

MSG No. 13.73 P_A2/c [Type IV, monoclinic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: -1

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

Table 6: Wyckoff site: $4\mathbf{f}$, site symmetry: -1

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

Table 7: Wyckoff site: $4\mathbf{g}$, site symmetry: 2

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

Table 8: Wyckoff site: $4\mathbf{h}$, site symmetry: 2

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

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

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

Table 10: Wyckoff site: $8\mathbf{j}$, site symmetry: 1

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

continued ...

Table 10

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