

MSG No. 16.3 $P2'2'2$ [Type III, orthorhombic]

Table 1: Wyckoff site: **1a**, site symmetry: $2'2'2$

| No. | position | mapping |
|-----|-------------|----------------|
| 1 | $[0, 0, 0]$ | $[1, 2, 3, 4]$ |

Table 2: Wyckoff site: **1b**, site symmetry: $2'2'2$

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

Table 3: Wyckoff site: **1c**, site symmetry: $2'2'2$

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

Table 4: Wyckoff site: **1d**, site symmetry: $2'2'2$

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

Table 5: Wyckoff site: **1e**, site symmetry: $2'2'2$

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

Table 6: Wyckoff site: **1f**, site symmetry: $2'2'2$

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

Table 7: Wyckoff site: $1\mathbf{g}$, site symmetry: $2'2'2$

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

Table 8: Wyckoff site: $1\mathbf{h}$, site symmetry: $2'2'2$

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

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

| No. | position | mapping |
|-----|--------------|----------|
| 1 | $[x, 0, 0]$ | $[1, 3]$ |
| 2 | $[-x, 0, 0]$ | $[2, 4]$ |

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

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

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

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

Table 12: Wyckoff site: $2\mathbf{l}$, site symmetry: $2'..$

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

Table 13: Wyckoff site: $2\mathfrak{m}$, site symmetry: $.2'$.

| No. | position | mapping |
|-----|--------------|----------|
| 1 | $[0, y, 0]$ | $[1, 4]$ |
| 2 | $[0, -y, 0]$ | $[2, 3]$ |

Table 14: Wyckoff site: $2\mathfrak{n}$, site symmetry: $.2'$.

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

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

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

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

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

Table 17: Wyckoff site: $2\mathfrak{q}$, site symmetry: $..2$

| No. | position | mapping |
|-----|--------------|----------|
| 1 | $[0, 0, z]$ | $[1, 2]$ |
| 2 | $[0, 0, -z]$ | $[3, 4]$ |

Table 18: Wyckoff site: $2\mathfrak{r}$, site symmetry: $..2$

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

Table 19: Wyckoff site: $2\mathbf{s}$, site symmetry: $\dots 2$

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

Table 20: Wyckoff site: $2\mathbf{t}$, site symmetry: $\dots 2$

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

Table 21: Wyckoff site: $4\mathbf{u}$, site symmetry: 1

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