MSG No. 129.417 $P4/nm'm'$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: `2b`, site symmetry: `-4m'2'`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 9

No.	position	mapping
8	$\left[\frac{3}{4}, y+\frac{1}{2}, -z\right]$	[8,10]

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

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

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

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