

MSG No. 64.475 $Cmc'a'$ [Type III, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: $.2'$.

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

Table 7: Wyckoff site: **16g**, 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 | $[\frac{1}{2} - x, y, \frac{1}{2} - z]$ | [5] |
| 6 | $[\frac{1}{2} - x, -y, z + \frac{1}{2}]$ | [6] |
| 7 | $[x + \frac{1}{2}, -y, z + \frac{1}{2}]$ | [7] |
| 8 | $[x + \frac{1}{2}, y, \frac{1}{2} - z]$ | [8] |
| 9 | $[x + \frac{1}{2}, y + \frac{1}{2}, z]$ | [9] |
| 10 | $[x + \frac{1}{2}, \frac{1}{2} - y, -z]$ | [10] |
| 11 | $[\frac{1}{2} - x, \frac{1}{2} - y, -z]$ | [11] |
| 12 | $[\frac{1}{2} - x, y + \frac{1}{2}, z]$ | [12] |
| 13 | $[-x, y + \frac{1}{2}, \frac{1}{2} - z]$ | [13] |
| 14 | $[-x, \frac{1}{2} - y, z + \frac{1}{2}]$ | [14] |
| 15 | $[x, \frac{1}{2} - y, z + \frac{1}{2}]$ | [15] |
| 16 | $[x, y + \frac{1}{2}, \frac{1}{2} - z]$ | [16] |