

MSG No. 165.95 $P\bar{3}c'1$ [Type III, trigonal]

Table 1: Wyckoff site: 2a, site symmetry: $32'$.

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

Table 2: Wyckoff site: 2b, site symmetry: $-3..$

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

Table 3: Wyckoff site: 4c, site symmetry: $3..$

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

Table 4: Wyckoff site: 4d, 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 | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$ | [7, 8, 9] |
| 4 | $[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$ | [10, 11, 12] |

Table 5: Wyckoff site: 6e, site symmetry: -1

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

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

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

Table 7: Wyckoff site: 12g, site symmetry: 1

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