

PG No. 35  $C_{3v}(1)$   $3m$  (31m setting) [ trigonal ]

\* Wyckoff site: 1a, site symmetry: 3.m

Table 1: Wyckoff bond: 1a@1a

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

Table 2: Wyckoff bond: 3b@1a

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

Table 3: Wyckoff bond: 3c@1a

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

Table 4: Wyckoff bond: 6d@1a

| 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: .m

Table 5: Wyckoff bond: 3a@3b

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

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

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

Table 7: Wyckoff bond: **6c@3b**

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

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

Table 8: 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   | $[-X, -X + Y, Z]$ | $[-x, -x + y, z]$ | $[6]$   |