SG No. 164 D^3_{3d} $P\bar{3}m1$ [trigonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `1a`, site symmetry: `-3m.`

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	$[X, -X, Z]$	$[0, 0, 0]$	`[1,-4,-7,10]`
2	$[X, 2X, Z]$	$[0, 0, 0]$	`[2,-6,-8,12]`
3	$[-2X, -X, Z]$	$[0, 0, 0]$	`[3,-5,-9,11]`

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

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

Table 4: Wyckoff bond: `6d@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	$[Y, X, -Z]$	$[0, 0, 0]$	`[4,-10]`
5	$[X-Y, -Y, -Z]$	$[0, 0, 0]$	`[5,-11]`
6	$[-X, -X+Y, -Z]$	$[0, 0, 0]$	`[6,-12]`

* Wyckoff site: `1b`, site symmetry: `-3m.`

Table 5: 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 6: Wyckoff bond: `3b@1b`

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

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

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

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

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

* Wyckoff site: `2c`, site symmetry: `3m.`

Table 9: Wyckoff bond: `2a@2c`

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

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

No.	vector	center	mapping
1	$[X, -X, Z]$	$[0, 0, z]$	`[1,10]`
2	$[X, 2X, Z]$	$[0, 0, z]$	`[2,12]`
3	$[-2X, -X, Z]$	$[0, 0, z]$	`[3,11]`
4	$[-X, X, -Z]$	$[0, 0, -z]$	`[4,7]`
5	$[2X, X, -Z]$	$[0, 0, -z]$	`[5,9]`

continued ...

Table 10

No.	vector	center	mapping
6	$[-X, -2X, -Z]$	$[0, 0, -z]$	`[6,8]`

Table 11: Wyckoff bond: `6c@2c`

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

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

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]`
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	$[-Y, -X, Z]$	$[0, 0, z]$	`[10]`
11	$[-X+Y, Y, Z]$	$[0, 0, z]$	`[11]`
12	$[X, X-Y, Z]$	$[0, 0, z]$	`[12]`

* Wyckoff site: `2d`, site symmetry: `3m`.

Table 13: Wyckoff bond: `2a@2d`

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

Table 14: Wyckoff bond: `6b@2d`

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

Table 15: Wyckoff bond: `6c@2d`

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

Table 16: Wyckoff bond: `12d@2d`

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	$[Y, X, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	`[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]`
7	$[-X, -Y, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	`[7]`
8	$[Y, -X+Y, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	`[8]`
9	$[X-Y, X, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	`[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: `3e`, site symmetry: `.2/m.`

Table 17: Wyckoff bond: `3a@3e`

No.	vector	center	mapping
1	$[X, 2X, Z]$	$\left[\frac{1}{2}, 0, 0\right]$	`[1,-5,-7,11]`

continued ...

Table 17

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

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

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

Table 19: Wyckoff bond: `6c@3e`

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

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

Table 20: Wyckoff bond: `3a@3f`

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

Table 21: Wyckoff bond: `3b@3f`

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

Table 22: Wyckoff bond: `6c@3f`

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	$[Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	`[4,-10]`
5	$[X-Y, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	`[5,-11]`
6	$[-X, -X+Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	`[6,-12]`

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

Table 23: Wyckoff bond: `6a@6g`

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

Table 24: Wyckoff bond: `6b@6g`

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

Table 25: Wyckoff bond: `12c@6g`

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

continued ...

Table 25

No.	vector	center	mapping
8	$[Y,\ -X+Y,\ -Z]$	$[0,\ -x,\ 0]$	`[8]`
9	$[X-Y,\ X,\ -Z]$	$[x,\ x,\ 0]$	`[9]`
10	$[-Y,\ -X,\ Z]$	$[0,\ -x,\ 0]$	`[10]`
11	$[-X+Y,\ Y,\ Z]$	$[-x,\ 0,\ 0]$	`[11]`
12	$[X,\ X-Y,\ Z]$	$[x,\ x,\ 0]$	`[12]`

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

Table 26: Wyckoff bond: `6a@6h`

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

Table 27: Wyckoff bond: `6b@6h`

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

Table 28: Wyckoff bond: `12c@6h`

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

continued ...

Table 28

No.	vector	center	mapping
10	$[-Y, -X, Z]$	$\left[0, -x, \frac{1}{2}\right]$	`[10]`
11	$[-X+Y, Y, Z]$	$\left[-x, 0, \frac{1}{2}\right]$	`[11]`
12	$[X, X-Y, Z]$	$\left[x, x, \frac{1}{2}\right]$	`[12]`

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

Table 29: Wyckoff bond: `6a@6i`

No.	vector	center	mapping
1	$[X, -X, Z]$	$[x, -x, z]$	`[1,10]`
2	$[X, 2X, Z]$	$[x, 2x, z]$	`[2,12]`
3	$[-2X, -X, Z]$	$[-2x, -x, z]$	`[3,11]`
4	$[-X, X, -Z]$	$[-x, x, -z]$	`[4,7]`
5	$[2X, X, -Z]$	$[2x, x, -z]$	`[5,9]`
6	$[-X, -2X, -Z]$	$[-x, -2x, -z]$	`[6,8]`

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

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

Table 31: Wyckoff bond: `12c@6i`

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

continued ...

Table 31

No.	vector	center	mapping
12	$[X,\ X-Y,\ Z]$	$[x,\ 2x,\ z]$	[12]

* Wyckoff site: 12j, site symmetry: 1

Table 32: Wyckoff bond: 12a@12j

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]
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	$[-Y,\ -X,\ Z]$	$[-y,\ -x,\ z]$	[10]
11	$[-X+Y,\ Y,\ Z]$	$[-x+y,\ y,\ z]$	[11]
12	$[X,\ X-Y,\ Z]$	$[x,\ x-y,\ z]$	[12]