

SG No. 150 D_3^2 $P321$ [trigonal]

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

* Wyckoff site: **1a**, site symmetry: **32**.

Table 1: Wyckoff bond: **1a@1a**

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

Table 2: Wyckoff bond: **3b@1a**

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

Table 3: Wyckoff bond: **3c@1a**

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

Table 4: Wyckoff bond: **6d@1a**

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

* Wyckoff site: **1b**, site symmetry: **32**.

Table 5: Wyckoff bond: **1a@1b**

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

Table 6: Wyckoff bond: **3b@1b**

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

Table 7: Wyckoff bond: **3c@1b**

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

Table 8: Wyckoff bond: **6d@1b**

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

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

Table 9: Wyckoff bond: **2a@2c**

| 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 10: Wyckoff bond: **6b@2c**

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

continued ...

Table 10

| No. | vector | center | mapping |
|-----|--------------------|--------------|---------|
| 6 | $[-X, -X + Y, -Z]$ | $[0, 0, -z]$ | [6] |

* Wyckoff site: 2d, site symmetry: $3.$

Table 11: Wyckoff bond: 2a@2d

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

Table 12: Wyckoff bond: 6b@2d

| 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 | $[Y, X, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, -z]$ | [4] |
| 5 | $[X - Y, -Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, -z]$ | [5] |
| 6 | $[-X, -X + Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, -z]$ | [6] |

* Wyckoff site: 3e, site symmetry: $.2.$

Table 13: Wyckoff bond: 3a@3e

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

Table 14: Wyckoff bond: 3b@3e

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

Table 15: Wyckoff bond: **6c@3e**

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

* Wyckoff site: **3f**, site symmetry: $.2$.

Table 16: Wyckoff bond: **3a@3f**

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

Table 17: Wyckoff bond: **3b@3f**

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

Table 18: Wyckoff bond: **6c@3f**

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

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

Table 19: Wyckoff bond: **6a@6g**

| 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] |