MSG No. 49.268   *Pccm′*   [Type III, orthorhombic]

Table 1: Wyckoff site: `2a`, site symmetry: `..2/m'`

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: `..2/m'`

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 3: Wyckoff site: `2c`, site symmetry: `..2/m'`

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/m'`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 14: Wyckoff site: `4n`, site symmetry: `..2`

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

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

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

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

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

Table 17: Wyckoff site: `4q`, site symmetry: `..m'`

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

Table 18: Wyckoff site: `8r`, site symmetry: `1`

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