

Table 1: Wyckoff site: 8a, site symmetry: $\dots 2'$

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

Table 2: Wyckoff site: 16b, site symmetry: 1

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