

SG No. 79 C_4^5 $I4$ [tetragonal]

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

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

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

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

| No. | position | mapping |
|-----|-----------------------|----------|
| 1 | $[0, \frac{1}{2}, z]$ | $[1, 2]$ |
| 2 | $[\frac{1}{2}, 0, z]$ | $[3, 4]$ |

Table 3: Wyckoff site: 8c, site symmetry: 1

| No. | position | mapping |
|-----|---------------|---------|
| 1 | $[x, y, z]$ | $[1]$ |
| 2 | $[-x, -y, z]$ | $[2]$ |
| 3 | $[-y, x, z]$ | $[3]$ |
| 4 | $[y, -x, z]$ | $[4]$ |