

Table 1: Wyckoff site: 16a, site symmetry: $\dots 2$

| No. | position | mapping |
|-----|---|---------|
| 1 | $[0, 0, z]$ | [1,2] |
| 2 | $[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{4}]$ | [3,4] |
| 3 | $[0, \frac{1}{2}, z + \frac{1}{2}]$ | [5,6] |
| 4 | $[\frac{1}{4}, \frac{3}{4}, z + \frac{3}{4}]$ | [7,8] |
| 5 | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | [9,10] |
| 6 | $[\frac{3}{4}, \frac{1}{4}, z + \frac{3}{4}]$ | [11,12] |
| 7 | $[\frac{1}{2}, \frac{1}{2}, z]$ | [13,14] |
| 8 | $[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{4}]$ | [15,16] |
| 9 | $[0, 0, z + \frac{1}{2}]$ | [17,18] |
| 10 | $[\frac{1}{4}, \frac{1}{4}, z + \frac{3}{4}]$ | [19,20] |
| 11 | $[0, \frac{1}{2}, z]$ | [21,22] |
| 12 | $[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{4}]$ | [23,24] |
| 13 | $[\frac{1}{2}, 0, z]$ | [25,26] |
| 14 | $[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{4}]$ | [27,28] |
| 15 | $[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | [29,30] |
| 16 | $[\frac{3}{4}, \frac{3}{4}, z + \frac{3}{4}]$ | [31,32] |

Table 2: Wyckoff site: 16b, site symmetry: $\dots 2'$

| No. | position | mapping |
|-----|---|---------|
| 1 | $[0, \frac{1}{4}, z]$ | [1,22] |
| 2 | $[0, \frac{3}{4}, z]$ | [2,21] |
| 3 | $[\frac{1}{4}, \frac{1}{2}, z + \frac{1}{4}]$ | [3,24] |
| 4 | $[\frac{1}{4}, 0, z + \frac{1}{4}]$ | [4,23] |
| 5 | $[0, \frac{3}{4}, z + \frac{1}{2}]$ | [5,18] |
| 6 | $[0, \frac{1}{4}, z + \frac{1}{2}]$ | [6,17] |
| 7 | $[\frac{1}{4}, 0, z + \frac{3}{4}]$ | [7,20] |
| 8 | $[\frac{1}{4}, \frac{1}{2}, z + \frac{3}{4}]$ | [8,19] |
| 9 | $[\frac{1}{2}, \frac{1}{4}, z + \frac{1}{2}]$ | [9,30] |
| 10 | $[\frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$ | [10,29] |
| 11 | $[\frac{3}{4}, \frac{1}{2}, z + \frac{3}{4}]$ | [11,32] |
| 12 | $[\frac{3}{4}, 0, z + \frac{3}{4}]$ | [12,31] |
| 13 | $[\frac{1}{2}, \frac{3}{4}, z]$ | [13,26] |
| 14 | $[\frac{1}{2}, \frac{1}{4}, z]$ | [14,25] |
| 15 | $[\frac{3}{4}, 0, z + \frac{1}{4}]$ | [15,28] |
| 16 | $[\frac{3}{4}, \frac{1}{2}, z + \frac{1}{4}]$ | [16,27] |

Table 3: Wyckoff site: 32c, site symmetry: 1

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[-x, -y, z]$ | [2] |
| 3 | $[\frac{1}{4} - x, y + \frac{1}{4}, z + \frac{1}{4}]$ | [3] |
| 4 | $[x + \frac{1}{4}, \frac{1}{4} - y, z + \frac{1}{4}]$ | [4] |
| 5 | $[x, y + \frac{1}{2}, z + \frac{1}{2}]$ | [5] |
| 6 | $[-x, \frac{1}{2} - y, z + \frac{1}{2}]$ | [6] |
| 7 | $[\frac{1}{4} - x, y + \frac{3}{4}, z + \frac{3}{4}]$ | [7] |
| 8 | $[x + \frac{1}{4}, \frac{3}{4} - y, z + \frac{3}{4}]$ | [8] |
| 9 | $[x + \frac{1}{2}, y, z + \frac{1}{2}]$ | [9] |
| 10 | $[\frac{1}{2} - x, -y, z + \frac{1}{2}]$ | [10] |
| 11 | $[\frac{3}{4} - x, y + \frac{1}{4}, z + \frac{3}{4}]$ | [11] |
| 12 | $[x + \frac{3}{4}, \frac{1}{4} - y, z + \frac{3}{4}]$ | [12] |
| 13 | $[x + \frac{1}{2}, y + \frac{1}{2}, z]$ | [13] |
| 14 | $[\frac{1}{2} - x, \frac{1}{2} - y, z]$ | [14] |
| 15 | $[\frac{3}{4} - x, y + \frac{3}{4}, z + \frac{1}{4}]$ | [15] |
| 16 | $[x + \frac{3}{4}, \frac{3}{4} - y, z + \frac{1}{4}]$ | [16] |
| 17 | $[x, y, z + \frac{1}{2}]$ | [17] |
| 18 | $[-x, -y, z + \frac{1}{2}]$ | [18] |
| 19 | $[\frac{1}{4} - x, y + \frac{1}{4}, z + \frac{3}{4}]$ | [19] |
| 20 | $[x + \frac{1}{4}, \frac{1}{4} - y, z + \frac{3}{4}]$ | [20] |
| 21 | $[x, y + \frac{1}{2}, z]$ | [21] |
| 22 | $[-x, \frac{1}{2} - y, z]$ | [22] |
| 23 | $[\frac{1}{4} - x, y + \frac{3}{4}, z + \frac{1}{4}]$ | [23] |
| 24 | $[x + \frac{1}{4}, \frac{3}{4} - y, z + \frac{1}{4}]$ | [24] |
| 25 | $[x + \frac{1}{2}, y, z]$ | [25] |
| 26 | $[\frac{1}{2} - x, -y, z]$ | [26] |
| 27 | $[\frac{3}{4} - x, y + \frac{1}{4}, z + \frac{1}{4}]$ | [27] |
| 28 | $[x + \frac{3}{4}, \frac{1}{4} - y, z + \frac{1}{4}]$ | [28] |
| 29 | $[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$ | [29] |
| 30 | $[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$ | [30] |
| 31 | $[\frac{3}{4} - x, y + \frac{3}{4}, z + \frac{3}{4}]$ | [31] |
| 32 | $[x + \frac{3}{4}, \frac{3}{4} - y, z + \frac{3}{4}]$ | [32] |