

SG No. 96 D_4^8 $P4_3212$ [tetragonal]

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

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

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

Table 2: Wyckoff site: 8b, site symmetry: 1

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