

MSG No. 10.48 P_b2/m [Type IV, monoclinic]

Table 1: Wyckoff site: 2a, site symmetry: $2/m$

| No. | position | mapping |
|-----|-----------------------|----------------|
| 1 | $[0, 0, 0]$ | $[1, 2, 3, 4]$ |
| 2 | $[0, \frac{1}{2}, 0]$ | $[5, 6, 7, 8]$ |

Table 2: Wyckoff site: 2b, site symmetry: $2/m'$

| No. | position | mapping |
|-----|-----------------------|----------------|
| 1 | $[0, \frac{1}{4}, 0]$ | $[1, 2, 7, 8]$ |
| 2 | $[0, \frac{3}{4}, 0]$ | $[3, 4, 5, 6]$ |

Table 3: Wyckoff site: 2c, site symmetry: $2/m$

| No. | position | mapping |
|-----|---------------------------------|----------------|
| 1 | $[0, 0, \frac{1}{2}]$ | $[1, 2, 3, 4]$ |
| 2 | $[0, \frac{1}{2}, \frac{1}{2}]$ | $[5, 6, 7, 8]$ |

Table 4: Wyckoff site: 2d, site symmetry: $2/m$

| No. | position | mapping |
|-----|---------------------------------|----------------|
| 1 | $[\frac{1}{2}, 0, 0]$ | $[1, 2, 3, 4]$ |
| 2 | $[\frac{1}{2}, \frac{1}{2}, 0]$ | $[5, 6, 7, 8]$ |

Table 5: Wyckoff site: 2e, site symmetry: $2/m'$

| No. | position | mapping |
|-----|---------------------------------|----------------|
| 1 | $[\frac{1}{2}, \frac{1}{4}, 0]$ | $[1, 2, 7, 8]$ |
| 2 | $[\frac{1}{2}, \frac{3}{4}, 0]$ | $[3, 4, 5, 6]$ |

Table 6: Wyckoff site: 2f, site symmetry: $2/m'$

| No. | position | mapping |
|-----|---------------------------------|----------------|
| 1 | $[0, \frac{1}{4}, \frac{1}{2}]$ | $[1, 2, 7, 8]$ |
| 2 | $[0, \frac{3}{4}, \frac{1}{2}]$ | $[3, 4, 5, 6]$ |

Table 7: Wyckoff site: $2\mathbf{g}$, site symmetry: $2/m$

| No. | position | mapping |
|-----|---|----------------|
| 1 | $[\frac{1}{2}, 0, \frac{1}{2}]$ | $[1, 2, 3, 4]$ |
| 2 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | $[5, 6, 7, 8]$ |

Table 8: Wyckoff site: $2\mathbf{h}$, site symmetry: $2/m'$

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

Table 9: Wyckoff site: $4\mathbf{i}$, site symmetry: 2

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

Table 10: Wyckoff site: $4\mathbf{j}$, site symmetry: 2

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

Table 11: Wyckoff site: $4\mathbf{k}$, site symmetry: 2

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

Table 12: Wyckoff site: $4\bar{1}$, site symmetry: 2

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

Table 13: Wyckoff site: $4\bar{\mathbf{m}}$, site symmetry: $\bar{\mathbf{m}}$

| No. | position | mapping |
|-----|-------------------------|---------|
| 1 | $[x, 0, z]$ | [1, 4] |
| 2 | $[-x, 0, -z]$ | [2, 3] |
| 3 | $[x, \frac{1}{2}, z]$ | [5, 8] |
| 4 | $[-x, \frac{1}{2}, -z]$ | [6, 7] |

Table 14: Wyckoff site: $4\bar{\mathbf{n}}$, site symmetry: $\bar{\mathbf{m}}'$

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

Table 15: Wyckoff site: $8\bar{\mathbf{o}}$, site symmetry: 1

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