

MSG No. 74.558 $Im'm'a$ [Type III, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $2'/m'$. .

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $.2'/m'$.

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $m'm'2$

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

continued ...

Table 5

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

Table 6: Wyckoff site: $8f$, site symmetry: $2'$. .

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

Table 7: Wyckoff site: $8g$, site symmetry: $.2'$. .

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: $.m'$.

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

Table 10: Wyckoff site: 16j, 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	$[x, y + \frac{1}{2}, -z]$	[4]
5	$[x, -y, -z]$	[5]
6	$[-x, y + \frac{1}{2}, -z]$	[6]
7	$[-x, y, z]$	[7]
8	$[x, \frac{1}{2} - y, z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[10]
11	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[11]
12	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[12]
13	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[15]
16	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[16]