MSG No. 131.435 $P4_2/mmc$ [Type I, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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