

MSG No. 52.315 $P_b n n a$ [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $22'2'$

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

Table 2: Wyckoff site: 4b, site symmetry: $22'2'$

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

Table 3: Wyckoff site: 4c, site symmetry: $2'2'2$

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

Table 4: Wyckoff site: 4d, site symmetry: $2'2'2$

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

Table 5: Wyckoff site: 8e, site symmetry: $-1'$

| No. | position | mapping |
|-----|---|---------|
| 1 | $[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$ | [1,13] |
| 2 | $[\frac{1}{2}, \frac{1}{4}, 0]$ | [2,14] |

continued ...

Table 5

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

Table 6: Wyckoff site: **8f**, site symmetry: -1

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

Table 7: Wyckoff site: **8g**, site symmetry: $2..$

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

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

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, 0, \frac{3}{4}]$ | [1,10] |
| 2 | $[x, \frac{1}{2}, \frac{3}{4}]$ | [2,9] |
| 3 | $[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$ | [3,12] |
| 4 | $[\frac{1}{2} - x, 0, \frac{3}{4}]$ | [4,11] |
| 5 | $[-x, 0, \frac{1}{4}]$ | [5,14] |

continued ...

Table 8

| No. | position | mapping |
|-----|---|---------|
| 6 | $[-x, \frac{1}{2}, \frac{1}{4}]$ | [6,13] |
| 7 | $[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$ | [7,16] |
| 8 | $[x + \frac{1}{2}, 0, \frac{1}{4}]$ | [8,15] |

Table 9: Wyckoff site: 8i, site symmetry: $\dots 2'$

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

Table 10: Wyckoff site: 8j, site symmetry: $\dots 2$

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

Table 11: Wyckoff site: 8k, site symmetry: $\dots 2'$

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

Table 12: Wyckoff site: **81**, site symmetry: $.2'$.

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

Table 13: Wyckoff site: **16m**, site symmetry: 1

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