MSG No. 191.241 $P6/m'm'm'$ [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	$\left[\frac{1}{3}, \frac{2}{3}, 0\right]$	`[1,3,5,10,11,12,14,16,18,19,20,21]`
2	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[2,4,6,7,8,9,13,15,17,22,23,24]`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	`[1,7,16,23]`

continued ...

Table 11

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

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

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

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

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

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

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

continued ...

Table 14

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	`[1,16]`

continued ...

Table 17

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

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	$[-x,\, -y,\, -z]$	[13]
14	$[-x+y,\, -x,\, -z]$	[14]
15	$[y,\, -x+y,\, -z]$	[15]
16	$[x,\, y,\, -z]$	[16]
17	$[x-y,\, x,\, -z]$	[17]
18	$[-y,\, x-y,\, -z]$	[18]
19	$[-x+y,\, y,\, z]$	[19]
20	$[-y,\, -x,\, z]$	[20]
21	$[x,\, x-y,\, z]$	[21]
22	$[-x,\, -x+y,\, z]$	[22]
23	$[x-y,\, -y,\, z]$	[23]
24	$[y,\, x,\, z]$	[24]