

MSG No. 18.23 $P_C2_12_12$ [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $2' \dots$

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

Table 6: Wyckoff site: **4f**, site symmetry: $2'..$

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

Table 7: Wyckoff site: **4g**, site symmetry: $.2'$

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

Table 8: Wyckoff site: **4h**, site symmetry: $.2'$

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

Table 9: Wyckoff site: **4i**, site symmetry: $..2$

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

Table 10: Wyckoff site: **4j**, site symmetry: $..2$

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

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

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

Table 12: Wyckoff site: $8l$, site symmetry: 1

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