

Table 1: Wyckoff site: 2a, site symmetry: $2.mm1'$

| No. | position | mapping |
|-----|---|--------------------------------|
| 1 | $[0, 0, z]$ | $[1, 4, 7, 8, 9, 12, 15, 16]$ |
| 2 | $[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | $[2, 3, 5, 6, 10, 11, 13, 14]$ |

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

| No. | position | mapping |
|-----|-------------------------------------|------------------|
| 1 | $[0, \frac{1}{2}, z]$ | $[1, 4, 9, 12]$ |
| 2 | $[0, \frac{1}{2}, z + \frac{1}{2}]$ | $[2, 3, 10, 11]$ |
| 3 | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | $[5, 6, 13, 14]$ |
| 4 | $[\frac{1}{2}, 0, z]$ | $[7, 8, 15, 16]$ |

Table 3: Wyckoff site: 4c, site symmetry: $..m1'$

| No. | position | mapping |
|-----|---|------------------|
| 1 | $[x, x, z]$ | $[1, 8, 9, 16]$ |
| 2 | $[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$ | $[2, 5, 10, 13]$ |
| 3 | $[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$ | $[3, 6, 11, 14]$ |
| 4 | $[-x, -x, z]$ | $[4, 7, 12, 15]$ |

Table 4: Wyckoff site: 8d, site symmetry: $11'$

| No. | position | mapping |
|-----|---|-----------|
| 1 | $[x, y, z]$ | $[1, 9]$ |
| 2 | $[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$ | $[2, 10]$ |
| 3 | $[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$ | $[3, 11]$ |
| 4 | $[-x, -y, z]$ | $[4, 12]$ |
| 5 | $[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$ | $[5, 13]$ |
| 6 | $[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$ | $[6, 14]$ |
| 7 | $[-y, -x, z]$ | $[7, 15]$ |
| 8 | $[y, x, z]$ | $[8, 16]$ |