

MSG No. 90.100 P_c42_12 [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

Table 2: Wyckoff site: 4b, site symmetry: 2.2'2'

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

Table 3: Wyckoff site: 4c, site symmetry: 4..

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: . . 2

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

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

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

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

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