

Table 1: Wyckoff site: $1o$, site symmetry: $4'/m'$

| No. | position | mapping |
|-----|-------------|----------------------------|
| 1 | $[0, 0, 0]$ | $[1, 2, 3, 4, 5, 6, 7, 8]$ |

Table 2: Wyckoff site: $2a$, site symmetry: $4'..$

| No. | position | mapping |
|-----|--------------|----------------|
| 1 | $[0, 0, z]$ | $[1, 2, 5, 6]$ |
| 2 | $[0, 0, -z]$ | $[3, 4, 7, 8]$ |

Table 3: Wyckoff site: $4b$, site symmetry: $m'..$

| No. | position | mapping |
|-----|---------------|----------|
| 1 | $[x, y, 0]$ | $[1, 8]$ |
| 2 | $[-x, -y, 0]$ | $[2, 7]$ |
| 3 | $[-y, x, 0]$ | $[4, 5]$ |
| 4 | $[y, -x, 0]$ | $[3, 6]$ |

Table 4: Wyckoff site: $8c$, site symmetry: 1

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