

SG No. 175 C_{6h}^1 $P6/m$ [hexagonal]

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

* Wyckoff site: **1a**, site symmetry: 6/m..

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

| No. | vector | center | mapping |
|-----|-------------|-------------|---|
| 1 | $[0, 0, Z]$ | $[0, 0, 0]$ | $[1, 2, 3, 4, 5, 6, -7, -8, -9, -10, -11, -12]$ |

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

| No. | vector | center | mapping |
|-----|-------------------|-------------|-------------------|
| 1 | $[X, Y, 0]$ | $[0, 0, 0]$ | $[1, -4, -7, 10]$ |
| 2 | $[-Y, X - Y, 0]$ | $[0, 0, 0]$ | $[2, -5, -8, 11]$ |
| 3 | $[-X + Y, -X, 0]$ | $[0, 0, 0]$ | $[3, -6, -9, 12]$ |

Table 3: Wyckoff bond: **6c@1a**

| No. | vector | center | mapping |
|-----|-------------------|-------------|------------|
| 1 | $[X, Y, Z]$ | $[0, 0, 0]$ | $[1, -7]$ |
| 2 | $[-Y, X - Y, Z]$ | $[0, 0, 0]$ | $[2, -8]$ |
| 3 | $[-X + Y, -X, Z]$ | $[0, 0, 0]$ | $[3, -9]$ |
| 4 | $[-X, -Y, Z]$ | $[0, 0, 0]$ | $[4, -10]$ |
| 5 | $[Y, -X + Y, Z]$ | $[0, 0, 0]$ | $[5, -11]$ |
| 6 | $[X - Y, X, Z]$ | $[0, 0, 0]$ | $[6, -12]$ |

* Wyckoff site: **1b**, site symmetry: 6/m..

Table 4: Wyckoff bond: **1a@1b**

| No. | vector | center | mapping |
|-----|-------------|-----------------------|---|
| 1 | $[0, 0, Z]$ | $[0, 0, \frac{1}{2}]$ | $[1, 2, 3, 4, 5, 6, -7, -8, -9, -10, -11, -12]$ |

Table 5: Wyckoff bond: **3b@1b**

| No. | vector | center | mapping |
|-----|-------------------|-----------------------|-------------------|
| 1 | $[X, Y, 0]$ | $[0, 0, \frac{1}{2}]$ | $[1, -4, -7, 10]$ |
| 2 | $[-Y, X - Y, 0]$ | $[0, 0, \frac{1}{2}]$ | $[2, -5, -8, 11]$ |
| 3 | $[-X + Y, -X, 0]$ | $[0, 0, \frac{1}{2}]$ | $[3, -6, -9, 12]$ |

Table 6: Wyckoff bond: 6c@1b

| No. | vector | center | mapping |
|-----|-------------------|-----------------------|----------|
| 1 | $[X, Y, Z]$ | $[0, 0, \frac{1}{2}]$ | [1, -7] |
| 2 | $[-Y, X - Y, Z]$ | $[0, 0, \frac{1}{2}]$ | [2, -8] |
| 3 | $[-X + Y, -X, Z]$ | $[0, 0, \frac{1}{2}]$ | [3, -9] |
| 4 | $[-X, -Y, Z]$ | $[0, 0, \frac{1}{2}]$ | [4, -10] |
| 5 | $[Y, -X + Y, Z]$ | $[0, 0, \frac{1}{2}]$ | [5, -11] |
| 6 | $[X - Y, X, Z]$ | $[0, 0, \frac{1}{2}]$ | [6, -12] |

* Wyckoff site: 2c, site symmetry: -6..

Table 7: Wyckoff bond: 2a@2c

| No. | vector | center | mapping |
|-----|-------------|---------------------------------|--------------------------|
| 1 | $[0, 0, Z]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [1, 2, 3, -10, -11, -12] |
| 2 | $[0, 0, Z]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [4, 5, 6, -7, -8, -9] |

Table 8: Wyckoff bond: 6b@2c

| No. | vector | center | mapping |
|-----|-------------------|---------------------------------|---------|
| 1 | $[X, Y, 0]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [1, 10] |
| 2 | $[-Y, X - Y, 0]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [2, 11] |
| 3 | $[-X + Y, -X, 0]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [3, 12] |
| 4 | $[-X, -Y, 0]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [4, 7] |
| 5 | $[Y, -X + Y, 0]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [5, 8] |
| 6 | $[X - Y, X, 0]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [6, 9] |

Table 9: Wyckoff bond: 12c@2c

| No. | vector | center | mapping |
|-----|-------------------|---------------------------------|---------|
| 1 | $[X, Y, Z]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [1] |
| 2 | $[-Y, X - Y, Z]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [2] |
| 3 | $[-X + Y, -X, Z]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [3] |
| 4 | $[-X, -Y, Z]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [4] |
| 5 | $[Y, -X + Y, Z]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [5] |
| 6 | $[X - Y, X, Z]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [6] |
| 7 | $[-X, -Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [7] |
| 8 | $[Y, -X + Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [8] |
| 9 | $[X - Y, X, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, 0]$ | [9] |
| 10 | $[X, Y, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [10] |
| 11 | $[-Y, X - Y, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [11] |

continued ...

Table 9

| No. | vector | center | mapping |
|-----|--------------------|---------------------------------|---------|
| 12 | $[-X + Y, -X, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, 0]$ | [12] |

* Wyckoff site: 2d, site symmetry: -6..

Table 10: Wyckoff bond: 2a@2d

| No. | vector | center | mapping |
|-----|-------------|---|---------------------|
| 1 | $[0, 0, Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [1,2,3,-10,-11,-12] |
| 2 | $[0, 0, Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [4,5,6,-7,-8,-9] |

Table 11: Wyckoff bond: 6b@2d

| No. | vector | center | mapping |
|-----|-------------------|---|---------|
| 1 | $[X, Y, 0]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [1,10] |
| 2 | $[-Y, X - Y, 0]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [2,11] |
| 3 | $[-X + Y, -X, 0]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [3,12] |
| 4 | $[-X, -Y, 0]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [4,7] |
| 5 | $[Y, -X + Y, 0]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [5,8] |
| 6 | $[X - Y, X, 0]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [6,9] |

Table 12: Wyckoff bond: 12c@2d

| No. | vector | center | mapping |
|-----|--------------------|---|---------|
| 1 | $[X, Y, Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [1] |
| 2 | $[-Y, X - Y, Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [2] |
| 3 | $[-X + Y, -X, Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [3] |
| 4 | $[-X, -Y, Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [4] |
| 5 | $[Y, -X + Y, Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [5] |
| 6 | $[X - Y, X, Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [6] |
| 7 | $[-X, -Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [7] |
| 8 | $[Y, -X + Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [8] |
| 9 | $[X - Y, X, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ | [9] |
| 10 | $[X, Y, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [10] |
| 11 | $[-Y, X - Y, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [11] |
| 12 | $[-X + Y, -X, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ | [12] |

* Wyckoff site: 2e, site symmetry: 6..

Table 13: Wyckoff bond: 2a@2e

| No. | vector | center | mapping |
|-----|------------|------------|------------------|
| 1 | [0, 0, Z] | [0, 0, z] | [1,2,3,4,5,6] |
| 2 | [0, 0, -Z] | [0, 0, -z] | [7,8,9,10,11,12] |

Table 14: Wyckoff bond: 6b@2e

| No. | vector | center | mapping |
|-----|-----------------|------------|---------|
| 1 | [X, Y, 0] | [0, 0, z] | [1,-4] |
| 2 | [-Y, X - Y, 0] | [0, 0, z] | [2,-5] |
| 3 | [-X + Y, -X, 0] | [0, 0, z] | [3,-6] |
| 4 | [-X, -Y, 0] | [0, 0, -z] | [7,-10] |
| 5 | [Y, -X + Y, 0] | [0, 0, -z] | [8,-11] |
| 6 | [X - Y, X, 0] | [0, 0, -z] | [9,-12] |

Table 15: Wyckoff bond: 12c@2e

| 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 | [-X, -Y, Z] | [0, 0, z] | [4] |
| 5 | [Y, -X + Y, Z] | [0, 0, z] | [5] |
| 6 | [X - Y, X, Z] | [0, 0, z] | [6] |
| 7 | [-X, -Y, -Z] | [0, 0, -z] | [7] |
| 8 | [Y, -X + Y, -Z] | [0, 0, -z] | [8] |
| 9 | [X - Y, X, -Z] | [0, 0, -z] | [9] |
| 10 | [X, Y, -Z] | [0, 0, -z] | [10] |
| 11 | [-Y, X - Y, -Z] | [0, 0, -z] | [11] |
| 12 | [-X + Y, -X, -Z] | [0, 0, -z] | [12] |

* Wyckoff site: 3f, site symmetry: 2/m..

Table 16: Wyckoff bond: 3a@3f

| No. | vector | center | mapping |
|-----|-----------------|-------------------------------|--------------|
| 1 | [X, Y, 0] | [\frac{1}{2}, 0, 0] | [1,-4,-7,10] |
| 2 | [-Y, X - Y, 0] | [0, \frac{1}{2}, 0] | [2,-5,-8,11] |
| 3 | [-X + Y, -X, 0] | [\frac{1}{2}, \frac{1}{2}, 0] | [3,-6,-9,12] |

Table 17: Wyckoff bond: 3b@3f

| No. | vector | center | mapping |
|-----|-----------|---------------------------------|--------------|
| 1 | [0, 0, Z] | $[\frac{1}{2}, 0, 0]$ | [1,4,-7,-10] |
| 2 | [0, 0, Z] | $[0, \frac{1}{2}, 0]$ | [2,5,-8,-11] |
| 3 | [0, 0, Z] | $[\frac{1}{2}, \frac{1}{2}, 0]$ | [3,6,-9,-12] |

Table 18: Wyckoff bond: 6c@3f

| No. | vector | center | mapping |
|-----|-----------------|---------------------------------|---------|
| 1 | [X, Y, Z] | $[\frac{1}{2}, 0, 0]$ | [1,-7] |
| 2 | [-Y, X - Y, Z] | $[0, \frac{1}{2}, 0]$ | [2,-8] |
| 3 | [-X + Y, -X, Z] | $[\frac{1}{2}, \frac{1}{2}, 0]$ | [3,-9] |
| 4 | [-X, -Y, Z] | $[\frac{1}{2}, 0, 0]$ | [4,-10] |
| 5 | [Y, -X + Y, Z] | $[0, \frac{1}{2}, 0]$ | [5,-11] |
| 6 | [X - Y, X, Z] | $[\frac{1}{2}, \frac{1}{2}, 0]$ | [6,-12] |

* Wyckoff site: 3g, site symmetry: 2/m..

Table 19: Wyckoff bond: 3a@3g

| No. | vector | center | mapping |
|-----|-----------------|---|--------------|
| 1 | [X, Y, 0] | $[\frac{1}{2}, 0, \frac{1}{2}]$ | [1,-4,-7,10] |
| 2 | [-Y, X - Y, 0] | $[0, \frac{1}{2}, \frac{1}{2}]$ | [2,-5,-8,11] |
| 3 | [-X + Y, -X, 0] | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [3,-6,-9,12] |

Table 20: Wyckoff bond: 3b@3g

| No. | vector | center | mapping |
|-----|-----------|---|--------------|
| 1 | [0, 0, Z] | $[\frac{1}{2}, 0, \frac{1}{2}]$ | [1,4,-7,-10] |
| 2 | [0, 0, Z] | $[0, \frac{1}{2}, \frac{1}{2}]$ | [2,5,-8,-11] |
| 3 | [0, 0, Z] | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [3,6,-9,-12] |

Table 21: Wyckoff bond: 6c@3g

| No. | vector | center | mapping |
|-----|-----------------|---|---------|
| 1 | [X, Y, Z] | $[\frac{1}{2}, 0, \frac{1}{2}]$ | [1,-7] |
| 2 | [-Y, X - Y, Z] | $[0, \frac{1}{2}, \frac{1}{2}]$ | [2,-8] |
| 3 | [-X + Y, -X, Z] | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [3,-9] |
| 4 | [-X, -Y, Z] | $[\frac{1}{2}, 0, \frac{1}{2}]$ | [4,-10] |

continued ...

Table 21

| No. | vector | center | mapping |
|-----|------------------|---|---------|
| 5 | $[Y, -X + Y, Z]$ | $[0, \frac{1}{2}, \frac{1}{2}]$ | [5,-11] |
| 6 | $[X - Y, X, Z]$ | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [6,-12] |

* Wyckoff site: 4h, site symmetry: 3..

Table 22: Wyckoff bond: 4a@4h

| 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] |
| 3 | $[0, 0, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, -z]$ | [7,8,9] |
| 4 | $[0, 0, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, -z]$ | [10,11,12] |

Table 23: Wyckoff bond: 12b@4h

| 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 | $[-X, -Y, Z]$ | $[\frac{2}{3}, \frac{1}{3}, z]$ | [4] |
| 5 | $[Y, -X + Y, Z]$ | $[\frac{2}{3}, \frac{1}{3}, z]$ | [5] |
| 6 | $[X - Y, X, Z]$ | $[\frac{2}{3}, \frac{1}{3}, z]$ | [6] |
| 7 | $[-X, -Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, -z]$ | [7] |
| 8 | $[Y, -X + Y, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, -z]$ | [8] |
| 9 | $[X - Y, X, -Z]$ | $[\frac{2}{3}, \frac{1}{3}, -z]$ | [9] |
| 10 | $[X, Y, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, -z]$ | [10] |
| 11 | $[-Y, X - Y, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, -z]$ | [11] |
| 12 | $[-X + Y, -X, -Z]$ | $[\frac{1}{3}, \frac{2}{3}, -z]$ | [12] |

* Wyckoff site: 6i, site symmetry: 2..

Table 24: Wyckoff bond: 6a@6i

| No. | vector | center | mapping |
|-----|-------------------|----------------------------------|---------|
| 1 | $[X, Y, 0]$ | $[\frac{1}{2}, 0, z]$ | [1,-4] |
| 2 | $[-Y, X - Y, 0]$ | $[0, \frac{1}{2}, z]$ | [2,-5] |
| 3 | $[-X + Y, -X, 0]$ | $[\frac{1}{2}, \frac{1}{2}, z]$ | [3,-6] |
| 4 | $[-X, -Y, 0]$ | $[\frac{1}{2}, 0, -z]$ | [7,-10] |
| 5 | $[Y, -X + Y, 0]$ | $[0, \frac{1}{2}, -z]$ | [8,-11] |
| 6 | $[X - Y, X, 0]$ | $[\frac{1}{2}, \frac{1}{2}, -z]$ | [9,-12] |

Table 25: Wyckoff bond: 6b@6i

| No. | vector | center | mapping |
|-----|------------|--------------------------------|---------|
| 1 | [0, 0, Z] | [\frac{1}{2}, 0, z] | [1,4] |
| 2 | [0, 0, Z] | [0, \frac{1}{2}, z] | [2,5] |
| 3 | [0, 0, Z] | [\frac{1}{2}, \frac{1}{2}, z] | [3,6] |
| 4 | [0, 0, -Z] | [\frac{1}{2}, 0, -z] | [7,10] |
| 5 | [0, 0, -Z] | [0, \frac{1}{2}, -z] | [8,11] |
| 6 | [0, 0, -Z] | [\frac{1}{2}, \frac{1}{2}, -z] | [9,12] |

Table 26: Wyckoff bond: 12c@6i

| No. | vector | center | mapping |
|-----|------------------|--------------------------------|---------|
| 1 | [X, Y, Z] | [\frac{1}{2}, 0, z] | [1] |
| 2 | [-Y, X - Y, Z] | [0, \frac{1}{2}, z] | [2] |
| 3 | [-X + Y, -X, Z] | [\frac{1}{2}, \frac{1}{2}, z] | [3] |
| 4 | [-X, -Y, Z] | [\frac{1}{2}, 0, z] | [4] |
| 5 | [Y, -X + Y, Z] | [0, \frac{1}{2}, z] | [5] |
| 6 | [X - Y, X, Z] | [\frac{1}{2}, \frac{1}{2}, z] | [6] |
| 7 | [-X, -Y, -Z] | [\frac{1}{2}, 0, -z] | [7] |
| 8 | [Y, -X + Y, -Z] | [0, \frac{1}{2}, -z] | [8] |
| 9 | [X - Y, X, -Z] | [\frac{1}{2}, \frac{1}{2}, -z] | [9] |
| 10 | [X, Y, -Z] | [\frac{1}{2}, 0, -z] | [10] |
| 11 | [-Y, X - Y, -Z] | [0, \frac{1}{2}, -z] | [11] |
| 12 | [-X + Y, -X, -Z] | [\frac{1}{2}, \frac{1}{2}, -z] | [12] |

* Wyckoff site: 6j, site symmetry: m..

Table 27: Wyckoff bond: 6a@6j

| No. | vector | center | mapping |
|-----|-----------------|-----------------|---------|
| 1 | [X, Y, 0] | [x, y, 0] | [1,10] |
| 2 | [-Y, X - Y, 0] | [-y, x - y, 0] | [2,11] |
| 3 | [-X + Y, -X, 0] | [-x + y, -x, 0] | [3,12] |
| 4 | [-X, -Y, 0] | [-x, -y, 0] | [4,7] |
| 5 | [Y, -X + Y, 0] | [y, -x + y, 0] | [5,8] |
| 6 | [X - Y, X, 0] | [x - y, x, 0] | [6,9] |

Table 28: Wyckoff bond: 6b@6j

| No. | vector | center | mapping |
|-----|-----------|-----------|---------|
| 1 | [0, 0, Z] | [x, y, 0] | [1,-10] |

continued ...

Table 28

| No. | vector | center | mapping |
|-----|-----------|-----------------|----------|
| 2 | [0, 0, Z] | [-y, x - y, 0] | [2, -11] |
| 3 | [0, 0, Z] | [-x + y, -x, 0] | [3, -12] |
| 4 | [0, 0, Z] | [-x, -y, 0] | [4, -7] |
| 5 | [0, 0, Z] | [y, -x + y, 0] | [5, -8] |
| 6 | [0, 0, Z] | [x - y, x, 0] | [6, -9] |

Table 29: Wyckoff bond: 12c@6j

| No. | vector | center | mapping |
|-----|------------------|-----------------|---------|
| 1 | [X, Y, Z] | [x, y, 0] | [1] |
| 2 | [-Y, X - Y, Z] | [-y, x - y, 0] | [2] |
| 3 | [-X + Y, -X, Z] | [-x + y, -x, 0] | [3] |
| 4 | [-X, -Y, Z] | [-x, -y, 0] | [4] |
| 5 | [Y, -X + Y, Z] | [y, -x + y, 0] | [5] |
| 6 | [X - Y, X, Z] | [x - y, x, 0] | [6] |
| 7 | [-X, -Y, -Z] | [-x, -y, 0] | [7] |
| 8 | [Y, -X + Y, -Z] | [y, -x + y, 0] | [8] |
| 9 | [X - Y, X, -Z] | [x - y, x, 0] | [9] |
| 10 | [X, Y, -Z] | [x, y, 0] | [10] |
| 11 | [-Y, X - Y, -Z] | [-y, x - y, 0] | [11] |
| 12 | [-X + Y, -X, -Z] | [-x + y, -x, 0] | [12] |

* Wyckoff site: 6k, site symmetry: m..

Table 30: Wyckoff bond: 6a@6k

| No. | vector | center | mapping |
|-----|-----------------|------------------------------|---------|
| 1 | [X, Y, 0] | [x, y, $\frac{1}{2}$] | [1, 10] |
| 2 | [-Y, X - Y, 0] | [-y, x - y, $\frac{1}{2}$] | [2, 11] |
| 3 | [-X + Y, -X, 0] | [-x + y, -x, $\frac{1}{2}$] | [3, 12] |
| 4 | [-X, -Y, 0] | [-x, -y, $\frac{1}{2}$] | [4, 7] |
| 5 | [Y, -X + Y, 0] | [y, -x + y, $\frac{1}{2}$] | [5, 8] |
| 6 | [X - Y, X, 0] | [x - y, x, $\frac{1}{2}$] | [6, 9] |

Table 31: Wyckoff bond: 6b@6k

| No. | vector | center | mapping |
|-----|-----------|------------------------------|----------|
| 1 | [0, 0, Z] | [x, y, $\frac{1}{2}$] | [1, -10] |
| 2 | [0, 0, Z] | [-y, x - y, $\frac{1}{2}$] | [2, -11] |
| 3 | [0, 0, Z] | [-x + y, -x, $\frac{1}{2}$] | [3, -12] |

continued ...

Table 31

| No. | vector | center | mapping |
|-----|-------------|----------------------------|---------|
| 4 | $[0, 0, Z]$ | $[-x, -y, \frac{1}{2}]$ | [4,-7] |
| 5 | $[0, 0, Z]$ | $[y, -x + y, \frac{1}{2}]$ | [5,-8] |
| 6 | $[0, 0, Z]$ | $[x - y, x, \frac{1}{2}]$ | [6,-9] |

Table 32: Wyckoff bond: 12c@6k

| No. | vector | center | mapping |
|-----|--------------------|-----------------------------|---------|
| 1 | $[X, Y, Z]$ | $[x, y, \frac{1}{2}]$ | [1] |
| 2 | $[-Y, X - Y, Z]$ | $[-y, x - y, \frac{1}{2}]$ | [2] |
| 3 | $[-X + Y, -X, Z]$ | $[-x + y, -x, \frac{1}{2}]$ | [3] |
| 4 | $[-X, -Y, Z]$ | $[-x, -y, \frac{1}{2}]$ | [4] |
| 5 | $[Y, -X + Y, Z]$ | $[y, -x + y, \frac{1}{2}]$ | [5] |
| 6 | $[X - Y, X, Z]$ | $[x - y, x, \frac{1}{2}]$ | [6] |
| 7 | $[-X, -Y, -Z]$ | $[-x, -y, \frac{1}{2}]$ | [7] |
| 8 | $[Y, -X + Y, -Z]$ | $[y, -x + y, \frac{1}{2}]$ | [8] |
| 9 | $[X - Y, X, -Z]$ | $[x - y, x, \frac{1}{2}]$ | [9] |
| 10 | $[X, Y, -Z]$ | $[x, y, \frac{1}{2}]$ | [10] |
| 11 | $[-Y, X - Y, -Z]$ | $[-y, x - y, \frac{1}{2}]$ | [11] |
| 12 | $[-X + Y, -X, -Z]$ | $[-x + y, -x, \frac{1}{2}]$ | [12] |

* Wyckoff site: 121, site symmetry: 1

Table 33: Wyckoff bond: 12a@121

| 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 | $[-X, -Y, Z]$ | $[-x, -y, z]$ | [4] |
| 5 | $[Y, -X + Y, Z]$ | $[y, -x + y, z]$ | [5] |
| 6 | $[X - Y, X, Z]$ | $[x - y, x, z]$ | [6] |
| 7 | $[-X, -Y, -Z]$ | $[-x, -y, -z]$ | [7] |
| 8 | $[Y, -X + Y, -Z]$ | $[y, -x + y, -z]$ | [8] |
| 9 | $[X - Y, X, -Z]$ | $[x - y, x, -z]$ | [9] |
| 10 | $[X, Y, -Z]$ | $[x, y, -z]$ | [10] |
| 11 | $[-Y, X - Y, -Z]$ | $[-y, x - y, -z]$ | [11] |
| 12 | $[-X + Y, -X, -Z]$ | $[-x + y, -x, -z]$ | [12] |