MSG No. 191.237 $P6'/mmm'$ [Type III, hexagonal]

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

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'/mmm'`

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: `-6m2`

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

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

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

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: `mmm'`

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

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

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

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	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[4,5,6,7,8,9]`
3	$\left[\frac{2}{3}, \frac{1}{3}, z\right]$	`[13,14,15,22,23,24]`
4	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	`[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	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[4,7,18,21]`
5	$\left[\frac{1}{2}, 0, -z\right]$	`[5,8,16,19]`
6	$\left[0, \frac{1}{2}, -z\right]$	`[6,9,17,20]`

Table 10: Wyckoff site: `6j`, site symmetry: `m2'm'`

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

Table 11: Wyckoff site: `6k`, site symmetry: `m2'm'`

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	`[1,8,16,23]`

continued ...

Table 11

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

Table 12: Wyckoff site: 6l, site symmetry: mm2

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

Table 13: Wyckoff site: 6m, site symmetry: mm2

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

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	$[x,\, x,\, -z]$	[4,21]
5	$[-x,\, 0,\, -z]$	[5,19]
6	$[0,\, -x,\, -z]$	[6,20]
7	$[-x,\, -x,\, -z]$	[7,18]
8	$[x,\, 0,\, -z]$	[8,16]
9	$[0,\, x,\, -z]$	[9,17]
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	$[x,\ -x,\ -z]$	`[4,7]`
5	$[x,\ 2x,\ -z]$	`[5,8]`
6	$[-2x,\ -x,\ -z]$	`[6,9]`
7	$[-x,\ x,\ z]$	`[13,22]`
8	$[-x,\ -2x,\ z]$	`[14,23]`
9	$[2x,\ x,\ z]$	`[15,24]`
10	$[-x,\ -2x,\ -z]$	`[16,19]`
11	$[2x,\ x,\ -z]$	`[17,20]`
12	$[-x,\ x,\ -z]$	`[18,21]`

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

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

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

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	`[1,8]`

continued ...

Table 17

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

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	$[-x+y,\, -x,\, -z]$	[7]
8	$[x,\, y,\, -z]$	[8]
9	$[-y,\, x-y,\, -z]$	[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	$[x-y,\, -y,\, -z]$	[16]
17	$[y,\, x,\, -z]$	[17]
18	$[-x,\, -x+y,\, -z]$	[18]
19	$[-x,\, -y,\, -z]$	[19]
20	$[y,\, -x+y,\, -z]$	[20]
21	$[x-y,\, x,\, -z]$	[21]
22	$[-x,\, -x+y,\, z]$	[22]
23	$[x-y,\, -y,\, z]$	[23]
24	$[y,\, x,\, z]$	[24]