MSG No. 129.416 $P4'/n'm'm$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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	$\left[\frac{1}{2} - x, -x, 0\right]$	`[5,14]`
6	$\left[x, x + \frac{1}{2}, 0\right]$	`[6,15]`
7	$\left[x + \frac{1}{2}, \frac{1}{2} - x, 0\right]$	`[7,16]`
8	$[-x, x, 0]$	`[8,13]`

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	$\left[\frac{1}{2} - x, -x, \frac{1}{2}\right]$	`[5,14]`
6	$\left[x, x + \frac{1}{2}, \frac{1}{2}\right]$	`[6,15]`
7	$\left[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}\right]$	`[7,16]`
8	$\left[-x, x, \frac{1}{2}\right]$	`[8,13]`

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

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

continued ...

Table 9

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

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

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

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

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