MSG No. 193.261 $P6_3/m'c'm'$ [Type III, hexagonal]

Table 1: Wyckoff site: `2a`, site symmetry: `-6'2m'`

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

Table 2: Wyckoff site: `2b`, site symmetry: `-3'.m'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `-6'..`

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

Table 4: Wyckoff site: `4d`, site symmetry: `3.2`

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, 2x, 0]$	`[1,11]`
2	$\left[-x, x, \frac{1}{2}\right]$	`[2,9]`
3	$[-2x, -x, 0]$	`[3,12]`
4	$\left[-x, -2x, \frac{1}{2}\right]$	`[4,7]`
5	$[x, -x, 0]$	`[5,10]`
6	$\left[2x, x, \frac{1}{2}\right]$	`[6,8]`
7	$[-x, -2x, 0]$	`[13,23]`

continued ...

Table 9

No.	position	mapping
8	$\left[x,\, -x,\, \frac{1}{2}\right]$	[14,21]
9	$[2x,\, x,\, 0]$	[15,24]
10	$\left[x,\, 2x,\, \frac{1}{2}\right]$	[16,19]
11	$[-x,\, x,\, 0]$	[17,22]
12	$\left[-2x,\, -x,\, \frac{1}{2}\right]$	[18,20]

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

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

Table 11: Wyckoff site: 12k, site symmetry: ..m'

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

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

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