

Table 1: Wyckoff site: 4a, site symmetry: 4. .

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: 2' . .

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

Table 4: Wyckoff site: 16d, site symmetry: 1

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[-y, x, z]$ | [2] |
| 3 | $[y, -x, z]$ | [3] |
| 4 | $[-x, -y, z]$ | [4] |
| 5 | $[-x, y, z + \frac{1}{2}]$ | [5] |
| 6 | $[x, -y, z + \frac{1}{2}]$ | [6] |
| 7 | $[-y, -x, z + \frac{1}{2}]$ | [7] |
| 8 | $[y, x, z + \frac{1}{2}]$ | [8] |
| 9 | $[x + \frac{1}{2}, y + \frac{1}{2}, z]$ | [9] |

continued ...

Table 4

| No. | position | mapping |
|-----|---|---------|
| 10 | $[\frac{1}{2} - y, x + \frac{1}{2}, z]$ | [10] |
| 11 | $[y + \frac{1}{2}, \frac{1}{2} - x, z]$ | [11] |
| 12 | $[\frac{1}{2} - x, \frac{1}{2} - y, z]$ | [12] |
| 13 | $[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$ | [13] |
| 14 | $[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$ | [14] |
| 15 | $[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$ | [15] |
| 16 | $[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$ | [16] |