

SG No. 175  $C_{6h}^1$   $P6/m$  [ hexagonal ]

\* plus set: + [0, 0, 0]

Table 1: Wyckoff site: 1a, site symmetry: 6/m..

| No. | position  | mapping                      |
|-----|-----------|------------------------------|
| 1   | [0, 0, 0] | [1,2,3,4,5,6,7,8,9,10,11,12] |

Table 2: Wyckoff site: 1b, site symmetry: 6/m..

| No. | position               | mapping                      |
|-----|------------------------|------------------------------|
| 1   | [0, 0, $\frac{1}{2}$ ] | [1,2,3,4,5,6,7,8,9,10,11,12] |

Table 3: Wyckoff site: 2c, site symmetry: -6..

| No. | position                             | mapping          |
|-----|--------------------------------------|------------------|
| 1   | [ $\frac{1}{3}$ , $\frac{2}{3}$ , 0] | [1,2,3,10,11,12] |
| 2   | [ $\frac{2}{3}$ , $\frac{1}{3}$ , 0] | [4,5,6,7,8,9]    |

Table 4: Wyckoff site: 2d, site symmetry: -6..

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

Table 5: Wyckoff site: 2e, site symmetry: 6..

| No. | position      | mapping          |
|-----|---------------|------------------|
| 1   | [0, 0, $z$ ]  | [1,2,3,4,5,6]    |
| 2   | [0, 0, $-z$ ] | [7,8,9,10,11,12] |

Table 6: Wyckoff site: 3f, site symmetry: 2/m..

| No. | position                | mapping    |
|-----|-------------------------|------------|
| 1   | [ $\frac{1}{2}$ , 0, 0] | [1,4,7,10] |
| 2   | [0, $\frac{1}{2}$ , 0]  | [2,5,8,11] |

|   |                                 |            |
|---|---------------------------------|------------|
| 3 | $[\frac{1}{2}, \frac{1}{2}, 0]$ | [3,6,9,12] |
|---|---------------------------------|------------|

Table 7: Wyckoff site: 3g, site symmetry: 2/m..

| No. | position                                  | mapping    |
|-----|---|------------|
| 1   | $[\frac{1}{2}, 0, \frac{1}{2}]$           | [1,4,7,10] |
| 2   | $[0, \frac{1}{2}, \frac{1}{2}]$           | [2,5,8,11] |
| 3   | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [3,6,9,12] |

Table 8: Wyckoff site: 4h, 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   | $[\frac{2}{3}, \frac{1}{3}, -z]$ | [7,8,9]    |
| 4   | $[\frac{1}{3}, \frac{2}{3}, -z]$ | [10,11,12] |

Table 9: Wyckoff site: 6i, site symmetry: 2..

| No. | position                         | mapping |
|-----|----------------------------------|---------|
| 1   | $[\frac{1}{2}, 0, z]$            | [1,4]   |
| 2   | $[0, \frac{1}{2}, z]$            | [2,5]   |
| 3   | $[\frac{1}{2}, \frac{1}{2}, z]$  | [3,6]   |
| 4   | $[\frac{1}{2}, 0, -z]$           | [7,10]  |
| 5   | $[0, \frac{1}{2}, -z]$           | [8,11]  |
| 6   | $[\frac{1}{2}, \frac{1}{2}, -z]$ | [9,12]  |

Table 10: Wyckoff site: 6j, site symmetry: m..

| No. | position          | mapping |
|-----|-------------------|---------|
| 1   | $[x, y, 0]$       | [1,10]  |
| 2   | $[-y, x - y, 0]$  | [2,11]  |
| 3   | $[-x + y, -x, 0]$ | [3,12]  |
| 4   | $[-x, -y, 0]$     | [4,7]   |
| 5   | $[y, -x + y, 0]$  | [5,8]   |
| 6   | $[x - y, x, 0]$   | [6,9]   |

Table 11: Wyckoff site: **6k**, site symmetry: **m..**

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

Table 12: Wyckoff site: **12l**, site symmetry: **1**

| No. | position           | mapping |
|-----|--------------------|---------|
| 1   | $[x, y, z]$        | [1]     |
| 2   | $[-y, x - y, z]$   | [2]     |
| 3   | $[-x + y, -x, z]$  | [3]     |
| 4   | $[-x, -y, z]$      | [4]     |
| 5   | $[y, -x + y, z]$   | [5]     |
| 6   | $[x - y, x, z]$    | [6]     |
| 7   | $[-x, -y, -z]$     | [7]     |
| 8   | $[y, -x + y, -z]$  | [8]     |
| 9   | $[x - y, x, -z]$   | [9]     |
| 10  | $[x, y, -z]$       | [10]    |
| 11  | $[-y, x - y, -z]$  | [11]    |
| 12  | $[-x + y, -x, -z]$ | [12]    |