

PG No. 6 D_2 222 [orthorhombic]

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

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 2b@2a

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

Table 3: Wyckoff bond: 4c@2a

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

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

Table 4: Wyckoff bond: 2a@2b

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

Table 5: Wyckoff bond: 2b@2b

| No. | vector | center | mapping |
|-----|--------------|--------------|----------|
| 1 | $[0, Y, 0]$ | $[0, y, 0]$ | $[1, 3]$ |
| 2 | $[0, -Y, 0]$ | $[0, -y, 0]$ | $[2, 4]$ |

Table 6: Wyckoff bond: **4c@2b**

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

* Wyckoff site: **2c**, site symmetry: $\dots 2$

Table 7: Wyckoff bond: **2a@2c**

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

Table 8: Wyckoff bond: **2b@2c**

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

Table 9: Wyckoff bond: **4c@2c**

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

* Wyckoff site: **4d**, site symmetry: 1

Table 10: Wyckoff bond: **4a@4d**

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