

Table 1: Wyckoff site: 2a, site symmetry: $-6'2m'$

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

Table 2: Wyckoff site: 2b, site symmetry: $-6'2m'$

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

Table 3: Wyckoff site: 4c, site symmetry: $-6'..$

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

Table 4: Wyckoff site: 4d, site symmetry: $-6'..$

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

Table 5: Wyckoff site: 4e, site symmetry: $3.m'$

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

Table 6: Wyckoff site: **6f**, site symmetry: $m'2m'$

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

Table 7: Wyckoff site: **6g**, site symmetry: $m2'm'$

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

Table 8: Wyckoff site: **8h**, site symmetry: $3..$

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

Table 9: Wyckoff site: **12i**, site symmetry: $..m'$

| No. | position | mapping |
|-----|-----------------------------|-----------|
| 1 | $[x, 0, z]$ | $[1, 23]$ |
| 2 | $[0, x, z]$ | $[2, 24]$ |
| 3 | $[-x, -x, z]$ | $[3, 22]$ |
| 4 | $[x, 0, -z]$ | $[4, 20]$ |
| 5 | $[0, x, -z]$ | $[5, 21]$ |
| 6 | $[-x, -x, -z]$ | $[6, 19]$ |
| 7 | $[-x, -x, \frac{1}{2} - z]$ | $[7, 18]$ |

continued ...

Table 9

| No. | position | mapping |
|-----|-----------------------------|---------|
| 8 | $[x, 0, \frac{1}{2} - z]$ | [8,16] |
| 9 | $[0, x, \frac{1}{2} - z]$ | [9,17] |
| 10 | $[-x, -x, z + \frac{1}{2}]$ | [10,15] |
| 11 | $[x, 0, z + \frac{1}{2}]$ | [11,13] |
| 12 | $[0, x, z + \frac{1}{2}]$ | [12,14] |

Table 10: Wyckoff site: 12j, site symmetry: $m'..$

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

Table 11: Wyckoff site: 12k, site symmetry: $m..$

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

Table 12: Wyckoff site: 241, site symmetry: 1

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