

MSG No. 64.475 $Cmc'd'$ [Type III, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: -1

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

Table 4: Wyckoff site: 8d, site symmetry: $2..$

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

Table 5: Wyckoff site: **8e**, site symmetry: $.2'$.

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

Table 6: Wyckoff site: **8f**, site symmetry: $m.$

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

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