MSG No. 194.264 $P6_3/mmc1'$ [Type II, hexagonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: -6m21'

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

Table 3: Wyckoff site: 2c, site symmetry: -6m21'

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

Table 4: Wyckoff site: 2d, site symmetry: -6m21'

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

Table 5: Wyckoff site: 4e, site symmetry: 3m.1'

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

Table 6: Wyckoff site: `4f`, site symmetry: `3m.1'`

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

Table 7: Wyckoff site: `6g`, site symmetry: `.2/m.1'`

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

Table 8: Wyckoff site: `6h`, site symmetry: `mm21'`

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

Table 9: Wyckoff site: `12i`, site symmetry: `.2.1'`

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

continued ...

Table 9

No.	position	mapping
12	$\left[0,\, x,\, \frac{1}{2}\right]$	[18,24,42,48]

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	$\left[x-y,\, -y,\, \frac{3}{4}\right]$	[7,23,31,47]
8	$\left[y,\, x,\, \frac{3}{4}\right]$	[8,24,32,48]
9	$\left[-x,\, -x+y,\, \frac{3}{4}\right]$	[9,22,33,46]
10	$\left[x,\, x-y,\, \frac{1}{4}\right]$	[10,21,34,45]
11	$\left[-x+y,\, y,\, \frac{1}{4}\right]$	[11,19,35,43]
12	$\left[-y,\, -x,\, \frac{1}{4}\right]$	[12,20,36,44]

Table 11: Wyckoff site: 12k, site symmetry: .m.1'

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

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]

continued ...

Table 12

No.	position	mapping
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	$[x-y,\ -y,\ -z]$	[7,31]
8	$[y,\ x,\ -z]$	[8,32]
9	$[-x,\ -x+y,\ -z]$	[9,33]
10	$\left[x,\ x-y,\ \frac{1}{2}-z\right]$	[10,34]
11	$\left[-x+y,\ y,\ \frac{1}{2}-z\right]$	[11,35]
12	$\left[-y,\ -x,\ \frac{1}{2}-z\right]$	[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	$[-x+y,\ y,\ z]$	[19,43]
20	$[-y,\ -x,\ z]$	[20,44]
21	$[x,\ x-y,\ z]$	[21,45]
22	$\left[-x,\ -x+y,\ z+\frac{1}{2}\right]$	[22,46]
23	$\left[x-y,\ -y,\ z+\frac{1}{2}\right]$	[23,47]
24	$\left[y,\ x,\ z+\frac{1}{2}\right]$	[24,48]