

MSG No. 47.249 *Pmmm* [Type I, orthorhombic]

Table 1: Wyckoff site: **1a**, site symmetry: **mmm**

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6,7,8]

Table 2: Wyckoff site: **1b**, site symmetry: **mmm**

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

Table 3: Wyckoff site: **1c**, site symmetry: **mmm**

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

Table 4: Wyckoff site: **1d**, site symmetry: **mmm**

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

Table 5: Wyckoff site: **1e**, site symmetry: **mmm**

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

Table 6: Wyckoff site: **1f**, site symmetry: **mmm**

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

Table 7: Wyckoff site: 1g, site symmetry: mmm

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

Table 8: Wyckoff site: 1h, site symmetry: mmm

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

Table 9: Wyckoff site: 2i, site symmetry: 2mm

No.	position	mapping
1	$[x, 0, 0]$	$[1,2,7,8]$
2	$[-x, 0, 0]$	$[3,4,5,6]$

Table 10: Wyckoff site: 2j, site symmetry: 2mm

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

Table 11: Wyckoff site: 2k, site symmetry: 2mm

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

Table 12: Wyckoff site: 2l, site symmetry: 2mm

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

Table 13: Wyckoff site: $2m$, site symmetry: $m2m$

No.	position	mapping
1	$[0, y, 0]$	$[1, 3, 6, 8]$
2	$[0, -y, 0]$	$[2, 4, 5, 7]$

Table 14: Wyckoff site: $2n$, site symmetry: $m2m$

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

Table 15: Wyckoff site: $2o$, site symmetry: $m2m$

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

Table 16: Wyckoff site: $2p$, site symmetry: $m2m$

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

Table 17: Wyckoff site: $2q$, site symmetry: $mm2$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 6, 7]$
2	$[0, 0, -z]$	$[2, 3, 5, 8]$

Table 18: Wyckoff site: $2r$, site symmetry: $mm2$

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

Table 19: Wyckoff site: 2s, site symmetry: mm2

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

Table 20: Wyckoff site: 2t, site symmetry: mm2

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

Table 21: Wyckoff site: 4u, site symmetry: m..

No.	position	mapping
1	$[0, y, z]$	[1,6]
2	$[0, -y, -z]$	[2,5]
3	$[0, y, -z]$	[3,8]
4	$[0, -y, z]$	[4,7]

Table 22: Wyckoff site: 4v, site symmetry: m..

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

Table 23: Wyckoff site: 4w, site symmetry: .m.

No.	position	mapping
1	$[x, 0, z]$	[1,7]
2	$[x, 0, -z]$	[2,8]
3	$[-x, 0, -z]$	[3,5]
4	$[-x, 0, z]$	[4,6]

Table 24: Wyckoff site: 4x, site symmetry: .m.

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

Table 25: Wyckoff site: 4y, site symmetry: . . m

No.	position	mapping
1	$[x, y, 0]$	[1,8]
2	$[x, -y, 0]$	[2,7]
3	$[-x, y, 0]$	[3,6]
4	$[-x, -y, 0]$	[4,5]

Table 26: Wyckoff site: 4z, site symmetry: . . m

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

Table 27: Wyckoff site: 8A, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -y, -z]$	[2]
3	$[-x, y, -z]$	[3]
4	$[-x, -y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[-x, y, z]$	[6]
7	$[x, -y, z]$	[7]
8	$[x, y, -z]$	[8]