SG No. 149 D_3^1 $P312$ [trigonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `1a`, site symmetry: `3.2`

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

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

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

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

Table 3: Wyckoff bond: `3c@1a`

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

Table 4: Wyckoff bond: `6d@1a`

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	$[-Y, -X, -Z]$	$[0, 0, 0]$	`[4]`
5	$[-X+Y, Y, -Z]$	$[0, 0, 0]$	`[5]`
6	$[X, X-Y, -Z]$	$[0, 0, 0]$	`[6]`

* Wyckoff site: `1b`, site symmetry: `3.2`

Table 5: Wyckoff bond: `1a@1b`

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

Table 6: Wyckoff bond: `3b@1b`

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

Table 7: Wyckoff bond: `3c@1b`

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

Table 8: Wyckoff bond: `6d@1b`

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

* Wyckoff site: `1c`, site symmetry: `3.2`

Table 9: Wyckoff bond: `1a@1c`

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

Table 10: Wyckoff bond: `3b@1c`

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

Table 11: Wyckoff bond: `3c@1c`

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

Table 12: Wyckoff bond: `6d@1c`

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	$[-Y, -X, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, 0\right]$	`[4]`
5	$[-X+Y, Y, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, 0\right]$	`[5]`
6	$[X, X-Y, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, 0\right]$	`[6]`

* Wyckoff site: `1d`, site symmetry: `3.2`

Table 13: Wyckoff bond: `1a@1d`

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

Table 14: Wyckoff bond: `3b@1d`

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

Table 15: Wyckoff bond: `3c@1d`

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

Table 16: Wyckoff bond: `6d@1d`

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

* Wyckoff site: `1e`, site symmetry: `3.2`

Table 17: Wyckoff bond: `1a@1e`

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

Table 18: Wyckoff bond: `3b@1e`

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

Table 19: Wyckoff bond: `3c@1e`

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

Table 20: Wyckoff bond: `6d@1e`

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	$[-Y, -X, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[4]`
5	$[-X+Y, Y, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[5]`
6	$[X, X-Y, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[6]`

* Wyckoff site: `1f`, site symmetry: `3.2`

Table 21: Wyckoff bond: `1a@1f`

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

Table 22: Wyckoff bond: `3b@1f`

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

Table 23: Wyckoff bond: `3c@1f`

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

Table 24: Wyckoff bond: `6d@1f`

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

* Wyckoff site: `2g`, site symmetry: `3..`

Table 25: Wyckoff bond: `2a@2g`

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

Table 26: Wyckoff bond: `6b@2g`

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	$[-Y,\ -X,\ -Z]$	$[0,\ 0,\ -z]$	`[4]`
5	$[-X+Y,\ Y,\ -Z]$	$[0,\ 0,\ -z]$	`[5]`
6	$[X,\ X-Y,\ -Z]$	$[0,\ 0,\ -z]$	`[6]`

* Wyckoff site: `2h`, site symmetry: `3..`

Table 27: Wyckoff bond: `2a@2h`

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

Table 28: Wyckoff bond: `6b@2h`

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	$[-Y,\ -X,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ -z\right]$	`[4]`
5	$[-X+Y,\ Y,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ -z\right]$	`[5]`
6	$[X,\ X-Y,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ -z\right]$	`[6]`

* Wyckoff site: `2i`, site symmetry: `3..`

Table 29: Wyckoff bond: `2a@2i`

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

Table 30: Wyckoff bond: `6b@2i`

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]`

continued ...

Table 30

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

* Wyckoff site: `3j`, site symmetry: `..2`

Table 31: Wyckoff bond: `3a@3j`

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

Table 32: Wyckoff bond: `3b@3j`

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

Table 33: Wyckoff bond: `6c@3j`

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	$[-Y,\, -X,\, -Z]$	$[x,\, -x,\, 0]$	`[4]`
5	$[-X+Y,\, Y,\, -Z]$	$[-2x,\, -x,\, 0]$	`[5]`
6	$[X,\, X-Y,\, -Z]$	$[x,\, 2x,\, 0]$	`[6]`

* Wyckoff site: `3k`, site symmetry: `..2`

Table 34: Wyckoff bond: `3a@3k`

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

continued ...

Table 34

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

Table 35: Wyckoff bond: `3b@3k`

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

Table 36: Wyckoff bond: `6c@3k`

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

* Wyckoff site: `6l`, site symmetry: `1`

Table 37: Wyckoff bond: `6a@6l`

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	$[-Y,\, -X,\, -Z]$	$[-y,\, -x,\, -z]$	`[4]`
5	$[-X+Y,\, Y,\, -Z]$	$[-x+y,\, y,\, -z]$	`[5]`
6	$[X,\, X-Y,\, -Z]$	$[x,\, x-y,\, -z]$	`[6]`