# SG No. 140 $D_{4h}^{18}$ $I4/mcm$ [ tetragonal ]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$
* Wyckoff site: `4a`, site symmetry: `422`

Table 1: Wyckoff bond: `4a@4a`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0,\ 0,\ Z]$ | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[1,2,3,4,-5,-6,-7,-8]` |
| 2 | $[0,\ 0,\ -Z]$ | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[9,10,11,12,-13,-14,-15,-16]` |

Table 2: Wyckoff bond: `8b@4a`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ 0,\ 0]$ | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[1,-2,-5,6]` |
| 2 | $[0,\ X,\ 0]$ | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[3,-4,7,-8]` |
| 3 | $[-X,\ 0,\ 0]$ | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[9,-10,-13,14]` |
| 4 | $[0,\ -X,\ 0]$ | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[11,-12,15,-16]` |

Table 3: Wyckoff bond: `8c@4a`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ X,\ 0]$ | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[1,-2,7,-8]` |
| 2 | $[-X,\ X,\ 0]$ | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[3,-4,5,-6]` |
| 3 | $[-X,\ -X,\ 0]$ | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[9,-10,15,-16]` |
| 4 | $[X,\ -X,\ 0]$ | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[11,-12,13,-14]` |

Table 4: Wyckoff bond: `16d@4a`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ 0,\ Z]$ | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[1,-5]` |
| 2 | $[-X,\ 0,\ Z]$ | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[2,-6]` |
| 3 | $[0,\ X,\ Z]$ | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[3,-8]` |
| 4 | $[0,\ -X,\ Z]$ | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[4,-7]` |
| 5 | $[-X,\ 0,\ -Z]$ | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[9,-13]` |
| 6 | $[X,\ 0,\ -Z]$ | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[10,-14]` |
| 7 | $[0,\ -X,\ -Z]$ | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[11,-16]` |
| 8 | $[0,\ X,\ -Z]$ | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[12,-15]` |

Table 5: Wyckoff bond: `16e@4a`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, X, Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[1,-8]` |
| 2 | $[-X, -X, Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[2,-7]` |
| 3 | $[-X, X, Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[3,-6]` |
| 4 | $[X, -X, Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[4,-5]` |
| 5 | $[-X, -X, -Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[9,-16]` |
| 6 | $[X, X, -Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[10,-15]` |
| 7 | $[X, -X, -Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[11,-14]` |
| 8 | $[-X, X, -Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[12,-13]` |

Table 6: Wyckoff bond: `16f@4a`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, 0]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[1,-2]` |
| 2 | $[-Y, X, 0]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[3,-4]` |
| 3 | $[-X, Y, 0]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[5,-6]` |
| 4 | $[Y, X, 0]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[7,-8]` |
| 5 | $[-X, -Y, 0]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[9,-10]` |
| 6 | $[Y, -X, 0]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[11,-12]` |
| 7 | $[X, -Y, 0]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[13,-14]` |
| 8 | $[-Y, -X, 0]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[15,-16]` |

Table 7: Wyckoff bond: `32g@4a`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[1]` |
| 2 | $[-X, -Y, Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[2]` |
| 3 | $[-Y, X, Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[3]` |
| 4 | $[Y, -X, Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[4]` |
| 5 | $[-X, Y, -Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[5]` |
| 6 | $[X, -Y, -Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[6]` |
| 7 | $[Y, X, -Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[7]` |
| 8 | $[-Y, -X, -Z]$ | $\left[0, 0, \frac{1}{4}\right]$ | `[8]` |
| 9 | $[-X, -Y, -Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[9]` |
| 10 | $[X, Y, -Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[10]` |
| 11 | $[Y, -X, -Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[11]` |
| 12 | $[-Y, X, -Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[12]` |
| 13 | $[X, -Y, Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[13]` |
| 14 | $[-X, Y, Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[14]` |
| 15 | $[-Y, -X, Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[15]` |
| 16 | $[Y, X, Z]$ | $\left[0, 0, \frac{3}{4}\right]$ | `[16]` |

* Wyckoff site: `4b`, site symmetry: `-42m`

Table 8: Wyckoff bond: `4a@4b`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0, 0, Z]$ | $[0, \frac{1}{2}, \frac{1}{4}]$ | `[1,2,-5,-6,-11,-12,15,16]` |
| 2 | $[0, 0, Z]$ | $[\frac{1}{2}, 0, \frac{1}{4}]$ | `[3,4,-7,-8,-9,-10,13,14]` |

Table 9: Wyckoff bond: `8b@4b`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, 0, 0]$ | $[0, \frac{1}{2}, \frac{1}{4}]$ | `[1,-2,-5,6]` |
| 2 | $[0, X, 0]$ | $[\frac{1}{2}, 0, \frac{1}{4}]$ | `[3,-4,7,-8]` |
| 3 | $[-X, 0, 0]$ | $[\frac{1}{2}, 0, \frac{1}{4}]$ | `[9,-10,-13,14]` |
| 4 | $[0, -X, 0]$ | $[0, \frac{1}{2}, \frac{1}{4}]$ | `[11,-12,15,-16]` |

Table 10: Wyckoff bond: `8c@4b`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, X, 0]$ | $[0, \frac{1}{2}, \frac{1}{4}]$ | `[1,-2,-15,16]` |
| 2 | $[-X, X, 0]$ | $[\frac{1}{2}, 0, \frac{1}{4}]$ | `[3,-4,-13,14]` |
| 3 | $[-X, X, 0]$ | $[0, \frac{1}{2}, \frac{1}{4}]$ | `[5,-6,-11,12]` |
| 4 | $[X, X, 0]$ | $[\frac{1}{2}, 0, \frac{1}{4}]$ | `[7,-8,-9,10]` |

Table 11: Wyckoff bond: `16d@4b`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, 0, Z]$ | $[0, \frac{1}{2}, \frac{1}{4}]$ | `[1,-5]` |
| 2 | $[-X, 0, Z]$ | $[0, \frac{1}{2}, \frac{1}{4}]$ | `[2,-6]` |
| 3 | $[0, X, Z]$ | $[\frac{1}{2}, 0, \frac{1}{4}]$ | `[3,-8]` |
| 4 | $[0, -X, Z]$ | $[\frac{1}{2}, 0, \frac{1}{4}]$ | `[4,-7]` |
| 5 | $[-X, 0, -Z]$ | $[\frac{1}{2}, 0, \frac{1}{4}]$ | `[9,-13]` |
| 6 | $[X, 0, -Z]$ | $[\frac{1}{2}, 0, \frac{1}{4}]$ | `[10,-14]` |
| 7 | $[0, -X, -Z]$ | $[0, \frac{1}{2}, \frac{1}{4}]$ | `[11,-16]` |
| 8 | $[0, X, -Z]$ | $[0, \frac{1}{2}, \frac{1}{4}]$ | `[12,-15]` |

Table 12: Wyckoff bond: `16e@4b`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ X,\ Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[1,16]` |
| 2 | $[-X,\ -X,\ Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[2,15]` |
| 3 | $[-X,\ X,\ Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[3,14]` |
| 4 | $[X,\ -X,\ Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[4,13]` |
| 5 | $[-X,\ X,\ -Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[5,12]` |
| 6 | $[X,\ -X,\ -Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[6,11]` |
| 7 | $[X,\ X,\ -Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[7,10]` |
| 8 | $[-X,\ -X,\ -Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[8,9]` |

Table 13: Wyckoff bond: `16f@4b`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ Y,\ 0]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[1,-2]` |
| 2 | $[-Y,\ X,\ 0]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[3,-4]` |
| 3 | $[-X,\ Y,\ 0]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[5,-6]` |
| 4 | $[Y,\ X,\ 0]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[7,-8]` |
| 5 | $[-X,\ -Y,\ 0]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[9,-10]` |
| 6 | $[Y,\ -X,\ 0]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[11,-12]` |
| 7 | $[X,\ -Y,\ 0]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[13,-14]` |
| 8 | $[-Y,\ -X,\ 0]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[15,-16]` |

Table 14: Wyckoff bond: `32g@4b`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ Y,\ Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[1]` |
| 2 | $[-X,\ -Y,\ Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[2]` |
| 3 | $[-Y,\ X,\ Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[3]` |
| 4 | $[Y,\ -X,\ Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[4]` |
| 5 | $[-X,\ Y,\ -Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[5]` |
| 6 | $[X,\ -Y,\ -Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[6]` |
| 7 | $[Y,\ X,\ -Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[7]` |
| 8 | $[-Y,\ -X,\ -Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[8]` |
| 9 | $[-X,\ -Y,\ -Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[9]` |
| 10 | $[X,\ Y,\ -Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[10]` |
| 11 | $[Y,\ -X,\ -Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[11]` |
| 12 | $[-Y,\ X,\ -Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[12]` |
| 13 | $[X,\ -Y,\ Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[13]` |
| 14 | $[-X,\ Y,\ Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[14]` |
| 15 | $[-Y,\ -X,\ Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[15]` |
| 16 | $[Y,\ X,\ Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[16]` |

* Wyckoff site: `4c`, site symmetry: `4/m..`

Table 15: Wyckoff bond: `4a@4c`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0, 0, Z]$ | $[0, 0, 0]$ | `[1,2,3,4,-9,-10,-11,-12]` |
| 2 | $[0, 0, -Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[5,6,7,8,-13,-14,-15,-16]` |

Table 16: Wyckoff bond: `8b@4c`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, 0]$ | $[0, 0, 0]$ | `[1,-2,-9,10]` |
| 2 | $[-Y, X, 0]$ | $[0, 0, 0]$ | `[3,-4,-11,12]` |
| 3 | $[-X, Y, 0]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[5,-6,-13,14]` |
| 4 | $[Y, X, 0]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[7,-8,-15,16]` |

Table 17: Wyckoff bond: `16c@4c`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, Z]$ | $[0, 0, 0]$ | `[1,-9]` |
| 2 | $[-X, -Y, Z]$ | $[0, 0, 0]$ | `[2,-10]` |
| 3 | $[-Y, X, Z]$ | $[0, 0, 0]$ | `[3,-11]` |
| 4 | $[Y, -X, Z]$ | $[0, 0, 0]$ | `[4,-12]` |
| 5 | $[-X, Y, -Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[5,-13]` |
| 6 | $[X, -Y, -Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[6,-14]` |
| 7 | $[Y, X, -Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[7,-15]` |
| 8 | $[-Y, -X, -Z]$ | $\left[0, 0, \frac{1}{2}\right]$ | `[8,-16]` |

* Wyckoff site: `4d`, site symmetry: `m.mm`

Table 18: Wyckoff bond: `4a@4d`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, X, 0]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[1,-2,7,-8,-9,10,-15,16]` |
| 2 | $[-X, X, 0]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[3,-4,5,-6,-11,12,-13,14]` |

Table 19: Wyckoff bond: `4b@4d`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, -X, 0]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[1,-2,-7,8,-9,10,15,-16]` |

*continued ...*

Table 19

| No. | vector | center | mapping |
|---|---|---|---|
| 2 | $[X, X, 0]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[3,-4,-5,6,-11,12,13,-14]` |

Table 20: Wyckoff bond: `4c@4d`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0, 0, Z]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[1,2,-7,-8,-9,-10,15,16]` |
| 2 | $[0, 0, Z]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[3,4,-5,-6,-11,-12,13,14]` |

Table 21: Wyckoff bond: `8d@4d`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, X, Z]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[1,-8,-9,16]` |
| 2 | $[-X, -X, Z]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[2,-7,-10,15]` |
| 3 | $[-X, X, Z]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[3,-6,-11,14]` |
| 4 | $[X, -X, Z]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[4,-5,-12,13]` |

Table 22: Wyckoff bond: `8e@4d`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, -X, Z]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[1,-7,-9,15]` |
| 2 | $[-X, X, Z]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[2,-8,-10,16]` |
| 3 | $[X, X, Z]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[3,-5,-11,13]` |
| 4 | $[-X, -X, Z]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[4,-6,-12,14]` |

Table 23: Wyckoff bond: `8f@4d`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, 0]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[1,-2,-9,10]` |
| 2 | $[-Y, X, 0]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[3,-4,-11,12]` |
| 3 | $[-X, Y, 0]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[5,-6,-13,14]` |
| 4 | $[Y, X, 0]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[7,-8,-15,16]` |

Table 24: Wyckoff bond: `16g@4d`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, Z]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[1,-9]` |
| 2 | $[-X, -Y, Z]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[2,-10]` |
| 3 | $[-Y, X, Z]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[3,-11]` |
| 4 | $[Y, -X, Z]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[4,-12]` |
| 5 | $[-X, Y, -Z]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[5,-13]` |
| 6 | $[X, -Y, -Z]$ | $\left[\frac{1}{2}, 0, 0\right]$ | `[6,-14]` |
| 7 | $[Y, X, -Z]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[7,-15]` |
| 8 | $[-Y, -X, -Z]$ | $\left[0, \frac{1}{2}, 0\right]$ | `[8,-16]` |

* Wyckoff site: `8e`, site symmetry: `..2/m`

Table 25: Wyckoff bond: `8a@8e`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, -X, Z]$ | $\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[1,-7,-9,15]` |
| 2 | $[-X, X, Z]$ | $\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[2,-8,-10,16]` |
| 3 | $[X, X, Z]$ | $\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[3,-5,-11,13]` |
| 4 | $[-X, -X, Z]$ | $\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[4,-6,-12,14]` |

Table 26: Wyckoff bond: `8b@8e`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, X, 0]$ | $\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[1,7,-9,-15]` |
| 2 | $[-X, -X, 0]$ | $\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[2,8,-10,-16]` |
| 3 | $[-X, X, 0]$ | $\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[3,5,-11,-13]` |
| 4 | $[X, -X, 0]$ | $\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[4,6,-12,-14]` |

Table 27: Wyckoff bond: `16c@8e`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, Z]$ | $\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[1,-9]` |
| 2 | $[-X, -Y, Z]$ | $\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[2,-10]` |
| 3 | $[-Y, X, Z]$ | $\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[3,-11]` |
| 4 | $[Y, -X, Z]$ | $\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[4,-12]` |
| 5 | $[-X, Y, -Z]$ | $\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[5,-13]` |
| 6 | $[X, -Y, -Z]$ | $\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[6,-14]` |
| 7 | $[Y, X, -Z]$ | $\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[7,-15]` |
| 8 | $[-Y, -X, -Z]$ | $\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[8,-16]` |

* Wyckoff site: 8f, site symmetry: 4..

Table 28: Wyckoff bond: 8a@8f

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0,\ 0,\ Z]$ | $[0,\ 0,\ z]$ | [1,2,3,4] |
| 2 | $[0,\ 0,\ -Z]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | [5,6,7,8] |
| 3 | $[0,\ 0,\ -Z]$ | $[0,\ 0,\ -z]$ | [9,10,11,12] |
| 4 | $[0,\ 0,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | [13,14,15,16] |

Table 29: Wyckoff bond: 16b@8f

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ Y,\ 0]$ | $[0,\ 0,\ z]$ | [1,-2] |
| 2 | $[-Y,\ X,\ 0]$ | $[0,\ 0,\ z]$ | [3,-4] |
| 3 | $[-X,\ Y,\ 0]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | [5,-6] |
| 4 | $[Y,\ X,\ 0]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | [7,-8] |
| 5 | $[-X,\ -Y,\ 0]$ | $[0,\ 0,\ -z]$ | [9,-10] |
| 6 | $[Y,\ -X,\ 0]$ | $[0,\ 0,\ -z]$ | [11,-12] |
| 7 | $[X,\ -Y,\ 0]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | [13,-14] |
| 8 | $[-Y,\ -X,\ 0]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | [15,-16] |

Table 30: Wyckoff bond: 32c@8f

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ Y,\ Z]$ | $[0,\ 0,\ z]$ | [1] |
| 2 | $[-X,\ -Y,\ Z]$ | $[0,\ 0,\ z]$ | [2] |
| 3 | $[-Y,\ X,\ Z]$ | $[0,\ 0,\ z]$ | [3] |
| 4 | $[Y,\ -X,\ Z]$ | $[0,\ 0,\ z]$ | [4] |
| 5 | $[-X,\ Y,\ -Z]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | [5] |
| 6 | $[X,\ -Y,\ -Z]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | [6] |
| 7 | $[Y,\ X,\ -Z]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | [7] |
| 8 | $[-Y,\ -X,\ -Z]$ | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | [8] |
| 9 | $[-X,\ -Y,\ -Z]$ | $[0,\ 0,\ -z]$ | [9] |
| 10 | $[X,\ Y,\ -Z]$ | $[0,\ 0,\ -z]$ | [10] |
| 11 | $[Y,\ -X,\ -Z]$ | $[0,\ 0,\ -z]$ | [11] |
| 12 | $[-Y,\ X,\ -Z]$ | $[0,\ 0,\ -z]$ | [12] |
| 13 | $[X,\ -Y,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | [13] |
| 14 | $[-X,\ Y,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | [14] |
| 15 | $[-Y,\ -X,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | [15] |
| 16 | $[Y,\ X,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | [16] |

* Wyckoff site: 8g, site symmetry: 2.mm

Table 31: Wyckoff bond: `8a@8g`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ X,\ 0]$ | $\left[0,\ \frac{1}{2},\ z\right]$ | `[1,-2,-15,16]` |
| 2 | $[-X,\ X,\ 0]$ | $\left[\frac{1}{2},\ 0,\ z\right]$ | `[3,-4,-13,14]` |
| 3 | $[-X,\ X,\ 0]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$ | `[5,-6,-11,12]` |
| 4 | $[X,\ X,\ 0]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$ | `[7,-8,-9,10]` |

Table 32: Wyckoff bond: `8b@8g`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0,\ 0,\ Z]$ | $\left[0,\ \frac{1}{2},\ z\right]$ | `[1,2,15,16]` |
| 2 | $[0,\ 0,\ Z]$ | $\left[\frac{1}{2},\ 0,\ z\right]$ | `[3,4,13,14]` |
| 3 | $[0,\ 0,\ -Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$ | `[5,6,11,12]` |
| 4 | $[0,\ 0,\ -Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$ | `[7,8,9,10]` |

Table 33: Wyckoff bond: `16c@8g`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ X,\ Z]$ | $\left[0,\ \frac{1}{2},\ z\right]$ | `[1,16]` |
| 2 | $[-X,\ -X,\ Z]$ | $\left[0,\ \frac{1}{2},\ z\right]$ | `[2,15]` |
| 3 | $[-X,\ X,\ Z]$ | $\left[\frac{1}{2},\ 0,\ z\right]$ | `[3,14]` |
| 4 | $[X,\ -X,\ Z]$ | $\left[\frac{1}{2},\ 0,\ z\right]$ | `[4,13]` |
| 5 | $[-X,\ X,\ -Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$ | `[5,12]` |
| 6 | $[X,\ -X,\ -Z]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$ | `[6,11]` |
| 7 | $[X,\ X,\ -Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$ | `[7,10]` |
| 8 | $[-X,\ -X,\ -Z]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$ | `[8,9]` |

Table 34: Wyckoff bond: `16d@8g`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ Y,\ 0]$ | $\left[0,\ \frac{1}{2},\ z\right]$ | `[1,-2]` |
| 2 | $[-Y,\ X,\ 0]$ | $\left[\frac{1}{2},\ 0,\ z\right]$ | `[3,-4]` |
| 3 | $[-X,\ Y,\ 0]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$ | `[5,-6]` |
| 4 | $[Y,\ X,\ 0]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$ | `[7,-8]` |
| 5 | $[-X,\ -Y,\ 0]$ | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$ | `[9,-10]` |
| 6 | $[Y,\ -X,\ 0]$ | $\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$ | `[11,-12]` |
| 7 | $[X,\ -Y,\ 0]$ | $\left[\frac{1}{2},\ 0,\ z\right]$ | `[13,-14]` |
| 8 | $[-Y,\ -X,\ 0]$ | $\left[0,\ \frac{1}{2},\ z\right]$ | `[15,-16]` |

Table 35: Wyckoff bond: `32e@8g`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, Z]$ | $\left[0, \frac{1}{2}, z\right]$ | `[1]` |
| 2 | $[-X, -Y, Z]$ | $\left[0, \frac{1}{2}, z\right]$ | `[2]` |
| 3 | $[-Y, X, Z]$ | $\left[\frac{1}{2}, 0, z\right]$ | `[3]` |
| 4 | $[Y, -X, Z]$ | $\left[\frac{1}{2}, 0, z\right]$ | `[4]` |
| 5 | $[-X, Y, -Z]$ | $\left[0, \frac{1}{2}, \frac{1}{2} - z\right]$ | `[5]` |
| 6 | $[X, -Y, -Z]$ | $\left[0, \frac{1}{2}, \frac{1}{2} - z\right]$ | `[6]` |
| 7 | $[Y, X, -Z]$ | $\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$ | `[7]` |
| 8 | $[-Y, -X, -Z]$ | $\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$ | `[8]` |
| 9 | $[-X, -Y, -Z]$ | $\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$ | `[9]` |
| 10 | $[X, Y, -Z]$ | $\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$ | `[10]` |
| 11 | $[Y, -X, -Z]$ | $\left[0, \frac{1}{2}, \frac{1}{2} - z\right]$ | `[11]` |
| 12 | $[-Y, X, -Z]$ | $\left[0, \frac{1}{2}, \frac{1}{2} - z\right]$ | `[12]` |
| 13 | $[X, -Y, Z]$ | $\left[\frac{1}{2}, 0, z\right]$ | `[13]` |
| 14 | $[-X, Y, Z]$ | $\left[\frac{1}{2}, 0, z\right]$ | `[14]` |
| 15 | $[-Y, -X, Z]$ | $\left[0, \frac{1}{2}, z\right]$ | `[15]` |
| 16 | $[Y, X, Z]$ | $\left[0, \frac{1}{2}, z\right]$ | `[16]` |

* Wyckoff site: `8h`, site symmetry: `m.2m`

Table 36: Wyckoff bond: `8a@8h`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, X, 0]$ | $\left[x, x + \frac{1}{2}, 0\right]$ | `[1,7,10,16]` |
| 2 | $[-X, -X, 0]$ | $\left[-x, \frac{1}{2} - x, 0\right]$ | `[2,8,9,15]` |
| 3 | $[-X, X, 0]$ | $\left[\frac{1}{2} - x, x, 0\right]$ | `[3,5,12,14]` |
| 4 | $[X, -X, 0]$ | $\left[x + \frac{1}{2}, -x, 0\right]$ | `[4,6,11,13]` |

Table 37: Wyckoff bond: `8b@8h`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, -X, 0]$ | $\left[x, x + \frac{1}{2}, 0\right]$ | `[1,-7,10,-16]` |
| 2 | $[-X, X, 0]$ | $\left[-x, \frac{1}{2} - x, 0\right]$ | `[2,-8,9,-15]` |
| 3 | $[X, X, 0]$ | $\left[\frac{1}{2} - x, x, 0\right]$ | `[3,-5,12,-14]` |
| 4 | $[-X, -X, 0]$ | $\left[x + \frac{1}{2}, -x, 0\right]$ | `[4,-6,11,-13]` |

Table 38: Wyckoff bond: `8c@8h`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0, 0, Z]$ | $\left[x, x + \frac{1}{2}, 0\right]$ | `[1,-7,-10,16]` |

*continued ...*

Table 38

| No. | vector | center | mapping |
|---|---|---|---|
| 2 | $[0,\, 0,\, Z]$ | $\left[-x,\, \frac{1}{2}-x,\, 0\right]$ | `[2,-8,-9,15]` |
| 3 | $[0,\, 0,\, Z]$ | $\left[\frac{1}{2}-x,\, x,\, 0\right]$ | `[3,-5,-12,14]` |
| 4 | $[0,\, 0,\, Z]$ | $\left[x+\frac{1}{2},\, -x,\, 0\right]$ | `[4,-6,-11,13]` |

Table 39: Wyckoff bond: `16d@8h`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\, X,\, Z]$ | $\left[x,\, x+\frac{1}{2},\, 0\right]$ | `[1,16]` |
| 2 | $[-X,\, -X,\, Z]$ | $\left[-x,\, \frac{1}{2}-x,\, 0\right]$ | `[2,15]` |
| 3 | $[-X,\, X,\, Z]$ | $\left[\frac{1}{2}-x,\, x,\, 0\right]$ | `[3,14]` |
| 4 | $[X,\, -X,\, Z]$ | $\left[x+\frac{1}{2},\, -x,\, 0\right]$ | `[4,13]` |
| 5 | $[-X,\, X,\, -Z]$ | $\left[\frac{1}{2}-x,\, x,\, 0\right]$ | `[5,12]` |
| 6 | $[X,\, -X,\, -Z]$ | $\left[x+\frac{1}{2},\, -x,\, 0\right]$ | `[6,11]` |
| 7 | $[X,\, X,\, -Z]$ | $\left[x,\, x+\frac{1}{2},\, 0\right]$ | `[7,10]` |
| 8 | $[-X,\, -X,\, -Z]$ | $\left[-x,\, \frac{1}{2}-x,\, 0\right]$ | `[8,9]` |

Table 40: Wyckoff bond: `16e@8h`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\, -X,\, Z]$ | $\left[x,\, x+\frac{1}{2},\, 0\right]$ | `[1,-7]` |
| 2 | $[-X,\, X,\, Z]$ | $\left[-x,\, \frac{1}{2}-x,\, 0\right]$ | `[2,-8]` |
| 3 | $[X,\, X,\, Z]$ | $\left[\frac{1}{2}-x,\, x,\, 0\right]$ | `[3,-5]` |
| 4 | $[-X,\, -X,\, Z]$ | $\left[x+\frac{1}{2},\, -x,\, 0\right]$ | `[4,-6]` |
| 5 | $[-X,\, X,\, -Z]$ | $\left[-x,\, \frac{1}{2}-x,\, 0\right]$ | `[9,-15]` |
| 6 | $[X,\, -X,\, -Z]$ | $\left[x,\, x+\frac{1}{2},\, 0\right]$ | `[10,-16]` |
| 7 | $[-X,\, -X,\, -Z]$ | $\left[x+\frac{1}{2},\, -x,\, 0\right]$ | `[11,-13]` |
| 8 | $[X,\, X,\, -Z]$ | $\left[\frac{1}{2}-x,\, x,\, 0\right]$ | `[12,-14]` |

Table 41: Wyckoff bond: `16f@8h`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\, Y,\, 0]$ | $\left[x,\, x+\frac{1}{2},\, 0\right]$ | `[1,10]` |
| 2 | $[-X,\, -Y,\, 0]$ | $\left[-x,\, \frac{1}{2}-x,\, 0\right]$ | `[2,9]` |
| 3 | $[-Y,\, X,\, 0]$ | $\left[\frac{1}{2}-x,\, x,\, 0\right]$ | `[3,12]` |
| 4 | $[Y,\, -X,\, 0]$ | $\left[x+\frac{1}{2},\, -x,\, 0\right]$ | `[4,11]` |
| 5 | $[-X,\, Y,\, 0]$ | $\left[\frac{1}{2}-x,\, x,\, 0\right]$ | `[5,14]` |
| 6 | $[X,\, -Y,\, 0]$ | $\left[x+\frac{1}{2},\, -x,\, 0\right]$ | `[6,13]` |
| 7 | $[Y,\, X,\, 0]$ | $\left[x,\, x+\frac{1}{2},\, 0\right]$ | `[7,16]` |
| 8 | $[-Y,\, -X,\, 0]$ | $\left[-x,\, \frac{1}{2}-x,\, 0\right]$ | `[8,15]` |

Table 42: Wyckoff bond: `32g@8h`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, Z]$ | $\left[x, x+\frac{1}{2}, 0\right]$ | `[1]` |
| 2 | $[-X, -Y, Z]$ | $\left[-x, \frac{1}{2}-x, 0\right]$ | `[2]` |
| 3 | $[-Y, X, Z]$ | $\left[\frac{1}{2}-x, x, 0\right]$ | `[3]` |
| 4 | $[Y, -X, Z]$ | $\left[x+\frac{1}{2}, -x, 0\right]$ | `[4]` |
| 5 | $[-X, Y, -Z]$ | $\left[\frac{1}{2}-x, x, 0\right]$ | `[5]` |
| 6 | $[X, -Y, -Z]$ | $\left[x+\frac{1}{2}, -x, 0\right]$ | `[6]` |
| 7 | $[Y, X, -Z]$ | $\left[x, x+\frac{1}{2}, 0\right]$ | `[7]` |
| 8 | $[-Y, -X, -Z]$ | $\left[-x, \frac{1}{2}-x, 0\right]$ | `[8]` |
| 9 | $[-X, -Y, -Z]$ | $\left[-x, \frac{1}{2}-x, 0\right]$ | `[9]` |
| 10 | $[X, Y, -Z]$ | $\left[x, x+\frac{1}{2}, 0\right]$ | `[10]` |
| 11 | $[Y, -X, -Z]$ | $\left[x+\frac{1}{2}, -x, 0\right]$ | `[11]` |
| 12 | $[-Y, X, -Z]$ | $\left[\frac{1}{2}-x, x, 0\right]$ | `[12]` |
| 13 | $[X, -Y, Z]$ | $\left[x+\frac{1}{2}, -x, 0\right]$ | `[13]` |
| 14 | $[-X, Y, Z]$ | $\left[\frac{1}{2}-x, x, 0\right]$ | `[14]` |
| 15 | $[-Y, -X, Z]$ | $\left[-x, \frac{1}{2}-x, 0\right]$ | `[15]` |
| 16 | $[Y, X, Z]$ | $\left[x, x+\frac{1}{2}, 0\right]$ | `[16]` |

* Wyckoff site: `16i`, site symmetry: `..2`

Table 43: Wyckoff bond: `16a@16i`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, -X, Z]$ | $\left[x, x, \frac{1}{4}\right]$ | `[1,-7]` |
| 2 | $[-X, X, Z]$ | $\left[-x, -x, \frac{1}{4}\right]$ | `[2,-8]` |
| 3 | $[X, X, Z]$ | $\left[-x, x, \frac{1}{4}\right]$ | `[3,-5]` |
| 4 | $[-X, -X, Z]$ | $\left[x, -x, \frac{1}{4}\right]$ | `[4,-6]` |
| 5 | $[-X, X, -Z]$ | $\left[-x, -x, \frac{3}{4}\right]$ | `[9,-15]` |
| 6 | $[X, -X, -Z]$ | $\left[x, x, \frac{3}{4}\right]$ | `[10,-16]` |
| 7 | $[-X, -X, -Z]$ | $\left[x, -x, \frac{3}{4}\right]$ | `[11,-13]` |
| 8 | $[X, X, -Z]$ | $\left[-x, x, \frac{3}{4}\right]$ | `[12,-14]` |

Table 44: Wyckoff bond: `16b@16i`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, X, 0]$ | $\left[x, x, \frac{1}{4}\right]$ | `[1,7]` |
| 2 | $[-X, -X, 0]$ | $\left[-x, -x, \frac{1}{4}\right]$ | `[2,8]` |
| 3 | $[-X, X, 0]$ | $\left[-x, x, \frac{1}{4}\right]$ | `[3,5]` |
| 4 | $[X, -X, 0]$ | $\left[x, -x, \frac{1}{4}\right]$ | `[4,6]` |
| 5 | $[-X, -X, 0]$ | $\left[-x, -x, \frac{3}{4}\right]$ | `[9,15]` |
| 6 | $[X, X, 0]$ | $\left[x, x, \frac{3}{4}\right]$ | `[10,16]` |
| 7 | $[X, -X, 0]$ | $\left[x, -x, \frac{3}{4}\right]$ | `[11,13]` |
| 8 | $[-X, X, 0]$ | $\left[-x, x, \frac{3}{4}\right]$ | `[12,14]` |

Table 45: Wyckoff bond: `32c@16i`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, Z]$ | $\left[x, x, \frac{1}{4}\right]$ | `[1]` |
| 2 | $[-X, -Y, Z]$ | $\left[-x, -x, \frac{1}{4}\right]$ | `[2]` |
| 3 | $[-Y, X, Z]$ | $\left[-x, x, \frac{1}{4}\right]$ | `[3]` |
| 4 | $[Y, -X, Z]$ | $\left[x, -x, \frac{1}{4}\right]$ | `[4]` |
| 5 | $[-X, Y, -Z]$ | $\left[-x, x, \frac{1}{4}\right]$ | `[5]` |
| 6 | $[X, -Y, -Z]$ | $\left[x, -x, \frac{1}{4}\right]$ | `[6]` |
| 7 | $[Y, X, -Z]$ | $\left[x, x, \frac{1}{4}\right]$ | `[7]` |
| 8 | $[-Y, -X, -Z]$ | $\left[-x, -x, \frac{1}{4}\right]$ | `[8]` |
| 9 | $[-X, -Y, -Z]$ | $\left[-x, -x, \frac{3}{4}\right]$ | `[9]` |
| 10 | $[X, Y, -Z]$ | $\left[x, x, \frac{3}{4}\right]$ | `[10]` |
| 11 | $[Y, -X, -Z]$ | $\left[x, -x, \frac{3}{4}\right]$ | `[11]` |
| 12 | $[-Y, X, -Z]$ | $\left[-x, x, \frac{3}{4}\right]$ | `[12]` |
| 13 | $[X, -Y, Z]$ | $\left[x, -x, \frac{3}{4}\right]$ | `[13]` |
| 14 | $[-X, Y, Z]$ | $\left[-x, x, \frac{3}{4}\right]$ | `[14]` |
| 15 | $[-Y, -X, Z]$ | $\left[-x, -x, \frac{3}{4}\right]$ | `[15]` |
| 16 | $[Y, X, Z]$ | $\left[x, x, \frac{3}{4}\right]$ | `[16]` |

* Wyckoff site: `16j`, site symmetry: `.2.`

Table 46: Wyckoff bond: `16a@16j`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0, X, Z]$ | $\left[x, 0, \frac{1}{4}\right]$ | `[1,-6]` |
| 2 | $[0, -X, Z]$ | $\left[-x, 0, \frac{1}{4}\right]$ | `[2,-5]` |
| 3 | $[-X, 0, Z]$ | $\left[0, x, \frac{1}{4}\right]$ | `[3,-7]` |
| 4 | $[X, 0, Z]$ | $\left[0, -x, \frac{1}{4}\right]$ | `[4,-8]` |
| 5 | $[0, -X, -Z]$ | $\left[-x, 0, \frac{3}{4}\right]$ | `[9,-14]` |
| 6 | $[0, X, -Z]$ | $\left[x, 0, \frac{3}{4}\right]$ | `[10,-13]` |
| 7 | $[X, 0, -Z]$ | $\left[0, -x, \frac{3}{4}\right]$ | `[11,-15]` |
| 8 | $[-X, 0, -Z]$ | $\left[0, x, \frac{3}{4}\right]$ | `[12,-16]` |

Table 47: Wyckoff bond: `16b@16j`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, 0, 0]$ | $\left[x, 0, \frac{1}{4}\right]$ | `[1,6]` |
| 2 | $[-X, 0, 0]$ | $\left[-x, 0, \frac{1}{4}\right]$ | `[2,5]` |
| 3 | $[0, X, 0]$ | $\left[0, x, \frac{1}{4}\right]$ | `[3,7]` |
| 4 | $[0, -X, 0]$ | $\left[0, -x, \frac{1}{4}\right]$ | `[4,8]` |
| 5 | $[-X, 0, 0]$ | $\left[-x, 0, \frac{3}{4}\right]$ | `[9,14]` |
| 6 | $[X, 0, 0]$ | $\left[x, 0, \frac{3}{4}\right]$ | `[10,13]` |

*continued ...*

Table 47

| No. | vector | center | mapping |
|---|---|---|---|
| 7 | $[0, -X, 0]$ | $\left[0, -x, \frac{3}{4}\right]$ | `[11,15]` |
| 8 | $[0, X, 0]$ | $\left[0, x, \frac{3}{4}\right]$ | `[12,16]` |

Table 48: Wyckoff bond: `32c@16j`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, Z]$ | $\left[x, 0, \frac{1}{4}\right]$ | `[1]` |
| 2 | $[-X, -Y, Z]$ | $\left[-x, 0, \frac{1}{4}\right]$ | `[2]` |
| 3 | $[-Y, X, Z]$ | $\left[0, x, \frac{1}{4}\right]$ | `[3]` |
| 4 | $[Y, -X, Z]$ | $\left[0, -x, \frac{1}{4}\right]$ | `[4]` |
| 5 | $[-X, Y, -Z]$ | $\left[-x, 0, \frac{1}{4}\right]$ | `[5]` |
| 6 | $[X, -Y, -Z]$ | $\left[x, 0, \frac{1}{4}\right]$ | `[6]` |
| 7 | $[Y, X, -Z]$ | $\left[0, x, \frac{1}{4}\right]$ | `[7]` |
| 8 | $[-Y, -X, -Z]$ | $\left[0, -x, \frac{1}{4}\right]$ | `[8]` |
| 9 | $[-X, -Y, -Z]$ | $\left[-x, 0, \frac{3}{4}\right]$ | `[9]` |
| 10 | $[X, Y, -Z]$ | $\left[x, 0, \frac{3}{4}\right]$ | `[10]` |
| 11 | $[Y, -X, -Z]$ | $\left[0, -x, \frac{3}{4}\right]$ | `[11]` |
| 12 | $[-Y, X, -Z]$ | $\left[0, x, \frac{3}{4}\right]$ | `[12]` |
| 13 | $[X, -Y, Z]$ | $\left[x, 0, \frac{3}{4}\right]$ | `[13]` |
| 14 | $[-X, Y, Z]$ | $\left[-x, 0, \frac{3}{4}\right]$ | `[14]` |
| 15 | $[-Y, -X, Z]$ | $\left[0, -x, \frac{3}{4}\right]$ | `[15]` |
| 16 | $[Y, X, Z]$ | $\left[0, x, \frac{3}{4}\right]$ | `[16]` |

* Wyckoff site: `16k`, site symmetry: `m..`

Table 49: Wyckoff bond: `16a@16k`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, 0]$ | $[x, y, 0]$ | `[1,10]` |
| 2 | $[-X, -Y, 0]$ | $[-x, -y, 0]$ | `[2,9]` |
| 3 | $[-Y, X, 0]$ | $[-y, x, 0]$ | `[3,12]` |
| 4 | $[Y, -X, 0]$ | $[y, -x, 0]$ | `[4,11]` |
| 5 | $[-X, Y, 0]$ | $\left[-x, y, \frac{1}{2}\right]$ | `[5,14]` |
| 6 | $[X, -Y, 0]$ | $\left[x, -y, \frac{1}{2}\right]$ | `[6,13]` |
| 7 | $[Y, X, 0]$ | $\left[y, x, \frac{1}{2}\right]$ | `[7,16]` |
| 8 | $[-Y, -X, 0]$ | $\left[-y, -x, \frac{1}{2}\right]$ | `[8,15]` |

Table 50: Wyckoff bond: `16b@16k`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[0,\ 0,\ Z]$ | $[x,\ y,\ 0]$ | `[1,-10]` |
| 2 | $[0,\ 0,\ Z]$ | $[-x,\ -y,\ 0]$ | `[2,-9]` |
| 3 | $[0,\ 0,\ Z]$ | $[-y,\ x,\ 0]$ | `[3,-12]` |
| 4 | $[0,\ 0,\ Z]$ | $[y,\ -x,\ 0]$ | `[4,-11]` |
| 5 | $[0,\ 0,\ -Z]$ | $\left[-x,\ y,\ \frac{1}{2}\right]$ | `[5,-14]` |
| 6 | $[0,\ 0,\ -Z]$ | $\left[x,\ -y,\ \frac{1}{2}\right]$ | `[6,-13]` |
| 7 | $[0,\ 0,\ -Z]$ | $\left[y,\ x,\ \frac{1}{2}\right]$ | `[7,-16]` |
| 8 | $[0,\ 0,\ -Z]$ | $\left[-y,\ -x,\ \frac{1}{2}\right]$ | `[8,-15]` |

Table 51: Wyckoff bond: `32c@16k`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ Y,\ Z]$ | $[x,\ y,\ 0]$ | `[1]` |
| 2 | $[-X,\ -Y,\ Z]$ | $[-x,\ -y,\ 0]$ | `[2]` |
| 3 | $[-Y,\ X,\ Z]$ | $[-y,\ x,\ 0]$ | `[3]` |
| 4 | $[Y,\ -X,\ Z]$ | $[y,\ -x,\ 0]$ | `[4]` |
| 5 | $[-X,\ Y,\ -Z]$ | $\left[-x,\ y,\ \frac{1}{2}\right]$ | `[5]` |
| 6 | $[X,\ -Y,\ -Z]$ | $\left[x,\ -y,\ \frac{1}{2}\right]$ | `[6]` |
| 7 | $[Y,\ X,\ -Z]$ | $\left[y,\ x,\ \frac{1}{2}\right]$ | `[7]` |
| 8 | $[-Y,\ -X,\ -Z]$ | $\left[-y,\ -x,\ \frac{1}{2}\right]$ | `[8]` |
| 9 | $[-X,\ -Y,\ -Z]$ | $[-x,\ -y,\ 0]$ | `[9]` |
| 10 | $[X,\ Y,\ -Z]$ | $[x,\ y,\ 0]$ | `[10]` |
| 11 | $[Y,\ -X,\ -Z]$ | $[y,\ -x,\ 0]$ | `[11]` |
| 12 | $[-Y,\ X,\ -Z]$ | $[-y,\ x,\ 0]$ | `[12]` |
| 13 | $[X,\ -Y,\ Z]$ | $\left[x,\ -y,\ \frac{1}{2}\right]$ | `[13]` |
| 14 | $[-X,\ Y,\ Z]$ | $\left[-x,\ y,\ \frac{1}{2}\right]$ | `[14]` |
| 15 | $[-Y,\ -X,\ Z]$ | $\left[-y,\ -x,\ \frac{1}{2}\right]$ | `[15]` |
| 16 | $[Y,\ X,\ Z]$ | $\left[y,\ x,\ \frac{1}{2}\right]$ | `[16]` |

* Wyckoff site: `16l`, site symmetry: `..m`

Table 52: Wyckoff bond: `16a@16l`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ X,\ Z]$ | $\left[x,\ x+\frac{1}{2},\ z\right]$ | `[1,16]` |
| 2 | $[-X,\ -X,\ Z]$ | $\left[-x,\ \frac{1}{2}-x,\ z\right]$ | `[2,15]` |
| 3 | $[-X,\ X,\ Z]$ | $\left[\frac{1}{2}-x,\ x,\ z\right]$ | `[3,14]` |
| 4 | $[X,\ -X,\ Z]$ | $\left[x+\frac{1}{2},\ -x,\ z\right]$ | `[4,13]` |
| 5 | $[-X,\ X,\ -Z]$ | $\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$ | `[5,12]` |
| 6 | $[X,\ -X,\ -Z]$ | $\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$ | `[6,11]` |
| 7 | $[X,\ X,\ -Z]$ | $\left[x+\frac{1}{2},\ x,\ \frac{1}{2}-z\right]$ | `[7,10]` |
| 8 | $[-X,\ -X,\ -Z]$ | $\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}-z\right]$ | `[8,9]` |

Table 53: Wyckoff bond: `16b@16l`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, -X, 0]$ | $\left[x, x+\frac{1}{2}, z\right]$ | `[1,-16]` |
| 2 | $[-X, X, 0]$ | $\left[-x, \frac{1}{2}-x, z\right]$ | `[2,-15]` |
| 3 | $[X, X, 0]$ | $\left[\frac{1}{2}-x, x, z\right]$ | `[3,-14]` |
| 4 | $[-X, -X, 0]$ | $\left[x+\frac{1}{2}, -x, z\right]$ | `[4,-13]` |
| 5 | $[-X, -X, 0]$ | $\left[-x, x+\frac{1}{2}, \frac{1}{2}-z\right]$ | `[5,-12]` |
| 6 | $[X, X, 0]$ | $\left[x, \frac{1}{2}-x, \frac{1}{2}-z\right]$ | `[6,-11]` |
| 7 | $[-X, X, 0]$ | $\left[x+\frac{1}{2}, x, \frac{1}{2}-z\right]$ | `[7,-10]` |
| 8 | $[X, -X, 0]$ | $\left[\frac{1}{2}-x, -x, \frac{1}{2}-z\right]$ | `[8,-9]` |

Table 54: Wyckoff bond: `32c@16l`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X, Y, Z]$ | $\left[x, x+\frac{1}{2}, z\right]$ | `[1]` |
| 2 | $[-X, -Y, Z]$ | $\left[-x, \frac{1}{2}-x, z\right]$ | `[2]` |
| 3 | $[-Y, X, Z]$ | $\left[\frac{1}{2}-x, x, z\right]$ | `[3]` |
| 4 | $[Y, -X, Z]$ | $\left[x+\frac{1}{2}, -x, z\right]$ | `[4]` |
| 5 | $[-X, Y, -Z]$ | $\left[-x, x+\frac{1}{2}, \frac{1}{2}-z\right]$ | `[5]` |
| 6 | $[X, -Y, -Z]$ | $\left[x, \frac{1}{2}-x, \frac{1}{2}-z\right]$ | `[6]` |
| 7 | $[Y, X, -Z]$ | $\left[x+\frac{1}{2}, x, \frac{1}{2}-z\right]$ | `[7]` |
| 8 | $[-Y, -X, -Z]$ | $\left[\frac{1}{2}-x, -x, \frac{1}{2}-z\right]$ | `[8]` |
| 9 | $[-X, -Y, -Z]$ | $\left[\frac{1}{2}-x, -x, \frac{1}{2}-z\right]$ | `[9]` |
| 10 | $[X, Y, -Z]$ | $\left[x+\frac{1}{2}, x, \frac{1}{2}-z\right]$ | `[10]` |
| 11 | $[Y, -X, -Z]$ | $\left[x, \frac{1}{2}-x, \frac{1}{2}-z\right]$ | `[11]` |
| 12 | $[-Y, X, -Z]$ | $\left[-x, x+\frac{1}{2}, \frac{1}{2}-z\right]$ | `[12]` |
| 13 | $[X, -Y, Z]$ | $\left[x+\frac{1}{2}, -x, z\right]$ | `[13]` |
| 14 | $[-X, Y, Z]$ | $\left[\frac{1}{2}-x, x, z\right]$ | `[14]` |
| 15 | $[-Y, -X, Z]$ | $\left[-x, \frac{1}{2}-x, z\right]$ | `[15]` |
| 16 | $[Y, X, Z]$ | $\left[x, x+\frac{1}{2}, z\right]$ | `[16]` |

* Wyckoff site: `32m`, site symmetry: `1`

Table 55: Wyckoff bond: `32a@32m`

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

*continued ...*

Table 55

| No. | vector | center | mapping |
|---|---|---|---|
| 7 | $[Y,\, X,\, -Z]$ | $\left[y,\, x,\, \frac{1}{2}-z\right]$ | [7] |
| 8 | $[-Y,\, -X,\, -Z]$ | $\left[-y,\, -x,\, \frac{1}{2}-z\right]$ | [8] |
| 9 | $[-X,\, -Y,\, -Z]$ | $[-x,\, -y,\, -z]$ | [9] |
| 10 | $[X,\, Y,\, -Z]$ | $[x,\, y,\, -z]$ | [10] |
| 11 | $[Y,\, -X,\, -Z]$ | $[y,\, -x,\, -z]$ | [11] |
| 12 | $[-Y,\, X,\, -Z]$ | $[-y,\, x,\, -z]$ | [12] |
| 13 | $[X,\, -Y,\, Z]$ | $\left[x,\, -y,\, z+\frac{1}{2}\right]$ | [13] |
| 14 | $[-X,\, Y,\, Z]$ | $\left[-x,\, y,\, z+\frac{1}{2}\right]$ | [14] |
| 15 | $[-Y,\, -X,\, Z]$ | $\left[-y,\, -x,\, z+\frac{1}{2}\right]$ | [15] |
| 16 | $[Y,\, X,\, Z]$ | $\left[y,\, x,\, z+\frac{1}{2}\right]$ | [16] |