

MSG No. 176.145  $P6'_3/m$  [ Type III, hexagonal ]

Table 1: Wyckoff site: 2a, site symmetry: -6..

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 3..

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

Table 6: Wyckoff site: 4f, 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   | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [7,8,9]    |
| 4   | $[\frac{2}{3}, \frac{1}{3}, -z]$              | [10,11,12] |

Table 7: Wyckoff site: 6g, site symmetry: -1'

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

Table 8: Wyckoff site: 6h, site symmetry: m..

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

Table 9: Wyckoff site: 12i, site symmetry: 1

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

*continued ...*

Table 9

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