MSG No. 131.442 $P4'_2/m'mc'$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: m'mm.

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

Table 3: Wyckoff site: 2c, site symmetry: m'mm.

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

Table 4: Wyckoff site: 2d, site symmetry: m'mm.

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

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

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: `4j`, site symmetry: `m'2'm`.

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

Table 11: Wyckoff site: `4k`, site symmetry: `m'2'm`.

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

Table 12: Wyckoff site: `4l`, site symmetry: `m'2'm`.

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

Table 13: Wyckoff site: `4m`, site symmetry: `m'2'm`.

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

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

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

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

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

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

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

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

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

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

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