

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: -1

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

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

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

Table 5: Wyckoff site: **4e**, site symmetry: $2'$

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

continued ...

Table 5

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

Table 6: Wyckoff site: **8f**, site symmetry: **1**

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