

MSG No. 117.302 $P\bar{4}'b2'$ [Type III, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: $2.2'2'$

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

Table 4: Wyckoff site: 2d, site symmetry: $2.2'2'$

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

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

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

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 | $[0, \frac{1}{2}, -z]$ | [5,6] |
| 4 | $[\frac{1}{2}, 0, -z]$ | [7,8] |

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

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

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

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

Table 9: Wyckoff site: $8i$, site symmetry: 1

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