

SG No. 57 D_{2h}^{11} $Pbcm$ [orthorhombic]

* plus set: $+ [0, 0, 0]$

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: $..m$

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

Table 5: Wyckoff site: 8e, site symmetry: 1

| No. | position | mapping |
|-----|-------------|---------|
| 1 | $[x, y, z]$ | [1] |

continued ...

Table 5

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