

MSG No. 57.390 P_Bbcm [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $\dots 2'/m$

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

Table 2: Wyckoff site: 4b, site symmetry: $\dots 2'/m$

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: $\dots 2'$

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

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

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

Table 6: Wyckoff site: **8f**, site symmetry: $..m$

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

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

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