

MSG No. 181.175 $P6'_42'2$ [Type III, hexagonal]

Table 1: Wyckoff site: 3a, site symmetry: 2'2'2

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

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

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

Table 3: Wyckoff site: 3c, site symmetry: 2'2'2

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

Table 4: Wyckoff site: 3d, site symmetry: 2'2'2

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

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

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

Table 6: Wyckoff site: 6f, site symmetry: 2' .

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

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

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

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

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

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

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

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

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

Table 11: Wyckoff site: 12k, site symmetry: 1

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