MSG No. 123.339 $P4/mmm$ [Type I, tetragonal]

Table 1: Wyckoff site: `1a`, site symmetry: `4/mmm`

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

Table 2: Wyckoff site: `1b`, site symmetry: `4/mmm`

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

Table 3: Wyckoff site: `1c`, site symmetry: `4/mmm`

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

Table 4: Wyckoff site: `1d`, site symmetry: `4/mmm`

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

Table 5: Wyckoff site: `2e`, 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	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[2,3,7,8,10,11,15,16]`

Table 6: Wyckoff site: `2f`, site symmetry: `mmm.`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[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	$\left[-x,\ 0,\ \frac{1}{2}\right]$	`[5,6,9,12]`

Table 14: Wyckoff site: `4n`, site symmetry: `m2m.`

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ 0\right]$	`[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	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[5,6,9,12]`

Table 15: Wyckoff site: `4o`, site symmetry: `m2m.`

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

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

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,14]`
2	$[-y,\ x,\ 0]$	`[2,11]`
3	$[y,\ -x,\ 0]$	`[3,10]`
4	$[x,\ -y,\ 0]$	`[4,13]`

continued ...

Table 16

No.	position	mapping
5	$[-x,\ y,\ 0]$	`[5,12]`
6	$[-x,\ -y,\ 0]$	`[6,9]`
7	$[y,\ x,\ 0]$	`[7,16]`
8	$[-y,\ -x,\ 0]$	`[8,15]`

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

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	`[1,14]`
2	$\left[-y,\ x,\ \frac{1}{2}\right]$	`[2,11]`
3	$\left[y,\ -x,\ \frac{1}{2}\right]$	`[3,10]`
4	$\left[x,\ -y,\ \frac{1}{2}\right]$	`[4,13]`
5	$\left[-x,\ y,\ \frac{1}{2}\right]$	`[5,12]`
6	$\left[-x,\ -y,\ \frac{1}{2}\right]$	`[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: `8r`, site symmetry: `..m`

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

Table 19: Wyckoff site: `8s`, site symmetry: `.m.`

No.	position	mapping
1	$[x,\ 0,\ z]$	`[1,13]`
2	$[0,\ x,\ z]$	`[2,16]`
3	$[0,\ -x,\ z]$	`[3,15]`
4	$[x,\ 0,\ -z]$	`[4,14]`
5	$[-x,\ 0,\ -z]$	`[5,9]`
6	$[-x,\ 0,\ z]$	`[6,12]`
7	$[0,\ x,\ -z]$	`[7,11]`

continued ...

Table 19

No.	position	mapping
8	$[0, -x, -z]$	`[8,10]`

Table 20: Wyckoff site: `8t`, site symmetry: `.m.`

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

Table 21: Wyckoff site: `16u`, site symmetry: `1`

No.	position	mapping
1	$[x, y, z]$	`[1]`
2	$[-y, x, z]$	`[2]`
3	$[y, -x, z]$	`[3]`
4	$[x, -y, -z]$	`[4]`
5	$[-x, y, -z]$	`[5]`
6	$[-x, -y, z]$	`[6]`
7	$[y, x, -z]$	`[7]`
8	$[-y, -x, -z]$	`[8]`
9	$[-x, -y, -z]$	`[9]`
10	$[y, -x, -z]$	`[10]`
11	$[-y, x, -z]$	`[11]`
12	$[-x, y, z]$	`[12]`
13	$[x, -y, z]$	`[13]`
14	$[x, y, -z]$	`[14]`
15	$[-y, -x, z]$	`[15]`
16	$[y, x, z]$	`[16]`