

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: . . 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] |