

Table 1: Wyckoff site: 2a, site symmetry: $m'm'2$

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

Table 2: Wyckoff site: 2b, site symmetry: $m'm'2$

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

Table 3: Wyckoff site: 2c, site symmetry: $mm'2'$

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $.m'$

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

Table 6: Wyckoff site: **4f**, site symmetry: $.m'$.

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

Table 7: Wyckoff site: **4g**, site symmetry: m' .

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

Table 8: Wyckoff site: **4h**, site symmetry: m .

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

Table 9: Wyckoff site: **8i**, site symmetry: 1

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