

Table 1: Wyckoff site: 2a, site symmetry:  $-3'm'$ .

| 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:  $-6m'2'$

| 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: 2c, site symmetry:  $-6m'2'$

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

Table 4: Wyckoff site: 2d, site symmetry:  $-6m'2'$

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

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

| 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: 4f, site symmetry:  $3m'$ .

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

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

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

Table 8: Wyckoff site: 6h, site symmetry:  $mm'2'$ .

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

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

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

*continued ...*

Table 9

| No. | position    | mapping    |
|-----|-------------|------------|
| 12  | $[x, x, 0]$ | $[21, 24]$ |

Table 10: Wyckoff site: 12j, 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   | $[x - y, x, \frac{3}{4}]$   | $[13, 21]$ |
| 8   | $[-x, -y, \frac{3}{4}]$     | $[14, 19]$ |
| 9   | $[y, -x + y, \frac{3}{4}]$  | $[15, 20]$ |
| 10  | $[x, x - y, \frac{1}{4}]$   | $[16, 24]$ |
| 11  | $[-x + y, y, \frac{1}{4}]$  | $[17, 22]$ |
| 12  | $[-y, -x, \frac{1}{4}]$     | $[18, 23]$ |

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

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

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

| No. | position         | mapping |
|-----|------------------|---------|
| 1   | $[x, y, z]$      | $[1]$   |
| 2   | $[-y, x - y, z]$ | $[2]$   |

*continued ...*

Table 12

| No. | position                        | mapping |
|-----|---------------------------------|---------|
| 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  | $[x - y, x, z + \frac{1}{2}]$   | [13]    |
| 14  | $[-x, -y, z + \frac{1}{2}]$     | [14]    |
| 15  | $[y, -x + y, z + \frac{1}{2}]$  | [15]    |
| 16  | $[x, x - y, \frac{1}{2} - z]$   | [16]    |
| 17  | $[-x + y, y, \frac{1}{2} - z]$  | [17]    |
| 18  | $[-y, -x, \frac{1}{2} - z]$     | [18]    |
| 19  | $[-x, -y, -z]$                  | [19]    |
| 20  | $[y, -x + y, -z]$               | [20]    |
| 21  | $[x - y, x, -z]$                | [21]    |
| 22  | $[-x + y, y, z]$                | [22]    |
| 23  | $[-y, -x, z]$                   | [23]    |
| 24  | $[x, x - y, z]$                 | [24]    |