# SG No. 188 $D_{3h}^2$ $P\bar{6}c2$ [ hexagonal ]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `2a`, site symmetry: `3.2`

Table 1: Wyckoff bond: `2a@2a`

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

Table 2: Wyckoff bond: `6b@2a`

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

Table 3: Wyckoff bond: `6c@2a`

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

Table 4: Wyckoff bond: `12d@2a`

| 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 | $[X, Y, -Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[4]` |
| 5 | $[-Y, X-Y, -Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[5]` |
| 6 | $[-X+Y, -X, -Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[6]` |
| 7 | $[-Y, -X, Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[7]` |
| 8 | $[-X+Y, Y, Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[8]` |
| 9 | $[X, X-Y, Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[9]` |

*continued ...*

Table 4

| No. | vector | center | mapping |
|---|---|---|---|
| 10 | $[-Y, -X, -Z]$ | $[0, 0, 0]$ | `[10]` |
| 11 | $[-X+Y, Y, -Z]$ | $[0, 0, 0]$ | `[11]` |
| 12 | $[X, X-Y, -Z]$ | $[0, 0, 0]$ | `[12]` |

* Wyckoff site: `2b`, site symmetry: `-6..`

Table 5: Wyckoff bond: `2a@2b`

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

Table 6: Wyckoff bond: `6b@2b`

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

Table 7: Wyckoff bond: `12c@2b`

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

* Wyckoff site: `2c`, site symmetry: `3.2`

Table 8: Wyckoff bond: `2a@2c`

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

Table 9: Wyckoff bond: `6b@2c`

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

Table 10: Wyckoff bond: `6c@2c`

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

Table 11: Wyckoff bond: `12d@2c`

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

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

Table 12: Wyckoff bond: 2a@2d

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

Table 13: Wyckoff bond: 6b@2d

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

Table 14: Wyckoff bond: 12c@2d

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

* Wyckoff site: 2e, site symmetry: 3.2

Table 15: Wyckoff bond: 2a@2e

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

Table 16: Wyckoff bond: `6b@2e`

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

Table 17: Wyckoff bond: `6c@2e`

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

Table 18: Wyckoff bond: `12d@2e`

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

* Wyckoff site: `2f`, site symmetry: `-6..`

Table 19: Wyckoff bond: `2a@2f`

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

*continued ...*

Table 19

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

Table 20: Wyckoff bond: `6b@2f`

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

Table 21: Wyckoff bond: `12c@2f`

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

* Wyckoff site: `4g`, site symmetry: `3..`

Table 22: Wyckoff bond: `4a@4g`

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

Table 23: Wyckoff bond: `12b@4g`

| 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 | $[X,\ Y,\ -Z]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | `[4]` |
| 5 | $[-Y,\ X-Y,\ -Z]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | `[5]` |
| 6 | $[-X+Y,\ -X,\ -Z]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | `[6]` |
| 7 | $[-Y,\ -X,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | `[7]` |
| 8 | $[-X+Y,\ Y,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | `[8]` |
| 9 | $[X,\ X-Y,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | `[9]` |
| 10 | $[-Y,\ -X,\ -Z]$ | $[0,\ 0,\ -z]$ | `[10]` |
| 11 | $[-X+Y,\ Y,\ -Z]$ | $[0,\ 0,\ -z]$ | `[11]` |
| 12 | $[X,\ X-Y,\ -Z]$ | $[0,\ 0,\ -z]$ | `[12]` |

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

Table 24: Wyckoff bond: `4a@4h`

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

Table 25: Wyckoff bond: `12b@4h`

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

* Wyckoff site: `4i`, site symmetry: `3..`

Table 26: Wyckoff bond: `4a@4i`

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

Table 27: Wyckoff bond: `12b@4i`

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

* Wyckoff site: `6j`, site symmetry: `..2`

Table 28: Wyckoff bond: `6a@6j`

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

Table 29: Wyckoff bond: `6b@6j`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ -X,\ 0]$ | $[x,\ -x,\ 0]$ | `[1,10]` |
| 2 | $[X,\ 2X,\ 0]$ | $[x,\ 2x,\ 0]$ | `[2,12]` |
| 3 | $[-2X,\ -X,\ 0]$ | $[-2x,\ -x,\ 0]$ | `[3,11]` |

*continued ...*

Table 29

| No. | vector | center | mapping |
|---|---|---|---|
| 4 | $[X, -X, 0]$ | $\left[x, -x, \frac{1}{2}\right]$ | `[4,7]` |
| 5 | $[X, 2X, 0]$ | $\left[x, 2x, \frac{1}{2}\right]$ | `[5,9]` |
| 6 | $[-2X, -X, 0]$ | $\left[-2x, -x, \frac{1}{2}\right]$ | `[6,8]` |

Table 30: Wyckoff bond: `12c@6j`

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

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

Table 31: Wyckoff bond: `6a@6k`

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

Table 32: Wyckoff bond: `6b@6k`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0, 0, Z]$ | $\left[x, y, \frac{1}{4}\right]$ | `[1,-4]` |
| 2 | $[0, 0, Z]$ | $\left[-y, x-y, \frac{1}{4}\right]$ | `[2,-5]` |
| 3 | $[0, 0, Z]$ | $\left[-x+y, -x, \frac{1}{4}\right]$ | `[3,-6]` |
| 4 | $[0, 0, Z]$ | $\left[-y, -x, \frac{3}{4}\right]$ | `[7,-10]` |
| 5 | $[0, 0, Z]$ | $\left[-x+y, y, \frac{3}{4}\right]$ | `[8,-11]` |

*continued ...*

Table 32

| No. | vector | center | mapping |
|---|---|---|---|
| 6 | $[0,\ 0,\ Z]$ | $\left[x,\ x-y,\ \frac{3}{4}\right]$ | `[9,-12]` |

Table 33: Wyckoff bond: `12c@6k`

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

* Wyckoff site: `12l`, site symmetry: `1`

Table 34: Wyckoff bond: `12a@12l`

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