

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $-3'$

| No. | position | mapping |
|-----|-------------|----------------------|
| 1 | $[0, 0, 0]$ | $[1, 2, 3, 4, 5, 6]$ |

Table 2: Wyckoff site: $2\mathbf{a}$, site symmetry: $3.$

| No. | position | mapping |
|-----|--------------|-------------|
| 1 | $[0, 0, z]$ | $[1, 2, 3]$ |
| 2 | $[0, 0, -z]$ | $[4, 5, 6]$ |

Table 3: Wyckoff site: $6\mathbf{b}$, site symmetry: 1

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