

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: 1

| No. | position | mapping |
|-----|----------------------------|---------|
| 1 | $[x, y, z]$ | $[1]$ |
| 2 | $[\frac{1}{2} - x, -y, z]$ | $[2]$ |

continued ...

Table 5

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