MSG No. 191.239 $P6'/m'mm'$ [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	$\left[\frac{1}{3}, \frac{2}{3}, 0\right]$	[1,2,3,10,11,12,16,17,18,19,20,21]
2	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	[4,5,6,7,8,9,13,14,15,22,23,24]

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

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: `6j`, 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 11: Wyckoff site: `6k`, site symmetry: `m'2m'`

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	`[1,4,20,23]`

continued ...

Table 11

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

Table 12: Wyckoff site: `6l`, 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 13: Wyckoff site: `6m`, site symmetry: `m'm2'`

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

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

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

continued ...

Table 14

No.	position	mapping
11	$[0,\ -x,\ z]$	`[11,15]`
12	$[x,\ x,\ z]$	`[12,13]`

Table 15: Wyckoff site: `12o`, 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	$[-x,\ -2x,\ -z]$	`[4,7]`
5	$[2x,\ x,\ -z]$	`[5,8]`
6	$[-x,\ x,\ -z]$	`[6,9]`
7	$[-x,\ x,\ z]$	`[13,22]`
8	$[-x,\ -2x,\ z]$	`[14,23]`
9	$[2x,\ x,\ z]$	`[15,24]`
10	$[x,\ -x,\ -z]$	`[16,19]`
11	$[x,\ 2x,\ -z]$	`[17,20]`
12	$[-2x,\ -x,\ -z]$	`[18,21]`

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

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	$\left[x-y,\, -y,\, \frac{1}{2}\right]$	[4,23]
5	$\left[y,\, x,\, \frac{1}{2}\right]$	[5,24]
6	$\left[-x,\, -x+y,\, \frac{1}{2}\right]$	[6,22]
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	$\left[-x+y,\, y,\, \frac{1}{2}\right]$	[10,17]
11	$\left[-y,\, -x,\, \frac{1}{2}\right]$	[11,18]
12	$\left[x,\, x-y,\, \frac{1}{2}\right]$	[12,16]

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	$[x-y,\, -y,\, -z]$	[4]
5	$[y,\, x,\, -z]$	[5]
6	$[-x,\, -x+y,\, -z]$	[6]
7	$[-x,\, -y,\, -z]$	[7]
8	$[y,\, -x+y,\, -z]$	[8]
9	$[x-y,\, x,\, -z]$	[9]
10	$[-x+y,\, y,\, z]$	[10]
11	$[-y,\, -x,\, z]$	[11]
12	$[x,\, x-y,\, z]$	[12]
13	$[x-y,\, x,\, z]$	[13]
14	$[-x,\, -y,\, z]$	[14]
15	$[y,\, -x+y,\, z]$	[15]
16	$[x,\, x-y,\, -z]$	[16]
17	$[-x+y,\, y,\, -z]$	[17]
18	$[-y,\, -x,\, -z]$	[18]
19	$[-x+y,\, -x,\, -z]$	[19]
20	$[x,\, y,\, -z]$	[20]
21	$[-y,\, x-y,\, -z]$	[21]
22	$[-x,\, -x+y,\, z]$	[22]
23	$[x-y,\, -y,\, z]$	[23]
24	$[y,\, x,\, z]$	[24]