MSG No. 127.389 $P4/m'bm$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4/m'..

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

Table 2: Wyckoff site: 2b, site symmetry: 4/m'..

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

Table 3: Wyckoff site: 2c, site symmetry: m'.mm

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

Table 4: Wyckoff site: 2d, site symmetry: m'.mm

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

Table 5: Wyckoff site: 4e, site symmetry: 4..

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

Table 6: Wyckoff site: `4f`, site symmetry: `2.mm`

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m'..`

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

Table 10: Wyckoff site: `8j`, site symmetry: `m'..`.

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

Table 11: Wyckoff site: `8k`, site symmetry: `..m`

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

Table 12: Wyckoff site: `16l`, site symmetry: `1`

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