

MSG No. 47.253  $Pm'm'm'$  [ Type III, orthorhombic ]

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

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

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

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

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

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

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

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:  $m'm'm'$

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

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

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:  $m'm'm'$ 

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:  $m'm'm'$ 

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:  $2m'm'$ 

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:  $2m'm'$ 

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:  $2m'm'$ 

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:  $2m'm'$ 

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:  $2\mathbf{m}$ , site symmetry:  $\mathbf{m}'2\mathbf{m}'$ 

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

Table 14: Wyckoff site:  $2\mathbf{n}$ , site symmetry:  $\mathbf{m}'2\mathbf{m}'$ 

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:  $2\mathbf{o}$ , site symmetry:  $\mathbf{m}'2\mathbf{m}'$ 

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:  $2\mathbf{p}$ , site symmetry:  $\mathbf{m}'2\mathbf{m}'$ 

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:  $2\mathbf{q}$ , site symmetry:  $\mathbf{m}'\mathbf{m}'2$ 

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

Table 18: Wyckoff site:  $2\mathbf{r}$ , site symmetry:  $\mathbf{m}'\mathbf{m}'2$ 

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:  $m'm'2$ 

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:  $m'm'2$ 

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:  $4\mathbf{x}$ , site symmetry:  $\bar{3}m'$ .

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:  $4\mathbf{y}$ , site symmetry:  $\bar{3}m'$ .

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:  $4\mathbf{z}$ , site symmetry:  $\bar{3}m'$ .

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:  $8\mathbf{A}$ , 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	$[x, y, -z]$	$[8]$