

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

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

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: -1

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

Table 5: Wyckoff site: $8e$, site symmetry: $2..$

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

Table 6: Wyckoff site: $8f$, site symmetry: $..2$

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

Table 7: Wyckoff site: $16g$, site symmetry: 1

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