

SG No. 159 C_{3v}^4 $P31c$ [trigonal]

* plus set: $+ [0, 0, 0]$

Table 1: Wyckoff site: 2a, site symmetry: $3..$

| No. | position | mapping |
|-----|---------------------------|-------------|
| 1 | $[0, 0, z]$ | $[1, 2, 3]$ |
| 2 | $[0, 0, z + \frac{1}{2}]$ | $[4, 5, 6]$ |

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

| No. | position | mapping |
|-----|---|-------------|
| 1 | $[\frac{1}{3}, \frac{2}{3}, z]$ | $[1, 2, 3]$ |
| 2 | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | $[4, 5, 6]$ |

Table 3: Wyckoff site: 6c, site symmetry: 1

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