

MSG No. 53.328 $Pm'na'$ [Type III, orthorhombic]

Table 1: Wyckoff site: **2a**, site symmetry: $2'/\mathfrak{m}'..$

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

Table 2: Wyckoff site: **2b**, site symmetry: $2'/\mathfrak{m}'..$

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

Table 3: Wyckoff site: **2c**, site symmetry: $2'/\mathfrak{m}'..$

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

Table 4: Wyckoff site: **2d**, site symmetry: $2'/\mathfrak{m}'..$

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

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

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

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

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

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

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

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

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

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

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