

MSG No. 109.240 $I4_1md1'$ [Type II, tetragonal]

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

No.	position	mapping
1	[0, 0, z]	[1,4,5,6,17,20,21,22]
2	[0, $\frac{1}{2}$, $z + \frac{1}{4}$]	[2,3,7,8,18,19,23,24]
3	[$\frac{1}{2}$, $\frac{1}{2}$, $z + \frac{1}{2}$]	[9,12,13,14,25,28,29,30]
4	[$\frac{1}{2}$, 0, $z + \frac{3}{4}$]	[10,11,15,16,26,27,31,32]

Table 2: Wyckoff site: 8b, site symmetry: .m.1'

No.	position	mapping
1	[0, y, z]	[1,5,17,21]
2	[$-y$, $\frac{1}{2}$, $z + \frac{1}{4}$]	[2,7,18,23]
3	[y, $\frac{1}{2}$, $z + \frac{1}{4}$]	[3,8,19,24]
4	[0, $-y$, z]	[4,6,20,22]
5	[$\frac{1}{2}$, $y + \frac{1}{2}$, $z + \frac{1}{2}$]	[9,13,25,29]
6	[$\frac{1}{2} - y$, 0, $z + \frac{3}{4}$]	[10,15,26,31]
7	[$y + \frac{1}{2}$, 0, $z + \frac{3}{4}$]	[11,16,27,32]
8	[$\frac{1}{2}$, $\frac{1}{2} - y$, $z + \frac{1}{2}$]	[12,14,28,30]

Table 3: Wyckoff site: 16c, site symmetry: 11'

No.	position	mapping
1	[x, y, z]	[1,17]
2	[$-y$, $x + \frac{1}{2}$, $z + \frac{1}{4}$]	[2,18]
3	[y, $\frac{1}{2} - x$, $z + \frac{1}{4}$]	[3,19]
4	[$-x$, $-y$, z]	[4,20]
5	[$-x$, y, z]	[5,21]
6	[x, $-y$, z]	[6,22]
7	[$-y$, $\frac{1}{2} - x$, $z + \frac{1}{4}$]	[7,23]
8	[y, $x + \frac{1}{2}$, $z + \frac{1}{4}$]	[8,24]
9	[$x + \frac{1}{2}$, $y + \frac{1}{2}$, $z + \frac{1}{2}$]	[9,25]
10	[$\frac{1}{2} - y$, x, $z + \frac{3}{4}$]	[10,26]
11	[$y + \frac{1}{2}$, $-x$, $z + \frac{3}{4}$]	[11,27]
12	[$\frac{1}{2} - x$, $\frac{1}{2} - y$, $z + \frac{1}{2}$]	[12,28]
13	[$\frac{1}{2} - x$, $y + \frac{1}{2}$, $z + \frac{1}{2}$]	[13,29]
14	[$x + \frac{1}{2}$, $\frac{1}{2} - y$, $z + \frac{1}{2}$]	[14,30]
15	[$\frac{1}{2} - y$, $-x$, $z + \frac{3}{4}$]	[15,31]
16	[$y + \frac{1}{2}$, x, $z + \frac{3}{4}$]	[16,32]