MSG No. 129.418 $P4'/n'mm'$ [Type III, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `-4m2`

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

Table 2: Wyckoff site: `2b`, site symmetry: `-4m2`

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

Table 3: Wyckoff site: `2c`, site symmetry: `4'mm'`

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `..2/m'`

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

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

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

Table 7: Wyckoff site: `8g`, site symmetry: `..2`

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

Table 8: Wyckoff site: `8h`, site symmetry: `..2`

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

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

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

continued ...

Table 9

No.	position	mapping
8	$\left[\frac{3}{4}, y+\frac{1}{2}, -z\right]$	[12,14]

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

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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