

Table 1: Wyckoff site: 4a, site symmetry: $2'..$

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, 0, \frac{1}{4}]$ | [1,6] |
| 2 | $[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$ | [2,5] |
| 3 | $[-x, \frac{1}{2}, \frac{1}{4}]$ | [3,8] |
| 4 | $[\frac{1}{2} - x, 0, \frac{3}{4}]$ | [4,7] |

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

| No. | position | mapping |
|-----|---|---------|
| 1 | $[\frac{1}{4}, y, 0]$ | [1,7] |
| 2 | $[\frac{3}{4}, \frac{1}{2} - y, 0]$ | [2,8] |
| 3 | $[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2}]$ | [3,5] |
| 4 | $[\frac{1}{4}, -y, \frac{1}{2}]$ | [4,6] |

Table 3: Wyckoff site: 4c, site symmetry: $..2'$

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

Table 4: Wyckoff site: 8d, site symmetry: 1

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