

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]