

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:  $\text{mmm}1'$ 

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:  $\text{mmm}1'$ 

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:  $2\text{mm}1'$ 

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:  $2\text{mm}1'$ 

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:  $2\text{mm}1'$ 

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:  $2\text{mm}1'$ 

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:  $2\bar{m}$ , site symmetry:  $\bar{m}2\bar{m}1'$ 

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:  $\bar{m}2\bar{m}1'$ 

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:  $\bar{m}2\bar{m}1'$ 

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:  $\bar{m}2\bar{m}1'$ 

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:  $\bar{m}\bar{m}21'$ 

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:  $\bar{m}\bar{m}21'$ 

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]