

MSG No. 48.257 $Pnnn$ [Type I, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: 222

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

Table 2: Wyckoff site: 2b, site symmetry: 222

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

Table 3: Wyckoff site: 2c, site symmetry: 222

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

Table 4: Wyckoff site: 2d, site symmetry: 222

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 11: Wyckoff site: $4k$, site symmetry: $\dots 2$

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

Table 12: Wyckoff site: $4l$, site symmetry: $\dots 2$

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

Table 13: Wyckoff site: $8m$, site symmetry: 1

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