MSG No. 131.439 $P4_2'/mmc'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: mmm.

No.	position	mapping
1	$[0, 0, 0]$	[1,2,3,4,5,6,7,8]
2	$\left[0, 0, \frac{1}{2}\right]$	[9,10,11,12,13,14,15,16]

Table 2: Wyckoff site: 2b, site symmetry: mmm.

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[1,2,3,4,5,6,7,8]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[9,10,11,12,13,14,15,16]

Table 3: Wyckoff site: 2c, site symmetry: mmm.

No.	position	mapping
1	$\left[0, \frac{1}{2}, 0\right]$	[1,2,3,4,5,6,7,8]
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[9,10,11,12,13,14,15,16]

Table 4: Wyckoff site: 2d, site symmetry: mmm.

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[1,2,3,4,5,6,7,8]
2	$\left[\frac{1}{2}, 0, 0\right]$	[9,10,11,12,13,14,15,16]

Table 5: Wyckoff site: 2e, site symmetry: -4'm2'

No.	position	mapping
1	$\left[0, 0, \frac{1}{4}\right]$	[1,4,6,7,11,12,13,14]
2	$\left[0, 0, \frac{3}{4}\right]$	[2,3,5,8,9,10,15,16]

Table 6: Wyckoff site: 2f, site symmetry: -4'm2'

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[1,4,6,7,11,12,13,14]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[2,3,5,8,9,10,15,16]

Table 7: Wyckoff site: `4g`, site symmetry: `2mm`.

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

Table 8: Wyckoff site: `4h`, site symmetry: `2mm`.

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[1,4,6,7]
2	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	[2,3,5,8]
3	$\left[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	[9,10,15,16]
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z\right]$	[11,12,13,14]

Table 9: Wyckoff site: `4i`, site symmetry: `2mm`.

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

Table 10: Wyckoff site: `4j`, site symmetry: `m2m`.

No.	position	mapping
1	$[x, 0, 0]$	[1,2,7,8]
2	$[-x, 0, 0]$	[3,4,5,6]
3	$\left[0, x, \frac{1}{2}\right]$	[9,11,14,16]
4	$\left[0, -x, \frac{1}{2}\right]$	[10,12,13,15]

Table 11: Wyckoff site: `4k`, site symmetry: `m2m`.

No.	position	mapping
1	$\left[x, \frac{1}{2}, \frac{1}{2}\right]$	[1,2,7,8]
2	$\left[-x, \frac{1}{2}, \frac{1}{2}\right]$	[3,4,5,6]
3	$\left[\frac{1}{2}, x, 0\right]$	[9,11,14,16]
4	$\left[\frac{1}{2}, -x, 0\right]$	[10,12,13,15]

Table 12: Wyckoff site: `4l`, site symmetry: `m2m`.

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

Table 13: Wyckoff site: `4m`, site symmetry: `m2m`.

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

Table 14: Wyckoff site: `8n`, site symmetry: `..2'`

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

Table 15: Wyckoff site: `8o`, site symmetry: `.m.`.

No.	position	mapping
1	$[0, y, z]$	`[1,6]`
2	$[0, -y, -z]$	`[2,5]`
3	$[0, y, -z]$	`[3,8]`
4	$[0, -y, z]$	`[4,7]`
5	$\left[-y, 0, z+\frac{1}{2}\right]$	`[9,15]`
6	$\left[y, 0, z+\frac{1}{2}\right]$	`[10,16]`
7	$\left[y, 0, \frac{1}{2}-z\right]$	`[11,13]`
8	$\left[-y, 0, \frac{1}{2}-z\right]$	`[12,14]`

Table 16: Wyckoff site: `8p`, site symmetry: `.m.`.

No.	position	mapping
1	$\left[\frac{1}{2},\, y,\, z\right]$	[1,6]
2	$\left[\frac{1}{2},\, -y,\, -z\right]$	[2,5]
3	$\left[\frac{1}{2},\, y,\, -z\right]$	[3,8]
4	$\left[\frac{1}{2},\, -y,\, z\right]$	[4,7]
5	$\left[-y,\, \frac{1}{2},\, z+\frac{1}{2}\right]$	[9,15]
6	$\left[y,\, \frac{1}{2},\, z+\frac{1}{2}\right]$	[10,16]
7	$\left[y,\, \frac{1}{2},\, \frac{1}{2}-z\right]$	[11,13]
8	$\left[-y,\, \frac{1}{2},\, \frac{1}{2}-z\right]$	[12,14]

Table 17: Wyckoff site: `8q`, site symmetry: `m..`.

No.	position	mapping
1	$[x,\, y,\, 0]$	[1,8]
2	$[x,\, -y,\, 0]$	[2,7]
3	$[-x,\, y,\, 0]$	[3,6]
4	$[-x,\, -y,\, 0]$	[4,5]
5	$\left[-y,\, x,\, \frac{1}{2}\right]$	[9,14]
6	$\left[y,\, -x,\, \frac{1}{2}\right]$	[10,13]
7	$\left[y,\, x,\, \frac{1}{2}\right]$	[11,16]
8	$\left[-y,\, -x,\, \frac{1}{2}\right]$	[12,15]

Table 18: Wyckoff site: `16r`, site symmetry: `1`

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