

SG No. 187 D_{3h}^1 $P\bar{6}m2$ [hexagonal]

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

Table 1: Wyckoff site: 1a, site symmetry: $-6m2$

| 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: $-6m2$

| 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: 1c, site symmetry: $-6m2$

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

Table 4: Wyckoff site: 1d, site symmetry: $-6m2$

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

Table 5: Wyckoff site: 1e, site symmetry: $-6m2$

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

Table 6: Wyckoff site: 1f, site symmetry: $-6m2$

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

Table 7: Wyckoff site: $2\mathbf{g}$, site symmetry: $3\mathbf{m}$.

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

Table 8: Wyckoff site: $2\mathbf{h}$, site symmetry: $3\mathbf{m}$.

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

Table 9: Wyckoff site: $2\mathbf{i}$, site symmetry: $3\mathbf{m}$.

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

Table 10: Wyckoff site: $3\mathbf{j}$, site symmetry: $\mathbf{mm}2$

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

Table 11: Wyckoff site: $3\mathbf{k}$, site symmetry: $\mathbf{mm}2$

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

Table 12: Wyckoff site: $6\mathbf{l}$, site symmetry: $\mathbf{m} . .$

| No. | position | mapping |
|-----|------------------|----------|
| 1 | $[x, y, 0]$ | $[1, 4]$ |
| 2 | $[-y, x - y, 0]$ | $[2, 5]$ |

continued ...

Table 12

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

Table 13: Wyckoff site: $6\bar{m}$, site symmetry: $m..$

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

Table 14: Wyckoff site: $6n$, site symmetry: $.m.$

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

Table 15: Wyckoff site: $12o$, 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 | $[-y, -x, z]$ | [7] |
| 8 | $[-x + y, y, z]$ | [8] |
| 9 | $[x, x - y, z]$ | [9] |
| 10 | $[-y, -x, -z]$ | [10] |
| 11 | $[-x + y, y, -z]$ | [11] |

continued ...

Table 15

| No. | position | mapping |
|-----|------------------|---------|
| 12 | $[x, x - y, -z]$ | [12] |