

SG No. 153 D_3^5 $P3_212$ [trigonal]

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

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

Table 1: Wyckoff bond: 3a@3a

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

Table 2: Wyckoff bond: 3b@3a

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

Table 3: Wyckoff bond: 6c@3a

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

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

Table 4: Wyckoff bond: 3a@3b

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

Table 5: Wyckoff bond: 3b@3b

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

Table 6: Wyckoff bond: 6c@3b

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