

MSG No. 109.239  $I4_1md$  [ Type I, tetragonal ]

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

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

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

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

Table 3: Wyckoff site: 16c, site symmetry: 1

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