

MSG No. 189.223 $P\bar{6}'2'm$ [Type III, hexagonal]

Table 1: Wyckoff site: 1a, site symmetry: $-6'2'm$

| 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: $-6'2'm$

| 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: 2c, site symmetry: $-6'..$

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

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

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

Table 5: Wyckoff site: 2e, site symmetry: $3.m$

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

Table 6: Wyckoff site: 3f, site symmetry: $m'2'm$

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

Table 7: Wyckoff site: $3g$, site symmetry: $m'2'm$

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

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

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

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

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

Table 10: Wyckoff site: $6j$, site symmetry: $m'..$

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

Table 11: Wyckoff site: $6k$, site symmetry: $m'..$

| No. | position | mapping |
|-----|-----------------------|-----------|
| 1 | $[x, y, \frac{1}{2}]$ | $[1, 11]$ |

continued ...

Table 11

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

Table 12: Wyckoff site: 121, 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 | $[x - y, -y, -z]$ | [7] |
| 8 | $[y, x, -z]$ | [8] |
| 9 | $[-x, -x + y, -z]$ | [9] |
| 10 | $[-x + y, -x, -z]$ | [10] |
| 11 | $[x, y, -z]$ | [11] |
| 12 | $[-y, x - y, -z]$ | [12] |