

Table 1: Wyckoff site: **4a**, site symmetry: $-1'$

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

Table 2: Wyckoff site: **4b**, site symmetry: $-1'$

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

Table 3: Wyckoff site: **4c**, site symmetry: $.m.$

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

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

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