

MPG No. 15.4.56 $4'/mm'm$ ($4'/\text{mm}'\text{m}$ setting) [Type III, tetragonal]

Table 1: Wyckoff site: 1o, site symmetry: $4'/\text{mm}'\text{m}$

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

Table 2: Wyckoff site: 2a, site symmetry: $4'\text{m}'\text{m}$

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

Table 3: Wyckoff site: 4b, site symmetry: $\text{m}.\text{m}2$

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

Table 4: Wyckoff site: 4c, site symmetry: $\text{m}2'\text{m}$.

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

Table 5: Wyckoff site: 8d, site symmetry: m..

| No. | position | mapping |
|-----|-------------|---------|
| 1 | [x, y, 0] | [1,6] |
| 2 | [-x, -y, 0] | [2,5] |
| 3 | [-y, x, 0] | [11,16] |
| 4 | [y, -x, 0] | [12,15] |
| 5 | [-x, y, 0] | [10,13] |
| 6 | [x, -y, 0] | [9,14] |
| 7 | [y, x, 0] | [4,7] |

continued ...

Table 5

| No. | position | mapping |
|-----|---------------|---------|
| 8 | $[-y, -x, 0]$ | [3,8] |

Table 6: Wyckoff site: 8e, site symmetry: . .m

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

Table 7: Wyckoff site: 8f, site symmetry: .m.

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

Table 8: Wyckoff site: 16g, site symmetry: 1

| No. | position | mapping |
|-----|----------------|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[-x, -y, z]$ | [2] |
| 3 | $[-y, x, z]$ | [11] |
| 4 | $[y, -x, z]$ | [12] |
| 5 | $[-x, y, -z]$ | [10] |
| 6 | $[x, -y, -z]$ | [9] |
| 7 | $[y, x, -z]$ | [4] |
| 8 | $[-y, -x, -z]$ | [3] |
| 9 | $[-x, -y, -z]$ | [5] |
| 10 | $[x, y, -z]$ | [6] |

continued ...

Table 8

| No. | position | mapping |
|-----|---------------|---------|
| 11 | $[y, -x, -z]$ | [15] |
| 12 | $[-y, x, -z]$ | [16] |
| 13 | $[x, -y, z]$ | [14] |
| 14 | $[-x, y, z]$ | [13] |
| 15 | $[-y, -x, z]$ | [8] |
| 16 | $[y, x, z]$ | [7] |