

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: 3.2

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $6'..$

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

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

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

Table 7: Wyckoff site: $6g$, site symmetry: $2'/m'$

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

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

| No. | position | mapping |
|-----|---|--------------|
| 1 | $[\frac{1}{3}, \frac{2}{3}, z]$ | [1, 2, 3] |
| 2 | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$ | [4, 5, 6] |
| 3 | $[\frac{2}{3}, \frac{1}{3}, -z]$ | [7, 8, 9] |
| 4 | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [10, 11, 12] |
| 5 | $[\frac{2}{3}, \frac{1}{3}, z]$ | [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 | $[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$ | [22, 23, 24] |

Table 9: Wyckoff site: $12i$, site symmetry: $2'..$

| No. | position | mapping |
|-----|---|---------|
| 1 | $[\frac{1}{2}, 0, z]$ | [1, 14] |
| 2 | $[0, \frac{1}{2}, z]$ | [2, 15] |
| 3 | $[\frac{1}{2}, \frac{1}{2}, z]$ | [3, 13] |
| 4 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$ | [4, 18] |
| 5 | $[\frac{1}{2}, 0, \frac{1}{2} - z]$ | [5, 16] |
| 6 | $[0, \frac{1}{2}, \frac{1}{2} - z]$ | [6, 17] |
| 7 | $[\frac{1}{2}, 0, -z]$ | [7, 20] |

continued ...

Table 9

| No. | position | mapping |
|-----|---|---------|
| 8 | $[0, \frac{1}{2}, -z]$ | [8,21] |
| 9 | $[\frac{1}{2}, \frac{1}{2}, -z]$ | [9,19] |
| 10 | $[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | [10,24] |
| 11 | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | [11,22] |
| 12 | $[0, \frac{1}{2}, z + \frac{1}{2}]$ | [12,23] |

Table 10: Wyckoff site: 12j, site symmetry: $.2'$.

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

Table 11: Wyckoff site: 12k, site symmetry: $..2$

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

Table 12: Wyckoff site: 12l, 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 | $[x, x - y, \frac{1}{2}]$ | [4,24] |
| 5 | $[-x + y, y, \frac{1}{2}]$ | [5,22] |
| 6 | $[-y, -x, \frac{1}{2}]$ | [6,23] |
| 7 | $[-x, -y, 0]$ | [7,14] |
| 8 | $[y, -x + y, 0]$ | [8,15] |
| 9 | $[x - y, x, 0]$ | [9,13] |
| 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 13: Wyckoff site: 24m, site symmetry: 1

| No. | position | mapping |
|-----|---------------------------------|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[-y, x - y, z]$ | [2] |
| 3 | $[-x + y, -x, z]$ | [3] |
| 4 | $[x, x - y, \frac{1}{2} - z]$ | [4] |
| 5 | $[-x + y, y, \frac{1}{2} - z]$ | [5] |
| 6 | $[-y, -x, \frac{1}{2} - z]$ | [6] |
| 7 | $[-x, -y, -z]$ | [7] |
| 8 | $[y, -x + y, -z]$ | [8] |
| 9 | $[x - y, x, -z]$ | [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 | $[x - y, x, z]$ | [13] |
| 14 | $[-x, -y, z]$ | [14] |
| 15 | $[y, -x + y, z]$ | [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 | $[-x + y, y, z + \frac{1}{2}]$ | [22] |
| 23 | $[-y, -x, z + \frac{1}{2}]$ | [23] |
| 24 | $[x, x - y, z + \frac{1}{2}]$ | [24] |