

PG No. 33 $D_{2d}(1)$ $\bar{4}2m$ (-4m2 setting) [tetragonal]

Table 1: Wyckoff site: 1o, site symmetry: $-4m2$

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

Table 2: Wyckoff site: 2a, site symmetry: $2mm$.

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

Table 3: Wyckoff site: 4b, site symmetry: $\dots 2$

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

Table 4: Wyckoff site: 4c, site symmetry: $\dots m$.

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

Table 5: Wyckoff site: 8d, 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] |

continued ...

Table 5

| No. | position | mapping |
|-----|----------------|---------|
| 8 | $[-y, -x, -z]$ | [8] |