MSG No. 194.268 $P6'_3/m'm'c$ [Type III, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: -3m'.

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

Table 2: Wyckoff site: 2b, site symmetry: -6'm'2

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

Table 3: Wyckoff site: 2c, site symmetry: -6'm'2

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

Table 5: Wyckoff site: 4e, site symmetry: 3m'.

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

Table 6: Wyckoff site: `4f`, site symmetry: `3m'.`

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

Table 7: Wyckoff site: `6g`, site symmetry: `.2'/m'.`

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

Table 8: Wyckoff site: `6h`, site symmetry: `m'm'2`

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

Table 9: Wyckoff site: `12i`, site symmetry: `.2'.`

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

continued ...

Table 9

No.	position	mapping
12	$\left[0,\, x,\, \frac{1}{2}\right]$	`[12,21]`

Table 10: Wyckoff site: `12j`, site symmetry: `m'..`

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

Table 11: Wyckoff site: `12k`, 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	$\left[x,\, -x,\, \frac{1}{2}-z\right]$	`[4,19]`
5	$\left[x,\, 2x,\, \frac{1}{2}-z\right]$	`[5,20]`
6	$\left[-2x,\, -x,\, \frac{1}{2}-z\right]$	`[6,21]`
7	$[-x,\, -2x,\, -z]$	`[7,16]`
8	$[2x,\, x,\, -z]$	`[8,17]`
9	$[-x,\, x,\, -z]$	`[9,18]`
10	$\left[-x,\, x,\, z+\frac{1}{2}\right]$	`[10,13]`
11	$\left[-x,\, -2x,\, z+\frac{1}{2}\right]$	`[11,14]`
12	$\left[2x,\, x,\, z+\frac{1}{2}\right]$	`[12,15]`

Table 12: Wyckoff site: `24l`, site symmetry: `1`

No.	position	mapping
1	$[x,\, y,\, z]$	`[1]`
2	$[-y,\, x-y,\, z]$	`[2]`

continued ...

Table 12

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