

Table 1: Wyckoff site: **6a**, site symmetry: **1**

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