

SG No. 154 D_3^6 $P3_221$ [trigonal]

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

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

Table 1: Wyckoff bond: 3a@3a

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

Table 2: Wyckoff bond: 3b@3a

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

Table 3: Wyckoff bond: 6c@3a

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

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

Table 4: Wyckoff bond: 3a@3b

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

Table 5: Wyckoff bond: **3b@3b**

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

Table 6: Wyckoff bond: **6c@3b**

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

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

Table 7: Wyckoff bond: **6a@6c**

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