

PG No. 31 $T_d \bar{4}3m$ [cubic]

Table 1: Wyckoff site: 1o, site symmetry: $\bar{4}3m$

| No. | position | mapping |
|-----|-------------|---|
| 1 | $[0, 0, 0]$ | $[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$ |

Table 2: Wyckoff site: 4a, site symmetry: $\bar{3}m$

| No. | position | mapping |
|-----|---------------|--------------------------|
| 1 | $[x, x, x]$ | $[1, 5, 9, 13, 17, 21]$ |
| 2 | $[-x, -x, x]$ | $[2, 7, 12, 14, 19, 24]$ |
| 3 | $[-x, x, -x]$ | $[3, 8, 10, 16, 18, 23]$ |
| 4 | $[x, -x, -x]$ | $[4, 6, 11, 15, 20, 22]$ |

Table 3: Wyckoff site: 6b, site symmetry: $2.mm$

| No. | position | mapping |
|-----|--------------|--------------------|
| 1 | $[x, 0, 0]$ | $[1, 4, 17, 20]$ |
| 2 | $[-x, 0, 0]$ | $[2, 3, 18, 19]$ |
| 3 | $[0, x, 0]$ | $[5, 8, 13, 16]$ |
| 4 | $[0, -x, 0]$ | $[6, 7, 14, 15]$ |
| 5 | $[0, 0, x]$ | $[9, 12, 21, 24]$ |
| 6 | $[0, 0, -x]$ | $[10, 11, 22, 23]$ |

Table 4: Wyckoff site: 12c, site symmetry: $\bar{3}.m$

| No. | position | mapping |
|-----|---------------|------------|
| 1 | $[x, x, z]$ | $[1, 13]$ |
| 2 | $[-x, -x, z]$ | $[2, 14]$ |
| 3 | $[-x, x, -z]$ | $[3, 16]$ |
| 4 | $[x, -x, -z]$ | $[4, 15]$ |
| 5 | $[z, x, x]$ | $[5, 21]$ |
| 6 | $[z, -x, -x]$ | $[6, 22]$ |
| 7 | $[-z, -x, x]$ | $[7, 24]$ |
| 8 | $[-z, x, -x]$ | $[8, 23]$ |
| 9 | $[x, z, x]$ | $[9, 17]$ |
| 10 | $[-x, z, -x]$ | $[10, 18]$ |
| 11 | $[x, -z, -x]$ | $[11, 20]$ |
| 12 | $[-x, -z, x]$ | $[12, 19]$ |

Table 5: Wyckoff site: 24d, site symmetry: 1

| No. | position | mapping |
|-----|---------------|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[-x, -y, z]$ | [2] |
| 3 | $[-x, y, -z]$ | [3] |
| 4 | $[x, -y, -z]$ | [4] |
| 5 | $[z, x, y]$ | [5] |
| 6 | $[z, -x, -y]$ | [6] |
| 7 | $[-z, -x, y]$ | [7] |
| 8 | $[-z, x, -y]$ | [8] |
| 9 | $[y, z, x]$ | [9] |
| 10 | $[-y, z, -x]$ | [10] |
| 11 | $[y, -z, -x]$ | [11] |
| 12 | $[-y, -z, x]$ | [12] |
| 13 | $[y, x, z]$ | [13] |
| 14 | $[-y, -x, z]$ | [14] |
| 15 | $[y, -x, -z]$ | [15] |
| 16 | $[-y, x, -z]$ | [16] |
| 17 | $[x, z, y]$ | [17] |
| 18 | $[-x, z, -y]$ | [18] |
| 19 | $[-x, -z, y]$ | [19] |
| 20 | $[x, -z, -y]$ | [20] |
| 21 | $[z, y, x]$ | [21] |
| 22 | $[z, -y, -x]$ | [22] |
| 23 | $[-z, y, -x]$ | [23] |
| 24 | $[-z, -y, x]$ | [24] |