

MSG No. 64.474 $Cm'c'a$ [Type III, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $2'/\text{m}'..$

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

Table 2: Wyckoff site: 4b, site symmetry: $2'/\text{m}'..$

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

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}, \frac{1}{2}]	[2,12]
3	[\frac{3}{4}, \frac{3}{4}, 0]	[3,9]
4	[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]	[4,10]
5	[\frac{1}{4}, \frac{3}{4}, 0]	[5,15]
6	[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]	[6,16]
7	[\frac{3}{4}, \frac{1}{4}, 0]	[7,13]
8	[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]	[8,14]

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

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

Table 5: Wyckoff site: 8e, site symmetry: .2¹.

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

Table 6: Wyckoff site: 8f, site symmetry: m'..

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

Table 7: Wyckoff site: 16g, site symmetry: 1

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