

MSG No. 62.450 $P_a nma$ [Type IV, orthorhombic]

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

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

Table 2: Wyckoff site: 4b, site symmetry: $2'mm'$

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: -1

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

Table 5: Wyckoff site: **8e**, site symmetry: $\bar{3}m'$

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

Table 6: Wyckoff site: **8f**, site symmetry: $\bar{3}m$.

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

Table 7: Wyckoff site: **16g**, site symmetry: $\bar{1}$

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