MSG No. 119.319 $I\bar{4}m'2'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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	$\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[9,10,15,16]`
4	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[11,12,13,14]`

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

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

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

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

Table 9: Wyckoff site: `8i`, 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	$\left[x+\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[9,16]`
6	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[10,15]`
7	$\left[\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	`[11,14]`

continued ...

Table 9

No.	position	mapping
8	$\left[\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}-z\right]$	`[12,13]`

Table 10: Wyckoff site: `16j`, 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	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	`[9]`
10	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	`[10]`
11	$\left[y+\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}-z\right]$	`[11]`
12	$\left[\frac{1}{2}-y, x+\frac{1}{2}, \frac{1}{2}-z\right]$	`[12]`
13	$\left[y+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}-z\right]$	`[13]`
14	$\left[\frac{1}{2}-y, \frac{1}{2}-x, \frac{1}{2}-z\right]$	`[14]`
15	$\left[\frac{1}{2}-x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	`[15]`
16	$\left[x+\frac{1}{2}, \frac{1}{2}-y, z+\frac{1}{2}\right]$	`[16]`