

MSG No. 76.7 $P4_1$ [Type I, tetragonal]Table 1: Wyckoff site: **4a**, site symmetry: **1**

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