

MSG No. 47.250 $Pmmm1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: 1a, site symmetry: $mmm1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]$

Table 2: Wyckoff site: 1b, site symmetry: $mmm1'$

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

Table 3: Wyckoff site: 1c, site symmetry: $mmm1'$

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

Table 4: Wyckoff site: 1d, site symmetry: $mmm1'$

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

Table 5: Wyckoff site: 1e, site symmetry: $mmm1'$

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

Table 6: Wyckoff site: 1f, site symmetry: $mmm1'$

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

Table 7: Wyckoff site: 1g, site symmetry: $mmm1'$

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

Table 8: Wyckoff site: 1h, site symmetry: $mmm1'$

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

Table 9: Wyckoff site: 2i, site symmetry: $2mm1'$

No.	position	mapping
1	$[x, 0, 0]$	[1,2,7,8,9,10,15,16]
2	$[-x, 0, 0]$	[3,4,5,6,11,12,13,14]

Table 10: Wyckoff site: 2j, site symmetry: $2mm1'$

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

Table 11: Wyckoff site: 2k, site symmetry: $2mm1'$

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

Table 12: Wyckoff site: 2l, site symmetry: $2mm1'$

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

Table 13: Wyckoff site: $2m$, site symmetry: $m2m1'$

No.	position	mapping
1	$[0, y, 0]$	$[1, 3, 6, 8, 9, 11, 14, 16]$
2	$[0, -y, 0]$	$[2, 4, 5, 7, 10, 12, 13, 15]$

Table 14: Wyckoff site: $2n$, site symmetry: $m2m1'$

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

Table 15: Wyckoff site: $2o$, site symmetry: $m2m1'$

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

Table 16: Wyckoff site: $2p$, site symmetry: $m2m1'$

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

Table 17: Wyckoff site: $2q$, site symmetry: $mm21'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 6, 7, 9, 12, 14, 15]$
2	$[0, 0, -z]$	$[2, 3, 5, 8, 10, 11, 13, 16]$

Table 18: Wyckoff site: $2r$, site symmetry: $mm21'$

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

Table 19: Wyckoff site: 2s, site symmetry: $mm21'$

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

Table 20: Wyckoff site: 2t, site symmetry: $mm21'$

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

Table 21: Wyckoff site: 4u, site symmetry: $m..1'$

No.	position	mapping
1	$[0, y, z]$	[1, 6, 9, 14]
2	$[0, -y, -z]$	[2, 5, 10, 13]
3	$[0, y, -z]$	[3, 8, 11, 16]
4	$[0, -y, z]$	[4, 7, 12, 15]

Table 22: Wyckoff site: 4v, site symmetry: $m..1'$

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

Table 23: Wyckoff site: 4w, site symmetry: $.m.1'$

No.	position	mapping
1	$[x, 0, z]$	[1, 7, 9, 15]
2	$[x, 0, -z]$	[2, 8, 10, 16]
3	$[-x, 0, -z]$	[3, 5, 11, 13]
4	$[-x, 0, z]$	[4, 6, 12, 14]

Table 24: Wyckoff site: 4x, site symmetry: $.m.1'$

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

Table 25: Wyckoff site: 4y, site symmetry: $..m1'$

No.	position	mapping
1	$[x, y, 0]$	[1,8,9,16]
2	$[x, -y, 0]$	[2,7,10,15]
3	$[-x, y, 0]$	[3,6,11,14]
4	$[-x, -y, 0]$	[4,5,12,13]

Table 26: Wyckoff site: 4z, site symmetry: $..m1'$

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

Table 27: Wyckoff site: 8A, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	[1,9]
2	$[x, -y, -z]$	[2,10]
3	$[-x, y, -z]$	[3,11]
4	$[-x, -y, z]$	[4,12]
5	$[-x, -y, -z]$	[5,13]
6	$[-x, y, z]$	[6,14]
7	$[x, -y, z]$	[7,15]
8	$[x, y, -z]$	[8,16]