

MSG No. 64.471 *Cm'ca* [Type III, orthorhombic]

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

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

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

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

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

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

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

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

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

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]	[1,8]
2	[0, -y, -z]	[2,7]
3	[$\frac{1}{2}, -y, z + \frac{1}{2}$]	[3,6]
4	[$\frac{1}{2}, y, \frac{1}{2} - z$]	[4,5]
5	[$\frac{1}{2}, y + \frac{1}{2}, z$]	[9,16]
6	[$\frac{1}{2}, \frac{1}{2} - y, -z$]	[10,15]
7	[0, $\frac{1}{2} - y, z + \frac{1}{2}$]	[11,14]
8	[0, $y + \frac{1}{2}, \frac{1}{2} - z$]	[12,13]

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

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