# MSG No. 177.151 $P6'2'2$ [ Type III, hexagonal ]

Table 1: Wyckoff site: `1a`, site symmetry: `6'2'2`

| 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: `6'2'2`

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

Table 3: Wyckoff site: `2c`, site symmetry: `3.2`

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

Table 4: Wyckoff site: `2d`, site symmetry: `3.2`

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

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

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

Table 6: Wyckoff site: `3f`, site symmetry: `2'2'2`

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

Table 7: Wyckoff site: `3g`, site symmetry: `2'2'2`

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

Table 8: Wyckoff site: `4h`, site symmetry: `3..`

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

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

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

Table 10: Wyckoff site: `6j`, site symmetry: `.2'.`

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

Table 11: Wyckoff site: `6k`, site symmetry: `.2'.`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x, 0, \frac{1}{2}\right]$ | `[1,10]` |

*continued ...*

Table 11

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

Table 12: Wyckoff site: `6l`, site symmetry: `..2`

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

Table 13: Wyckoff site: `6m`, site symmetry: `..2`

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

Table 14: Wyckoff site: `12n`, site symmetry: `1`

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

*continued ...*

Table 14

| No. | position | mapping |
|---|---|---|
| 11 | $[y,\, x,\, -z]$ | `[11]` |
| 12 | $[-x,\, -x+y,\, -z]$ | `[12]` |