

SG No. 87  $C_{4h}^5$   $I4/m$  [ tetragonal ]

\* plus set:  $+[0, 0, 0]$ ,  $+[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

Table 1: Wyckoff site: 2a, site symmetry: 4/m..

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

Table 2: Wyckoff site: 2b, site symmetry: 4/m..

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

Table 3: Wyckoff site: 4c, site symmetry: 2/m..

| 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: 4d, site symmetry: -4..

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

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

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

Table 6: Wyckoff site: 8f, site symmetry: -1

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

*continued ...*

Table 6

| No. | position   | mapping |
|-----|--|---------|
| 4   | $\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | [4,8]   |

Table 7: Wyckoff site: 8g, 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 8: Wyckoff site: 8h, site symmetry: m..

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

Table 9: Wyckoff site: 16i, 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   | $[-x, -y, -z]$ | [5]     |
| 6   | $[x, y, -z]$   | [6]     |
| 7   | $[y, -x, -z]$  | [7]     |
| 8   | $[-y, x, -z]$  | [8]     |