

MSG No. 71.535  $Im'mm$  [ Type III, orthorhombic ]

Table 1: Wyckoff site: 2a, site symmetry:  $m'mm$

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

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

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

Table 3: Wyckoff site: 2c, site symmetry:  $m'mm$

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

Table 4: Wyckoff site: 2d, site symmetry:  $m'mm$

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

Table 5: Wyckoff site: 4e, site symmetry:  $2mm$

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

Table 6: Wyckoff site: 4f, site symmetry:  $2mm$ 

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

Table 7: Wyckoff site: 4g, site symmetry:  $m'2'm$ 

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

Table 8: Wyckoff site: 4h, site symmetry:  $m'2'm$ 

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

Table 9: Wyckoff site: 4i, site symmetry:  $m'm2'$ 

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

Table 10: Wyckoff site: 4j, site symmetry:  $m'm2'$ 

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

Table 11: Wyckoff site:  $8k$ , site symmetry:  $-1'$ 

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

Table 12: Wyckoff site:  $8l$ , site symmetry:  $m'$ ...

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

Table 13: Wyckoff site:  $8m$ , site symmetry:  $.m$ .

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

Table 14: Wyckoff site:  $8n$ , site symmetry:  $..m$ 

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

*continued ...*

Table 14

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

Table 15: Wyckoff site: 16o, 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]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[10]
11	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[11]
12	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[12]
13	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[14]
15	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[15]
16	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[16]