MSG No. 123.346 $P4'/m'mm'$ [Type III, tetragonal]

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

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'mm'`

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'mm'`

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'mm'`

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'mm.`

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 12: Wyckoff site: `4l`, 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	$[0, x, 0]$	`[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	$\left[x, 0, \frac{1}{2}\right]$	`[1,8,11,14]`
2	$\left[-x, 0, \frac{1}{2}\right]$	`[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 14: Wyckoff site: `4n`, 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	$\left[\frac{1}{2}, x, 0\right]$	`[3,6,9,16]`
4	$\left[\frac{1}{2}, -x, 0\right]$	`[4,5,10,15]`

Table 15: Wyckoff site: `4o`, 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	$\left[\frac{1}{2}, x, \frac{1}{2}\right]$	`[3,6,9,16]`
4	$\left[\frac{1}{2}, -x, \frac{1}{2}\right]$	`[4,5,10,15]`

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

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

continued …

Table 16

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

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

No.	position	mapping
1	$\left[x, y, \frac{1}{2}\right]$	[1,14]
2	$\left[-x, -y, \frac{1}{2}\right]$	[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	$\left[-x, y, \frac{1}{2}\right]$	[7,12]
8	$\left[x, -y, \frac{1}{2}\right]$	[8,11]

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

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

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

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

continued …

Table 19

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

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

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

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[y, x, -z]$	[3]
4	$[-y, -x, -z]$	[4]
5	$[y, -x, -z]$	[5]
6	$[-y, x, -z]$	[6]
7	$[-x, y, z]$	[7]
8	$[x, -y, z]$	[8]
9	$[-y, x, z]$	[9]
10	$[y, -x, z]$	[10]
11	$[x, -y, -z]$	[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]