

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

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

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

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

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

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

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

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