MSG No. 17.13 P_B222_1 [Type IV, orthorhombic]

Table 1: Wyckoff site: `2a`, site symmetry: `22'2'`

No.	position	mapping
1	$\left[\frac{3}{4}, 0, 0\right]$	`[1,2,7,8]`
2	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	`[3,4,5,6]`

Table 2: Wyckoff site: `2b`, site symmetry: `22'2'`

No.	position	mapping
1	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	`[1,2,7,8]`
2	$\left[\frac{1}{4}, 0, 0\right]$	`[3,4,5,6]`

Table 3: Wyckoff site: `2c`, site symmetry: `22'2'`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	`[1,2,7,8]`
2	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}\right]$	`[3,4,5,6]`

Table 4: Wyckoff site: `2d`, site symmetry: `22'2'`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	`[1,2,7,8]`
2	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right]$	`[3,4,5,6]`

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

No.	position	mapping
1	$[x, 0, 0]$	`[1,2]`
2	$\left[-x, 0, \frac{1}{2}\right]$	`[3,4]`
3	$\left[x+\frac{1}{2}, 0, \frac{1}{2}\right]$	`[5,6]`
4	$\left[\frac{1}{2}-x, 0, 0\right]$	`[7,8]`

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

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ 0\right]$	`[1,2]`
2	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[3,4]`
3	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[5,6]`
4	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ 0\right]$	`[7,8]`

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

No.	position	mapping
1	$\left[\frac{3}{4},\ 0,\ z\right]$	`[1,8]`
2	$\left[\frac{3}{4},\ 0,\ -z\right]$	`[2,7]`
3	$\left[\frac{1}{4},\ 0,\ \frac{1}{2}-z\right]$	`[3,6]`
4	$\left[\frac{1}{4},\ 0,\ z+\frac{1}{2}\right]$	`[4,5]`

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

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{1}{2},\ z\right]$	`[1,8]`
2	$\left[\frac{3}{4},\ \frac{1}{2},\ -z\right]$	`[2,7]`
3	$\left[\frac{1}{4},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[3,6]`
4	$\left[\frac{1}{4},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[4,5]`

Table 9: Wyckoff site: `4i`, site symmetry: `.2'.`

No.	position	mapping
1	$\left[\frac{3}{4},\ y,\ 0\right]$	`[1,7]`
2	$\left[\frac{3}{4},\ -y,\ 0\right]$	`[2,8]`
3	$\left[\frac{1}{4},\ y,\ \frac{1}{2}\right]$	`[3,5]`
4	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}\right]$	`[4,6]`

Table 10: Wyckoff site: `4j`, site symmetry: `.2'.`

No.	position	mapping
1	$\left[\frac{3}{4},\ y,\ \frac{1}{2}\right]$	`[1,7]`
2	$\left[\frac{3}{4},\ -y,\ \frac{1}{2}\right]$	`[2,8]`
3	$\left[\frac{1}{4},\ y,\ 0\right]$	`[3,5]`
4	$\left[\frac{1}{4},\ -y,\ 0\right]$	`[4,6]`

Table 11: Wyckoff site: `4k`, site symmetry: `.2.`

No.	position	mapping
1	$\left[0,\, y,\, \frac{1}{4}\right]$	`[1,3]`
2	$\left[0,\, -y,\, \frac{3}{4}\right]$	`[2,4]`
3	$\left[\frac{1}{2},\, y,\, \frac{3}{4}\right]$	`[5,7]`
4	$\left[\frac{1}{2},\, -y,\, \frac{1}{4}\right]$	`[6,8]`

Table 12: Wyckoff site: `8l`, site symmetry: `1`

No.	position	mapping
1	$[x,\, y,\, z]$	`[1]`
2	$[x,\, -y,\, -z]$	`[2]`
3	$\left[-x,\, y,\, \frac{1}{2}-z\right]$	`[3]`
4	$\left[-x,\, -y,\, z+\frac{1}{2}\right]$	`[4]`
5	$\left[x+\frac{1}{2},\, y,\, z+\frac{1}{2}\right]$	`[5]`
6	$\left[x+\frac{1}{2},\, -y,\, \frac{1}{2}-z\right]$	`[6]`
7	$\left[\frac{1}{2}-x,\, y,\, -z\right]$	`[7]`
8	$\left[\frac{1}{2}-x,\, -y,\, z\right]$	`[8]`