

MSG No. 71.537 $Im'm'm'$ [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: $2m'm'$

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

Table 6: Wyckoff site: $4\mathbf{f}$, site symmetry: $2\mathbf{m}'\mathbf{m}'$

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

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

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

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

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

Table 9: Wyckoff site: $4\mathbf{i}$, site symmetry: $\mathbf{m}'\mathbf{m}'2$

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

Table 10: Wyckoff site: $4\mathbf{j}$, site symmetry: $\mathbf{m}'\mathbf{m}'2$

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

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

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

Table 12: Wyckoff site: $8l$, 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]
5	$[\frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9,14]
6	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[10,13]
7	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[11,16]
8	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[12,15]

Table 13: Wyckoff site: $8m$, 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]
5	$[x + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[9,15]
6	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[10,16]
7	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2} - z]$	[11,13]
8	$[\frac{1}{2} - x, \frac{1}{2}, z + \frac{1}{2}]$	[12,14]

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

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

continued ...

Table 14

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

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