

Table 1: Wyckoff site: **1a**, site symmetry: $3.m'$

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

Table 2: Wyckoff site: **3b**, site symmetry: $.m$

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

Table 3: Wyckoff site: **6c**, site symmetry: 1

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