

MSG No. 62.441 $Pnma$ [Type I, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: -1

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

Table 2: Wyckoff site: 4b, site symmetry: -1

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

Table 3: Wyckoff site: 4c, site symmetry: $.m$.

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

Table 4: Wyckoff site: 8d, site symmetry: 1

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