

MSG No. 59.412 P_bmmn [Type IV, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: $.2'/\mathbf{m}$.

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

Table 2: Wyckoff site: **4b**, site symmetry: $.2'/\mathbf{m'}$.

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

Table 3: Wyckoff site: **4c**, site symmetry: $.2'/\mathbf{m}$.

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

Table 4: Wyckoff site: **4d**, site symmetry: $.2'/\mathbf{m'}$.

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

Table 5: Wyckoff site: **4e**, site symmetry: $\mathbf{mm2}$

| No. | position | mapping |
|-----|----------------------------------|----------------|
| 1 | $[\frac{1}{4}, \frac{1}{4}, z]$ | $[1, 4, 6, 7]$ |
| 2 | $[\frac{3}{4}, \frac{3}{4}, -z]$ | $[2, 3, 5, 8]$ |

continued ...

Table 5

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

Table 6: Wyckoff site: 4f, site symmetry: mm'2'

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

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

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: .m.

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

Table 10: Wyckoff site: 8j, site symmetry: .m'.

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

Table 11: Wyckoff site: 8k, site symmetry: m..

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

Table 12: Wyckoff site: 16l, site symmetry: 1

| No. | position | mapping |
|-----|-----------------------------|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[x + \frac{1}{2}, -y, -z]$ | [2] |
| 3 | $[-x, y + \frac{1}{2}, -z]$ | [3] |

continued ...

Table 12

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