

PG No. 34 $D_3(1)$ 32 (312 setting) [trigonal]

* 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 | $[0, 0, -Z]$ | $[0, 0, -z]$ | $[4, 5, 6]$ |

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 | $[-Y, -X, -Z]$ | $[0, 0, -z]$ | $[4]$ |
| 5 | $[-X + Y, Y, -Z]$ | $[0, 0, -z]$ | $[5]$ |
| 6 | $[X, X - Y, -Z]$ | $[0, 0, -z]$ | $[6]$ |

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

Table 3: Wyckoff bond: 3a@3b

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

Table 4: Wyckoff bond: 3b@3b

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

Table 5: Wyckoff bond: 6c@3b

| No. | vector | center | mapping |
|-----|------------------|--------------|---------|
| 1 | $[X, Y, Z]$ | $[x, -x, 0]$ | $[1]$ |
| 2 | $[-Y, X - Y, Z]$ | $[x, 2x, 0]$ | $[2]$ |

continued ...

Table 5

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

* Wyckoff site: 6c, site symmetry: 1

Table 6: 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 | $[-Y, -X, -Z]$ | $[-y, -x, -z]$ | [4] |
| 5 | $[-X + Y, Y, -Z]$ | $[-x + y, y, -z]$ | [5] |
| 6 | $[X, X - Y, -Z]$ | $[x, x - y, -z]$ | [6] |