# MSG No. 164.87 $P\bar{3}'m1$ [ Type III, trigonal ]

Table 1: Wyckoff site: `1a`, site symmetry: `-3'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: `-3'm.`

| 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: `3m.`

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

Table 4: Wyckoff site: `2d`, site symmetry: `3m.`

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

Table 5: Wyckoff site: `3e`, site symmetry: `.2'/m.`

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

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

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

Table 7: Wyckoff site: `6g`, site symmetry: `.2'.`

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

Table 8: Wyckoff site: `6h`, site symmetry: `.2'.`

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

Table 9: Wyckoff site: `6i`, site symmetry: `.m.`

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

Table 10: Wyckoff site: `12j`, site symmetry: `1`

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

*continued ...*

Table 10

| No. | position | mapping |
|---|---|---|
| 10 | $[-x, -y, -z]$ | `[10]` |
| 11 | $[y, -x+y, -z]$ | `[11]` |
| 12 | $[x-y, x, -z]$ | `[12]` |