

MSG No. 51.297  $Pm'm'a'$  [ Type III, orthorhombic ]

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

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

Table 2: Wyckoff site: **2b**, site symmetry:  $.2/m'$ .

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

Table 3: Wyckoff site: **2c**, site symmetry:  $.2/m'$ .

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

Table 4: Wyckoff site: **2d**, site symmetry:  $.2/m'$ .

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

Table 5: Wyckoff site: **2e**, site symmetry:  $m'm'2$

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

Table 6: Wyckoff site: **2f**, site symmetry:  $m'm'2$

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

Table 7: Wyckoff site:  $4\mathbf{g}$ , site symmetry:  $.2$ .

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

Table 8: Wyckoff site:  $4\mathbf{h}$ , site symmetry:  $.2$ .

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

Table 9: Wyckoff site:  $4\mathbf{i}$ , site symmetry:  $.\mathbf{m}'$ .

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

Table 10: Wyckoff site:  $4\mathbf{j}$ , site symmetry:  $.\mathbf{m}'$ .

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

Table 11: Wyckoff site:  $4\mathbf{k}$ , site symmetry:  $\mathbf{m}'..$ 

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

Table 12: Wyckoff site: **81**, site symmetry: **1**

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