MSG No. 17.12 P_c222_1 [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `2e`, site symmetry: `22'2'`

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

Table 6: Wyckoff site: `2f`, site symmetry: `2'22'`

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

Table 7: Wyckoff site: `2g`, site symmetry: `2'22'`

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

Table 8: Wyckoff site: `2h`, site symmetry: `2'22'`

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

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

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

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

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

Table 11: Wyckoff site: `4k`, 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	$\left[x, \frac{1}{2}, \frac{1}{2}\right]$	`[5,6]`
4	$\left[-x, \frac{1}{2}, 0\right]$	`[7,8]`

Table 12: Wyckoff site: `4l`, site symmetry: `2'..`

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

Table 13: Wyckoff site: `4m`, site symmetry: `.2'.`

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

Table 14: Wyckoff site: `4n`, 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	$\left[0,\ y,\ \frac{3}{4}\right]$	`[5,7]`
4	$\left[0,\ -y,\ \frac{1}{4}\right]$	`[6,8]`

Table 15: Wyckoff site: `4o`, site symmetry: `.2'.`

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

Table 16: Wyckoff site: `4p`, site symmetry: `.2.`

No.	position	mapping
1	$\left[\frac{1}{2},\ y,\ \frac{1}{4}\right]$	`[1,3]`
2	$\left[\frac{1}{2},\ -y,\ \frac{3}{4}\right]$	`[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 17: Wyckoff site: `4q`, site symmetry: `..2'`

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

Table 18: Wyckoff site: `4r`, site symmetry: `..2'`

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

Table 19: Wyckoff site: `4s`, site symmetry: `..2'`

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

Table 20: Wyckoff site: `4t`, site symmetry: `..2'`

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

Table 21: Wyckoff site: `8u`, 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]`

continued ...

Table 21

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