

SG No. 220 T_d^6 $I\bar{4}3d$ [cubic]

* plus set: $+ [0, 0, 0], \quad + [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

Table 1: Wyckoff site: 12a, site symmetry: $-4..$

| No. | position | mapping |
|-----|---------------------------------|---------------|
| 1 | $[\frac{3}{8}, 0, \frac{1}{4}]$ | [1,4,18,19] |
| 2 | $[\frac{1}{8}, 0, \frac{3}{4}]$ | [2,3,17,20] |
| 3 | $[\frac{1}{4}, \frac{3}{8}, 0]$ | [5,8,14,15] |
| 4 | $[\frac{3}{4}, \frac{1}{8}, 0]$ | [6,7,13,16] |
| 5 | $[0, \frac{1}{4}, \frac{3}{8}]$ | [9,12,22,23] |
| 6 | $[0, \frac{3}{4}, \frac{1}{8}]$ | [10,11,21,24] |

Table 2: Wyckoff site: 12b, site symmetry: $-4..$

| No. | position | mapping |
|-----|---------------------------------|---------------|
| 1 | $[\frac{7}{8}, 0, \frac{1}{4}]$ | [1,4,18,19] |
| 2 | $[\frac{5}{8}, 0, \frac{3}{4}]$ | [2,3,17,20] |
| 3 | $[\frac{1}{4}, \frac{7}{8}, 0]$ | [5,8,14,15] |
| 4 | $[\frac{3}{4}, \frac{5}{8}, 0]$ | [6,7,13,16] |
| 5 | $[0, \frac{1}{4}, \frac{7}{8}]$ | [9,12,22,23] |
| 6 | $[0, \frac{3}{4}, \frac{5}{8}]$ | [10,11,21,24] |

Table 3: Wyckoff site: 16c, site symmetry: $.3..$

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

Table 4: Wyckoff site: 24d, site symmetry: $2..$

| No. | position | mapping |
|-----|-------------------------------------|---------|
| 1 | $[x, 0, \frac{1}{4}]$ | [1,4] |
| 2 | $[\frac{1}{2} - x, 0, \frac{3}{4}]$ | [2,3] |
| 3 | $[\frac{1}{4}, x, 0]$ | [5,8] |

continued ...

Table 4

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

Table 5: Wyckoff site: **48e**, site symmetry: 1

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