

MSG No. 95.140 P_c4_322 [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 2'2'2.

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

Table 2: Wyckoff site: 4b, site symmetry: 2'2'2.

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: 2'22'.

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

Table 5: Wyckoff site: 4e, site symmetry: 2.22

| No. | position | mapping |
|-----|------------------------|----------------|
| 1 | [0, 0, $\frac{1}{8}$] | [1, 7, 14, 16] |
| 2 | [0, 0, $\frac{7}{8}$] | [2, 5, 11, 12] |

continued ...

Table 5

| No. | position | mapping |
|-----|-----------------------|-------------|
| 3 | $[0, 0, \frac{3}{8}]$ | [3,4,10,13] |
| 4 | $[0, 0, \frac{5}{8}]$ | [6,8,9,15] |

Table 6: Wyckoff site: 4f, site symmetry: 2.22

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

Table 7: Wyckoff site: 8g, site symmetry: 2'..

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: 2' ..

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

Table 10: Wyckoff site: 8j, site symmetry: .2.

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

Table 11: Wyckoff site: 8k, site symmetry: .2'.

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

Table 12: Wyckoff site: 8l, site symmetry: .2'.

| No. | position | mapping |
|-----|-----------------------|---------|
| 1 | $[0, y, \frac{1}{4}]$ | [1,13] |
| 2 | $[-y, 0, 0]$ | [2,16] |
| 3 | $[y, 0, \frac{1}{2}]$ | [3,15] |

continued ...

Table 12

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

Table 13: Wyckoff site: 8m, site symmetry: .2.

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

Table 14: Wyckoff site: 8n, site symmetry: ..2'

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

Table 15: Wyckoff site: 8o, site symmetry: ...2

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

continued ...

Table 15

| No. | position | mapping |
|-----|-------------------------|---------|
| 7 | $[-x, -x, \frac{1}{8}]$ | [11,13] |
| 8 | $[-x, x, \frac{3}{8}]$ | [14,15] |

Table 16: Wyckoff site: 16p, site symmetry: 1

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