

SG No. 173  $C_6^6 P6_3$  [ hexagonal ]

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

\* Wyckoff site: 2a, site symmetry: 3 . .

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 6b@2a

| No. | vector          | center                     | mapping |
|-----|-----------------|----------------------------|---------|
| 1   | [X, Y, Z]       | [0, 0, z]                  | [1]     |
| 2   | [-Y, X - Y, Z]  | [0, 0, z]                  | [2]     |
| 3   | [-X + Y, -X, Z] | [0, 0, z]                  | [3]     |
| 4   | [-X, -Y, Z]     | [0, 0, $z + \frac{1}{2}$ ] | [4]     |
| 5   | [Y, -X + Y, Z]  | [0, 0, $z + \frac{1}{2}$ ] | [5]     |
| 6   | [X - Y, X, Z]   | [0, 0, $z + \frac{1}{2}$ ] | [6]     |

\* Wyckoff site: 2b, site symmetry: 3 . .

Table 3: Wyckoff bond: 2a@2b

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

Table 4: Wyckoff bond: 6b@2b

| No. | vector          | center  | mapping |
|-----|-----------------|---|---------|
| 1   | [X, Y, Z]       | $[\frac{1}{3}, \frac{2}{3}, z]$               | [1]     |
| 2   | [-Y, X - Y, Z]  | $[\frac{1}{3}, \frac{2}{3}, z]$               | [2]     |
| 3   | [-X + Y, -X, Z] | $[\frac{1}{3}, \frac{2}{3}, z]$               | [3]     |
| 4   | [-X, -Y, Z]     | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [4]     |
| 5   | [Y, -X + Y, Z]  | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [5]     |
| 6   | [X - Y, X, Z]   | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$ | [6]     |

\* Wyckoff site: 6c, site symmetry: 1

Table 5: Wyckoff bond: **6a@6c**

| No. | vector            | center                         | mapping |
|-----|-------------------|--------------------------------|---------|
| 1   | $[X, Y, Z]$       | $[x, y, z]$                    | [1]     |
| 2   | $[-Y, X - Y, Z]$  | $[-y, x - y, z]$               | [2]     |
| 3   | $[-X + Y, -X, Z]$ | $[-x + y, -x, z]$              | [3]     |
| 4   | $[-X, -Y, Z]$     | $[-x, -y, z + \frac{1}{2}]$    | [4]     |
| 5   | $[Y, -X + Y, Z]$  | $[y, -x + y, z + \frac{1}{2}]$ | [5]     |
| 6   | $[X - Y, X, Z]$   | $[x - y, x, z + \frac{1}{2}]$  | [6]     |