

MSG No. 16.4 P_a222 [Type IV, orthorhombic]

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

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

Table 2: Wyckoff site: 2b, site symmetry: $22'2'$

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

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

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

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

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

Table 5: Wyckoff site: 2e, site symmetry: $22'2'$

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

Table 6: Wyckoff site: 2f, site symmetry: $22'2'$

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

Table 7: Wyckoff site: $2\mathbf{g}$, site symmetry: 222

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

Table 8: Wyckoff site: $2\mathbf{h}$, site symmetry: $22'2'$

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

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

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

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

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

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

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

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

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

Table 13: Wyckoff site: $4\bar{\mathbf{m}}$, site symmetry: $.2.$

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

Table 14: Wyckoff site: $4\bar{\mathbf{n}}$, site symmetry: $.2.$

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

Table 15: Wyckoff site: $4\mathbf{o}$, site symmetry: $.2'.$

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

Table 16: Wyckoff site: $4\mathbf{p}$, site symmetry: $.2'.$

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

Table 17: Wyckoff site: $4q$, site symmetry: $\dots 2$

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

Table 18: Wyckoff site: $4r$, site symmetry: $\dots 2'$

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

Table 19: Wyckoff site: $4s$, site symmetry: $\dots 2$

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

Table 20: Wyckoff site: $4t$, site symmetry: $\dots 2'$

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

Table 21: Wyckoff site: $8u$, site symmetry: 1

| No. | position | mapping |
|-----|---------------|---------|
| 1 | $[x, y, z]$ | $[1]$ |
| 2 | $[x, -y, -z]$ | $[2]$ |
| 3 | $[-x, y, -z]$ | $[3]$ |
| 4 | $[-x, -y, z]$ | $[4]$ |

continued ...

Table 21

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