MSG No. 193.254 $P6_3/mcm1'$ [Type II, hexagonal]

Table 1: Wyckoff site: `2a`, site symmetry: `-62m1'`

No.	position	mapping
1	$\left[0,\ 0,\ \frac{1}{4}\right]$	[1,3,5,7,8,9,14,16,18,22,23,24,25,27,29,31,32,33,38,40,42,46,47,48]
2	$\left[0,\ 0,\ \frac{3}{4}\right]$	[2,4,6,10,11,12,13,15,17,19,20,21,26,28,30,34,35,36,37,39,41,43,44,45]

Table 2: Wyckoff site: `2b`, site symmetry: `-3.m1'`

No.	position	mapping
1	$[0,\ 0,\ 0]$	[1,3,5,10,11,12,13,15,17,22,23,24,25,27,29,34,35,36,37,39,41,46,47,48]
2	$\left[0,\ 0,\ \frac{1}{2}\right]$	[2,4,6,7,8,9,14,16,18,19,20,21,26,28,30,31,32,33,38,40,42,43,44,45]

Table 3: Wyckoff site: `4c`, site symmetry: `-6..1'`

No.	position	mapping
1	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{4}\right]$	[1,3,5,14,16,18,25,27,29,38,40,42]
2	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	[2,4,6,13,15,17,26,28,30,37,39,41]
3	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{4}\right]$	[7,8,9,22,23,24,31,32,33,46,47,48]
4	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{3}{4}\right]$	[10,11,12,19,20,21,34,35,36,43,44,45]

Table 4: Wyckoff site: `4d`, site symmetry: `3.21'`

No.	position	mapping
1	$\left[\frac{1}{3},\ \frac{2}{3},\ 0\right]$	[1,3,5,10,11,12,25,27,29,34,35,36]
2	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{2}\right]$	[2,4,6,7,8,9,26,28,30,31,32,33]
3	$\left[\frac{2}{3},\ \frac{1}{3},\ 0\right]$	[13,15,17,22,23,24,37,39,41,46,47,48]
4	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}\right]$	[14,16,18,19,20,21,38,40,42,43,44,45]

Table 5: Wyckoff site: `4e`, site symmetry: `3.m1'`

No.	position	mapping
1	$[0,\ 0,\ z]$	[1,3,5,22,23,24,25,27,29,46,47,48]
2	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	[2,4,6,19,20,21,26,28,30,43,44,45]
3	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	[7,8,9,14,16,18,31,32,33,38,40,42]
4	$[0,\ 0,\ -z]$	[10,11,12,13,15,17,34,35,36,37,39,41]

Table 6: Wyckoff site: `6f`, site symmetry: `..2/m1'`

No.	position	mapping
1	$\left[\frac{1}{2}, 0, 0\right]$	`[1,11,13,23,25,35,37,47]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[2,9,14,21,26,33,38,45]`
3	$\left[0, \frac{1}{2}, 0\right]$	`[3,12,15,24,27,36,39,48]`
4	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[4,7,16,19,28,31,40,43]`
5	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[5,10,17,22,29,34,41,46]`
6	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[6,8,18,20,30,32,42,44]`

Table 7: Wyckoff site: `6g`, site symmetry: `m2m1'`

No.	position	mapping
1	$\left[x, 0, \frac{1}{4}\right]$	`[1,7,16,23,25,31,40,47]`
2	$\left[x, x, \frac{3}{4}\right]$	`[2,10,17,21,26,34,41,45]`
3	$\left[0, x, \frac{1}{4}\right]$	`[3,8,18,24,27,32,42,48]`
4	$\left[-x, 0, \frac{3}{4}\right]$	`[4,11,13,19,28,35,37,43]`
5	$\left[-x, -x, \frac{1}{4}\right]$	`[5,9,14,22,29,33,38,46]`
6	$\left[0, -x, \frac{3}{4}\right]$	`[6,12,15,20,30,36,39,44]`

Table 8: Wyckoff site: `8h`, site symmetry: `3..1'`

No.	position	mapping
1	$\left[\frac{1}{3}, \frac{2}{3}, z\right]$	`[1,3,5,25,27,29]`
2	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[2,4,6,26,28,30]`
3	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}-z\right]$	`[7,8,9,31,32,33]`
4	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[10,11,12,34,35,36]`
5	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	`[13,15,17,37,39,41]`
6	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}-z\right]$	`[14,16,18,38,40,42]`
7	$\left[\frac{1}{3}, \frac{2}{3}, z+\frac{1}{2}\right]$	`[19,20,21,43,44,45]`
8	$\left[\frac{2}{3}, \frac{1}{3}, z\right]$	`[22,23,24,46,47,48]`

Table 9: Wyckoff site: `12i`, site symmetry: `..21'`

No.	position	mapping
1	$[x, 2x, 0]$	`[1,11,25,35]`
2	$\left[-x, x, \frac{1}{2}\right]$	`[2,9,26,33]`
3	$[-2x, -x, 0]$	`[3,12,27,36]`
4	$\left[-x, -2x, \frac{1}{2}\right]$	`[4,7,28,31]`
5	$[x, -x, 0]$	`[5,10,29,34]`
6	$\left[2x, x, \frac{1}{2}\right]$	`[6,8,30,32]`
7	$[-x, -2x, 0]$	`[13,23,37,47]`

continued ...

Table 9

No.	position	mapping
8	$\left[x,\, -x,\, \frac{1}{2}\right]$	`[14,21,38,45]`
9	$[2x,\, x,\, 0]$	`[15,24,39,48]`
10	$\left[x,\, 2x,\, \frac{1}{2}\right]$	`[16,19,40,43]`
11	$[-x,\, x,\, 0]$	`[17,22,41,46]`
12	$\left[-2x,\, -x,\, \frac{1}{2}\right]$	`[18,20,42,44]`

Table 10: Wyckoff site: `12j`, site symmetry: `m..1'`

No.	position	mapping
1	$\left[x,\, y,\, \frac{1}{4}\right]$	`[1,16,25,40]`
2	$\left[x-y,\, x,\, \frac{3}{4}\right]$	`[2,17,26,41]`
3	$\left[-y,\, x-y,\, \frac{1}{4}\right]$	`[3,18,27,42]`
4	$\left[-x,\, -y,\, \frac{3}{4}\right]$	`[4,13,28,37]`
5	$\left[-x+y,\, -x,\, \frac{1}{4}\right]$	`[5,14,29,38]`
6	$\left[y,\, -x+y,\, \frac{3}{4}\right]$	`[6,15,30,39]`
7	$\left[x-y,\, -y,\, \frac{1}{4}\right]$	`[7,23,31,47]`
8	$\left[y,\, x,\, \frac{1}{4}\right]$	`[8,24,32,48]`
9	$\left[-x,\, -x+y,\, \frac{1}{4}\right]$	`[9,22,33,46]`
10	$\left[x,\, x-y,\, \frac{3}{4}\right]$	`[10,21,34,45]`
11	$\left[-x+y,\, y,\, \frac{3}{4}\right]$	`[11,19,35,43]`
12	$\left[-y,\, -x,\, \frac{3}{4}\right]$	`[12,20,36,44]`

Table 11: Wyckoff site: `12k`, site symmetry: `..m1'`

No.	position	mapping
1	$[x,\, 0,\, z]$	`[1,23,25,47]`
2	$\left[x,\, x,\, z+\frac{1}{2}\right]$	`[2,21,26,45]`
3	$[0,\, x,\, z]$	`[3,24,27,48]`
4	$\left[-x,\, 0,\, z+\frac{1}{2}\right]$	`[4,19,28,43]`
5	$[-x,\, -x,\, z]$	`[5,22,29,46]`
6	$\left[0,\, -x,\, z+\frac{1}{2}\right]$	`[6,20,30,44]`
7	$\left[x,\, 0,\, \frac{1}{2}-z\right]$	`[7,16,31,40]`
8	$\left[0,\, x,\, \frac{1}{2}-z\right]$	`[8,18,32,42]`
9	$\left[-x,\, -x,\, \frac{1}{2}-z\right]$	`[9,14,33,38]`
10	$[x,\, x,\, -z]$	`[10,17,34,41]`
11	$[-x,\, 0,\, -z]$	`[11,13,35,37]`
12	$[0,\, -x,\, -z]$	`[12,15,36,39]`

Table 12: Wyckoff site: `24l`, site symmetry: `11'`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1,25]`
2	$\left[x-y,\ x,\ z+\frac{1}{2}\right]$	`[2,26]`
3	$[-y,\ x-y,\ z]$	`[3,27]`
4	$\left[-x,\ -y,\ z+\frac{1}{2}\right]$	`[4,28]`
5	$[-x+y,\ -x,\ z]$	`[5,29]`
6	$\left[y,\ -x+y,\ z+\frac{1}{2}\right]$	`[6,30]`
7	$\left[x-y,\ -y,\ \frac{1}{2}-z\right]$	`[7,31]`
8	$\left[y,\ x,\ \frac{1}{2}-z\right]$	`[8,32]`
9	$\left[-x,\ -x+y,\ \frac{1}{2}-z\right]$	`[9,33]`
10	$[x,\ x-y,\ -z]$	`[10,34]`
11	$[-x+y,\ y,\ -z]$	`[11,35]`
12	$[-y,\ -x,\ -z]$	`[12,36]`
13	$[-x,\ -y,\ -z]$	`[13,37]`
14	$\left[-x+y,\ -x,\ \frac{1}{2}-z\right]$	`[14,38]`
15	$[y,\ -x+y,\ -z]$	`[15,39]`
16	$\left[x,\ y,\ \frac{1}{2}-z\right]$	`[16,40]`
17	$[x-y,\ x,\ -z]$	`[17,41]`
18	$\left[-y,\ x-y,\ \frac{1}{2}-z\right]$	`[18,42]`
19	$\left[-x+y,\ y,\ z+\frac{1}{2}\right]$	`[19,43]`
20	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	`[20,44]`
21	$\left[x,\ x-y,\ z+\frac{1}{2}\right]$	`[21,45]`
22	$[-x,\ -x+y,\ z]$	`[22,46]`
23	$[x-y,\ -y,\ z]$	`[23,47]`
24	$[y,\ x,\ z]$	`[24,48]`