

MSG No. 109.242  $I4'_1md'$  [ Type III, tetragonal ]

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

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

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

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

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

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