# MSG No. 194.267 $P6'_3/mmc'$ [ Type III, hexagonal ]

Table 1: Wyckoff site: `2a`, site symmetry: `-3'm.`

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ 0,\ 0]$ | `[1,2,3,10,11,12,16,17,18,19,20,21]` |
| 2 | $\left[0,\ 0,\ \frac{1}{2}\right]$ | `[4,5,6,7,8,9,13,14,15,22,23,24]` |

Table 2: Wyckoff site: `2b`, site symmetry: `-6m2`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[1,2,3,4,5,6,7,8,9,10,11,12]` |
| 2 | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[13,14,15,16,17,18,19,20,21,22,23,24]` |

Table 3: Wyckoff site: `2c`, site symmetry: `-6m2`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{4}\right]$ | `[1,2,3,4,5,6,7,8,9,10,11,12]` |
| 2 | $\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$ | `[13,14,15,16,17,18,19,20,21,22,23,24]` |

Table 4: Wyckoff site: `2d`, site symmetry: `-6m2`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{3},\ \frac{2}{3},\ \frac{3}{4}\right]$ | `[1,2,3,4,5,6,7,8,9,10,11,12]` |
| 2 | $\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{4}\right]$ | `[13,14,15,16,17,18,19,20,21,22,23,24]` |

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

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ 0,\ z]$ | `[1,2,3,10,11,12]` |
| 2 | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | `[4,5,6,7,8,9]` |
| 3 | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | `[13,14,15,22,23,24]` |
| 4 | $[0,\ 0,\ -z]$ | `[16,17,18,19,20,21]` |

Table 6: Wyckoff site: `4f`, site symmetry: `3m.`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{3},\ \frac{2}{3},\ z\right]$ | `[1,2,3,10,11,12]` |
| 2 | $\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}-z\right]$ | `[4,5,6,7,8,9]` |
| 3 | $\left[\frac{2}{3},\ \frac{1}{3},\ z+\frac{1}{2}\right]$ | `[13,14,15,22,23,24]` |
| 4 | $\left[\frac{2}{3},\ \frac{1}{3},\ -z\right]$ | `[16,17,18,19,20,21]` |

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

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{2},\ 0,\ 0\right]$ | `[1,10,16,19]` |
| 2 | $\left[0,\ \frac{1}{2},\ 0\right]$ | `[2,11,17,20]` |
| 3 | $\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$ | `[3,12,18,21]` |
| 4 | $\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[4,7,13,22]` |
| 5 | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$ | `[5,8,14,23]` |
| 6 | $\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[6,9,15,24]` |

Table 8: Wyckoff site: `6h`, site symmetry: `mm2`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ 2x,\ \frac{1}{4}\right]$ | `[1,5,8,10]` |
| 2 | $\left[-2x,\ -x,\ \frac{1}{4}\right]$ | `[2,6,9,11]` |
| 3 | $\left[x,\ -x,\ \frac{1}{4}\right]$ | `[3,4,7,12]` |
| 4 | $\left[-x,\ x,\ \frac{3}{4}\right]$ | `[13,18,21,22]` |
| 5 | $\left[-x,\ -2x,\ \frac{3}{4}\right]$ | `[14,16,19,23]` |
| 6 | $\left[2x,\ x,\ \frac{3}{4}\right]$ | `[15,17,20,24]` |

Table 9: Wyckoff site: `12i`, site symmetry: `.2'.`

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ 0,\ 0]$ | `[1,16]` |
| 2 | $[0,\ x,\ 0]$ | `[2,17]` |
| 3 | $[-x,\ -x,\ 0]$ | `[3,18]` |
| 4 | $\left[x,\ x,\ \frac{1}{2}\right]$ | `[4,13]` |
| 5 | $\left[-x,\ 0,\ \frac{1}{2}\right]$ | `[5,14]` |
| 6 | $\left[0,\ -x,\ \frac{1}{2}\right]$ | `[6,15]` |
| 7 | $\left[-x,\ -x,\ \frac{1}{2}\right]$ | `[7,22]` |
| 8 | $\left[x,\ 0,\ \frac{1}{2}\right]$ | `[8,23]` |
| 9 | $\left[0,\ x,\ \frac{1}{2}\right]$ | `[9,24]` |
| 10 | $[-x,\ 0,\ 0]$ | `[10,19]` |
| 11 | $[0,\ -x,\ 0]$ | `[11,20]` |

*continued ...*

Table 9

| No. | position | mapping |
|---|---|---|
| 12 | $[x,\, x,\, 0]$ | `[12,21]` |

Table 10: Wyckoff site: `12j`, site symmetry: `m..`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\, y,\, \frac{1}{4}\right]$ | `[1,8]` |
| 2 | $\left[-y,\, x-y,\, \frac{1}{4}\right]$ | `[2,9]` |
| 3 | $\left[-x+y,\, -x,\, \frac{1}{4}\right]$ | `[3,7]` |
| 4 | $\left[x,\, x-y,\, \frac{1}{4}\right]$ | `[4,12]` |
| 5 | $\left[-x+y,\, y,\, \frac{1}{4}\right]$ | `[5,10]` |
| 6 | $\left[-y,\, -x,\, \frac{1}{4}\right]$ | `[6,11]` |
| 7 | $\left[x-y,\, x,\, \frac{3}{4}\right]$ | `[13,21]` |
| 8 | $\left[-x,\, -y,\, \frac{3}{4}\right]$ | `[14,19]` |
| 9 | $\left[y,\, -x+y,\, \frac{3}{4}\right]$ | `[15,20]` |
| 10 | $\left[x-y,\, -y,\, \frac{3}{4}\right]$ | `[16,23]` |
| 11 | $\left[y,\, x,\, \frac{3}{4}\right]$ | `[17,24]` |
| 12 | $\left[-x,\, -x+y,\, \frac{3}{4}\right]$ | `[18,22]` |

Table 11: Wyckoff site: `12k`, site symmetry: `.m.`

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\, 2x,\, z]$ | `[1,10]` |
| 2 | $[-2x,\, -x,\, z]$ | `[2,11]` |
| 3 | $[x,\, -x,\, z]$ | `[3,12]` |
| 4 | $\left[x,\, -x,\, \frac{1}{2}-z\right]$ | `[4,7]` |
| 5 | $\left[x,\, 2x,\, \frac{1}{2}-z\right]$ | `[5,8]` |
| 6 | $\left[-2x,\, -x,\, \frac{1}{2}-z\right]$ | `[6,9]` |
| 7 | $\left[-x,\, x,\, z+\frac{1}{2}\right]$ | `[13,22]` |
| 8 | $\left[-x,\, -2x,\, z+\frac{1}{2}\right]$ | `[14,23]` |
| 9 | $\left[2x,\, x,\, z+\frac{1}{2}\right]$ | `[15,24]` |
| 10 | $[-x,\, -2x,\, -z]$ | `[16,19]` |
| 11 | $[2x,\, x,\, -z]$ | `[17,20]` |
| 12 | $[-x,\, x,\, -z]$ | `[18,21]` |

Table 12: Wyckoff site: `24l`, site symmetry: `1`

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\, y,\, z]$ | `[1]` |
| 2 | $[-y,\, x-y,\, z]$ | `[2]` |

*continued ...*

Table 12

| No. | position | mapping |
|---|---|---|
| 3 | $[-x+y,\ -x,\ z]$ | [3] |
| 4 | $\left[x,\ x-y,\ \frac{1}{2}-z\right]$ | [4] |
| 5 | $\left[-x+y,\ y,\ \frac{1}{2}-z\right]$ | [5] |
| 6 | $\left[-y,\ -x,\ \frac{1}{2}-z\right]$ | [6] |
| 7 | $\left[-x+y,\ -x,\ \frac{1}{2}-z\right]$ | [7] |
| 8 | $\left[x,\ y,\ \frac{1}{2}-z\right]$ | [8] |
| 9 | $\left[-y,\ x-y,\ \frac{1}{2}-z\right]$ | [9] |
| 10 | $[-x+y,\ y,\ z]$ | [10] |
| 11 | $[-y,\ -x,\ z]$ | [11] |
| 12 | $[x,\ x-y,\ z]$ | [12] |
| 13 | $\left[x-y,\ x,\ z+\frac{1}{2}\right]$ | [13] |
| 14 | $\left[-x,\ -y,\ z+\frac{1}{2}\right]$ | [14] |
| 15 | $\left[y,\ -x+y,\ z+\frac{1}{2}\right]$ | [15] |
| 16 | $[x-y,\ -y,\ -z]$ | [16] |
| 17 | $[y,\ x,\ -z]$ | [17] |
| 18 | $[-x,\ -x+y,\ -z]$ | [18] |
| 19 | $[-x,\ -y,\ -z]$ | [19] |
| 20 | $[y,\ -x+y,\ -z]$ | [20] |
| 21 | $[x-y,\ x,\ -z]$ | [21] |
| 22 | $\left[-x,\ -x+y,\ z+\frac{1}{2}\right]$ | [22] |
| 23 | $\left[x-y,\ -y,\ z+\frac{1}{2}\right]$ | [23] |
| 24 | $\left[y,\ x,\ z+\frac{1}{2}\right]$ | [24] |