

MSG No. 163.83 $P\bar{3}1c'$ [Type III, trigonal]

Table 1: Wyckoff site: 2a, site symmetry: $3.2'$

| 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: 2c, site symmetry: $3.2'$

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

Table 4: Wyckoff site: 2d, site symmetry: $3.2'$

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

Table 5: Wyckoff site: 4e, 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 6: Wyckoff site: 4f, 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 | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$ | [7, 8, 9] |
| 4 | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [10, 11, 12] |

Table 7: Wyckoff site: 6g, 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 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [7, 10] |
| 5 | $[\frac{1}{2}, 0, \frac{1}{2}]$ | [8, 11] |
| 6 | $[0, \frac{1}{2}, \frac{1}{2}]$ | [9, 12] |

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

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

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

continued ...

Table 9

| No. | position | mapping |
|-----|---------------------------|---------|
| 12 | $[y, x, z + \frac{1}{2}]$ | [12] |