

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry:  $3.2'$

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

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

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

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

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

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

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

Table 8: Wyckoff site: **8h**, site symmetry:  $3\bar{.}$ 

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

Table 9: Wyckoff site: **12i**, site symmetry:  $\dots 2'$ 

| No. | position                 | mapping   |
|-----|--------------------------|-----------|
| 1   | $[x, 2x, 0]$             | $[1, 17]$ |
| 2   | $[-2x, -x, 0]$           | $[2, 18]$ |
| 3   | $[x, -x, 0]$             | $[3, 16]$ |
| 4   | $[-x, -2x, \frac{1}{2}]$ | $[4, 14]$ |
| 5   | $[2x, x, \frac{1}{2}]$   | $[5, 15]$ |
| 6   | $[-x, x, \frac{1}{2}]$   | $[6, 13]$ |
| 7   | $[-x, -2x, 0]$           | $[7, 23]$ |

*continued ...*

Table 9

| No. | position                 | mapping    |
|-----|--------------------------|------------|
| 8   | $[2x, x, 0]$             | $[8, 24]$  |
| 9   | $[-x, x, 0]$             | $[9, 22]$  |
| 10  | $[x, 2x, \frac{1}{2}]$   | $[10, 20]$ |
| 11  | $[-2x, -x, \frac{1}{2}]$ | $[11, 21]$ |
| 12  | $[x, -x, \frac{1}{2}]$   | $[12, 19]$ |

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

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

Table 11: Wyckoff site: 12k, 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   | $[x, 0, \frac{1}{2} - z]$   | $[4, 20]$  |
| 5   | $[0, x, \frac{1}{2} - z]$   | $[5, 21]$  |
| 6   | $[-x, -x, \frac{1}{2} - z]$ | $[6, 19]$  |
| 7   | $[-x, 0, -z]$               | $[7, 17]$  |
| 8   | $[0, -x, -z]$               | $[8, 18]$  |
| 9   | $[x, x, -z]$                | $[9, 16]$  |
| 10  | $[-x, 0, z + \frac{1}{2}]$  | $[10, 14]$ |
| 11  | $[0, -x, z + \frac{1}{2}]$  | $[11, 15]$ |
| 12  | $[x, x, z + \frac{1}{2}]$   | $[12, 13]$ |

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   | $[x - y, -y, \frac{1}{2} - z]$  | [4]     |
| 5   | $[y, x, \frac{1}{2} - z]$       | [5]     |
| 6   | $[-x, -x + y, \frac{1}{2} - z]$ | [6]     |
| 7   | $[-x, -y, -z]$                  | [7]     |
| 8   | $[y, -x + y, -z]$               | [8]     |
| 9   | $[x - y, x, -z]$                | [9]     |
| 10  | $[-x + y, y, z + \frac{1}{2}]$  | [10]    |
| 11  | $[-y, -x, z + \frac{1}{2}]$     | [11]    |
| 12  | $[x, x - y, z + \frac{1}{2}]$   | [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  | $[x, x - y, -z]$                | [16]    |
| 17  | $[-x + y, y, -z]$               | [17]    |
| 18  | $[-y, -x, -z]$                  | [18]    |
| 19  | $[-x + y, -x, \frac{1}{2} - z]$ | [19]    |
| 20  | $[x, y, \frac{1}{2} - z]$       | [20]    |
| 21  | $[-y, x - y, \frac{1}{2} - z]$  | [21]    |
| 22  | $[-x, -x + y, z]$               | [22]    |
| 23  | $[x - y, -y, z]$                | [23]    |
| 24  | $[y, x, z]$                     | [24]    |