SG No. 121 D_{2d}^{11} $I\bar{4}2m$ [tetragonal]

* plus set: $+[0, 0, 0]$, $+\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$
* Wyckoff site: `2a`, site symmetry: `-42m`

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, 0]$	`[1,2,-3,-4,-5,-6,7,8]`

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

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, 0]$	`[1,-2,-5,6]`
2	$[0, -X, 0]$	$[0, 0, 0]$	`[3,-4,7,-8]`

Table 3: Wyckoff bond: `4c@2a`

No.	vector	center	mapping
1	$[X, X, 0]$	$[0, 0, 0]$	`[1,-2,-7,8]`
2	$[X, -X, 0]$	$[0, 0, 0]$	`[3,-4,-5,6]`

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

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, 0]$	`[1,-5]`
2	$[-X, 0, Z]$	$[0, 0, 0]$	`[2,-6]`
3	$[0, -X, -Z]$	$[0, 0, 0]$	`[3,-8]`
4	$[0, X, -Z]$	$[0, 0, 0]$	`[4,-7]`

Table 5: Wyckoff bond: `8e@2a`

No.	vector	center	mapping
1	$[X, X, Z]$	$[0, 0, 0]$	`[1,8]`
2	$[-X, -X, Z]$	$[0, 0, 0]$	`[2,7]`
3	$[X, -X, -Z]$	$[0, 0, 0]$	`[3,6]`
4	$[-X, X, -Z]$	$[0, 0, 0]$	`[4,5]`

Table 6: Wyckoff bond: `8f@2a`

No.	vector	center	mapping
1	$[X, Y, 0]$	[0, 0, 0]	`[1,-2]`
2	$[Y, -X, 0]$	[0, 0, 0]	`[3,-4]`
3	$[-X, Y, 0]$	[0, 0, 0]	`[5,-6]`
4	$[-Y, -X, 0]$	[0, 0, 0]	`[7,-8]`

Table 7: Wyckoff bond: `16g@2a`

No.	vector	center	mapping
1	$[X, Y, Z]$	[0, 0, 0]	`[1]`
2	$[-X, -Y, Z]$	[0, 0, 0]	`[2]`
3	$[Y, -X, -Z]$	[0, 0, 0]	`[3]`
4	$[-Y, X, -Z]$	[0, 0, 0]	`[4]`
5	$[-X, Y, -Z]$	[0, 0, 0]	`[5]`
6	$[X, -Y, -Z]$	[0, 0, 0]	`[6]`
7	$[-Y, -X, Z]$	[0, 0, 0]	`[7]`
8	$[Y, X, Z]$	[0, 0, 0]	`[8]`

* Wyckoff site: `2b`, site symmetry: `-42m`

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

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

Table 9: Wyckoff bond: `4b@2b`

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

Table 10: Wyckoff bond: `4c@2b`

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

Table 11: Wyckoff bond: `8d@2b`

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

Table 12: Wyckoff bond: `8e@2b`

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

Table 13: Wyckoff bond: `8f@2b`

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

Table 14: Wyckoff bond: `16g@2b`

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

* Wyckoff site: `4c`, site symmetry: `222.`

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

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

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

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

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

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

Table 18: Wyckoff bond: `8d@4c`

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

Table 19: Wyckoff bond: `8e@4c`

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

Table 20: Wyckoff bond: `8f@4c`

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

Table 21: Wyckoff bond: `16g@4c`

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

* Wyckoff site: `4d`, site symmetry: `-4..`

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

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

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

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

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

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[1]`

continued ...

Table 24

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

* Wyckoff site: `4e`, site symmetry: `2.mm`

Table 25: Wyckoff bond: `4a@4e`

No.	vector	center	mapping
1	$[X, X, 0]$	$[0, 0, z]$	`[1,-2,-7,8]`
2	$[X, -X, 0]$	$[0, 0, -z]$	`[3,-4,-5,6]`

Table 26: Wyckoff bond: `4b@4e`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	`[1,2,7,8]`
2	$[0, 0, -Z]$	$[0, 0, -z]$	`[3,4,5,6]`

Table 27: Wyckoff bond: `8c@4e`

No.	vector	center	mapping
1	$[X, X, Z]$	$[0, 0, z]$	`[1,8]`
2	$[-X, -X, Z]$	$[0, 0, z]$	`[2,7]`
3	$[X, -X, -Z]$	$[0, 0, -z]$	`[3,6]`
4	$[-X, X, -Z]$	$[0, 0, -z]$	`[4,5]`

Table 28: Wyckoff bond: `8d@4e`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	`[1,-2]`
2	$[Y, -X, 0]$	$[0, 0, -z]$	`[3,-4]`
3	$[-X, Y, 0]$	$[0, 0, -z]$	`[5,-6]`
4	$[-Y, -X, 0]$	$[0, 0, z]$	`[7,-8]`

Table 29: Wyckoff bond: `16e@4e`

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	$[-X, Y, -Z]$	$[0, 0, -z]$	`[5]`
6	$[X, -Y, -Z]$	$[0, 0, -z]$	`[6]`
7	$[-Y, -X, Z]$	$[0, 0, z]$	`[7]`
8	$[Y, X, Z]$	$[0, 0, z]$	`[8]`

* Wyckoff site: `8f`, site symmetry: `.2.`

Table 30: Wyckoff bond: `8a@8f`

No.	vector	center	mapping
1	$[0, X, Z]$	$[x, 0, 0]$	`[1,-6]`
2	$[0, -X, Z]$	$[-x, 0, 0]$	`[2,-5]`
3	$[X, 0, -Z]$	$[0, -x, 0]$	`[3,-7]`
4	$[-X, 0, -Z]$	$[0, x, 0]$	`[4,-8]`

Table 31: Wyckoff bond: `8b@8f`

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	`[1,6]`
2	$[-X, 0, 0]$	$[-x, 0, 0]$	`[2,5]`
3	$[0, -X, 0]$	$[0, -x, 0]$	`[3,7]`
4	$[0, X, 0]$	$[0, x, 0]$	`[4,8]`

Table 32: Wyckoff bond: `16c@8f`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, 0]$	`[1]`
2	$[-X, -Y, Z]$	$[-x, 0, 0]$	`[2]`
3	$[Y, -X, -Z]$	$[0, -x, 0]$	`[3]`
4	$[-Y, X, -Z]$	$[0, x, 0]$	`[4]`
5	$[-X, Y, -Z]$	$[-x, 0, 0]$	`[5]`
6	$[X, -Y, -Z]$	$[x, 0, 0]$	`[6]`
7	$[-Y, -X, Z]$	$[0, -x, 0]$	`[7]`
8	$[Y, X, Z]$	$[0, x, 0]$	`[8]`

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

Table 33: Wyckoff bond: 8a@8g

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

Table 34: Wyckoff bond: 8b@8g

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

Table 35: Wyckoff bond: 16c@8g

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

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

Table 36: Wyckoff bond: 8a@8h

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	$[-X,\ Y,\ 0]$	$\left[0,\ \frac{1}{2},\ -z\right]$	[5,-6]
4	$[-Y,\ -X,\ 0]$	$\left[\frac{1}{2},\ 0,\ z\right]$	[7,-8]

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

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

Table 38: Wyckoff bond: `16c@8h`

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

* Wyckoff site: `8i`, site symmetry: `..m`

Table 39: Wyckoff bond: `8a@8i`

No.	vector	center	mapping
1	$[X,\ X,\ Z]$	$[x,\ x,\ z]$	`[1,8]`
2	$[-X,\ -X,\ Z]$	$[-x,\ -x,\ z]$	`[2,7]`
3	$[X,\ -X,\ -Z]$	$[x,\ -x,\ -z]$	`[3,6]`
4	$[-X,\ X,\ -Z]$	$[-x,\ x,\ -z]$	`[4,5]`

Table 40: Wyckoff bond: `8b@8i`

No.	vector	center	mapping
1	$[X,\ -X,\ 0]$	$[x,\ x,\ z]$	`[1,-8]`
2	$[-X,\ X,\ 0]$	$[-x,\ -x,\ z]$	`[2,-7]`
3	$[-X,\ -X,\ 0]$	$[x,\ -x,\ -z]$	`[3,-6]`
4	$[X,\ X,\ 0]$	$[-x,\ x,\ -z]$	`[4,-5]`

Table 41: Wyckoff bond: `16c@8i`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, z]$	`[1]`
2	$[-X, -Y, Z]$	$[-x, -x, z]$	`[2]`
3	$[Y, -X, -Z]$	$[x, -x, -z]$	`[3]`
4	$[-Y, X, -Z]$	$[-x, x, -z]$	`[4]`
5	$[-X, Y, -Z]$	$[-x, x, -z]$	`[5]`
6	$[X, -Y, -Z]$	$[x, -x, -z]$	`[6]`
7	$[-Y, -X, Z]$	$[-x, -x, z]$	`[7]`
8	$[Y, X, Z]$	$[x, x, z]$	`[8]`

* Wyckoff site: `16j`, site symmetry: `1`

Table 42: Wyckoff bond: `16a@16j`

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	$[-X, Y, -Z]$	$[-x, y, -z]$	`[5]`
6	$[X, -Y, -Z]$	$[x, -y, -z]$	`[6]`
7	$[-Y, -X, Z]$	$[-y, -x, z]$	`[7]`
8	$[Y, X, Z]$	$[y, x, z]$	`[8]`