MSG No. 191.238 $P6'/m'm'm$ [Type III, hexagonal]

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

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'm'2`

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

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

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

Table 5: Wyckoff site: `2e`, 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 6: Wyckoff site: `3f`, site symmetry: `m'm'm`

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

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

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

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

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

Table 9: Wyckoff site: 6i, site symmetry: 2'm'm

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

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

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

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

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	[1,11,16,20]

continued ...

Table 11

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

Table 12: Wyckoff site: 6l, site symmetry: m'm'2

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

Table 13: Wyckoff site: 6m, site symmetry: m'm'2

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

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

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

continued ...

Table 14

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

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

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

Table 16: Wyckoff site: `12p`, 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	$[x,\ x-y,\ 0]$	`[4,24]`
5	$[-x+y,\ y,\ 0]$	`[5,22]`
6	$[-y,\ -x,\ 0]$	`[6,23]`
7	$[-x,\ -y,\ 0]$	`[7,14]`
8	$[y,\ -x+y,\ 0]$	`[8,15]`
9	$[x-y,\ x,\ 0]$	`[9,13]`
10	$[-x,\ -x+y,\ 0]$	`[10,18]`
11	$[x-y,\ -y,\ 0]$	`[11,16]`
12	$[y,\ x,\ 0]$	`[12,17]`

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

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	`[1,20]`

continued ...

Table 17

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

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

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