

SG No. 186  $C_{6v}^4$   $P6_3mc$  [ hexagonal ]

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

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

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

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

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

Table 3: Wyckoff site: 6c, site symmetry: .m.

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

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