MSG No. 123.344 $P4'/m'm'm$ [Type III, tetragonal]

Table 1: Wyckoff site: `1a`, site symmetry: `4'/m'm'm`

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'/m'm'm`

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'/m'm'm`

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'/m'm'm`

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: `m'm'm'`.

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

Table 6: Wyckoff site: `2f`, site symmetry: `m'm'm'`.

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

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

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: 2m'm'.

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

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

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

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	$\left[x,\ -x,\ \frac{1}{2}\right]$	[2,5,10,15]
3	$\left[-x,\ x,\ \frac{1}{2}\right]$	[3,6,9,14]
4	$\left[-x,\ -x,\ \frac{1}{2}\right]$	[4,7,12,13]

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

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

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

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

Table 14: Wyckoff site: 4n, site symmetry: m'2m'.

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

Table 15: Wyckoff site: 4o, site symmetry: m'2m'.

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

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

No.	position	mapping
1	$[x,\ y,\ 0]$	[1,16]
2	$[x,\ -y,\ 0]$	[2,15]
3	$[-x,\ y,\ 0]$	[3,14]
4	$[-x,\ -y,\ 0]$	[4,13]

continued ...

Table 16

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

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

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

Table 18: Wyckoff site: `8r`, site symmetry: `..m`

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

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

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

continued ...

Table 19

No.	position	mapping
8	$[0,\, x,\, z]$	`[8,9]`

Table 20: Wyckoff site: `8t`, site symmetry: `.m'.`

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

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	$[y,\, -x,\, -z]$	`[5]`
6	$[-y,\, x,\, -z]$	`[6]`
7	$[-y,\, -x,\, z]$	`[7]`
8	$[y,\, x,\, z]$	`[8]`
9	$[-y,\, x,\, z]$	`[9]`
10	$[y,\, -x,\, z]$	`[10]`
11	$[y,\, x,\, -z]$	`[11]`
12	$[-y,\, -x,\, -z]$	`[12]`
13	$[-x,\, -y,\, -z]$	`[13]`
14	$[-x,\, y,\, z]$	`[14]`
15	$[x,\, -y,\, z]$	`[15]`
16	$[x,\, y,\, -z]$	`[16]`