

SG No. 77  $C_4^3$   $P4_2$  [ tetragonal ]

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

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: 1

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