

MSG No. 165.92 $P\bar{3}c11'$ [Type II, trigonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: -3..1'

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

Table 3: Wyckoff site: 4c, site symmetry: 3..1'

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

Table 4: Wyckoff site: 4d, site symmetry: 3..1'

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

Table 5: Wyckoff site: 6e, site symmetry: -11'

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

Table 6: Wyckoff site: 6f, site symmetry: .2.1'

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

Table 7: Wyckoff site: 12g, site symmetry: 11'

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