

MSG No. 71.536 $Im'm'm$ [Type III, orthorhombic]

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

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: $m'm'm$

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: $m'm'm$

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: $m'm'm$

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: $2'm'm$

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

Table 6: Wyckoff site: $4f$, site symmetry: $2'm'm$

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

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

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

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

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

Table 9: Wyckoff site: $4i$, site symmetry: $m'm'2$

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

Table 10: Wyckoff site: $4j$, site symmetry: $m'm'2$

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

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

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

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

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

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

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

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	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2}]$	[10, 11]
7	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[13, 16]
8	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[10]
11	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[11]
12	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[12]
13	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[15]
16	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[16]