'mm`

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

Table 8: Wyckoff site: `4h`, site symmetry: `3m`.

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

Table 9: Wyckoff site: `6i`, site symmetry: `2mm`

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

Table 10: Wyckoff site: `6j`, site symmetry: `m'2'm`

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

Table 11: Wyckoff site: `6k`, site symmetry: `m'2'm`

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	[1,11,13,22]

continued ...

Table 11

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

Table 12: Wyckoff site: `6l`, site symmetry: `m'm2'`

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

Table 13: Wyckoff site: `6m`, site symmetry: `m'm2'`

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

Table 14: Wyckoff site: `12n`, site symmetry: `..m`

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

continued ...

Table 14

No.	position	mapping
11	$[-x, 0, -z]$	[17,19]
12	$[0, -x, -z]$	[18,21]

Table 15: Wyckoff site: 12o, site symmetry: .m.

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

Table 16: Wyckoff site: 12p, site symmetry: m'..

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

Table 17: Wyckoff site: 12q, site symmetry: m'..

No.	position	mapping
1	$\left[x, y, \frac{1}{2}\right]$	[1,22]

continued ...

4

Table 17

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

Table 18: Wyckoff site: `24r`, site symmetry: `1`

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