

MSG No. 81.38 $P_7\bar{4}$ [Type IV, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $-4..$

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

Table 2: Wyckoff site: 2b, site symmetry: $-4..$

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

Table 3: Wyckoff site: 2c, site symmetry: $-4'..$

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $2..$

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

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

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

Table 7: Wyckoff site: **8g**, site symmetry: **1**

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