MSG No. 123.343 $P4'/mmm'$ [Type III, 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	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[1,2,3,4,5,6,7,8]`
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[9,10,11,12,13,14,15,16]`

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

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

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

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

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

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

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	$\left[\frac{1}{2},\ 0,\ z\right]$	[9,10,15,16]
4	$\left[\frac{1}{2},\ 0,\ -z\right]$	[11,12,13,14]

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

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

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

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

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

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

Table 15: Wyckoff site: `4o`, 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	$\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$	`[9,11,14,16]`
4	$\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[10,12,13,15]`

Table 16: Wyckoff site: `8p`, 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]`

continued ...

Table 16

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

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

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	`[1,8]`
2	$\left[x,\ -y,\ \frac{1}{2}\right]$	`[2,7]`
3	$\left[-x,\ y,\ \frac{1}{2}\right]$	`[3,6]`
4	$\left[-x,\ -y,\ \frac{1}{2}\right]$	`[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: `8r`, site symmetry: `..m'`

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

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

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

continued ...

Table 19

No.	position	mapping
8	$[0, -x, -z]$	`[12,13]`

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

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

Table 21: Wyckoff site: `16u`, 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	$[-y, x, z]$	`[9]`
10	$[y, -x, z]$	`[10]`
11	$[y, x, -z]$	`[11]`
12	$[-y, -x, -z]$	`[12]`
13	$[y, -x, -z]$	`[13]`
14	$[-y, x, -z]$	`[14]`
15	$[-y, -x, z]$	`[15]`
16	$[y, x, z]$	`[16]`