SG No. 163 D_{3d}^2 $P\bar{3}1c$ [trigonal]

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

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

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

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

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

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

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

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

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

continued ...

Table 4

No.	vector	center	mapping
10	$[Y,\ X,\ Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[10]`
11	$[X-Y,\ -Y,\ Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[11]`
12	$[-X,\ -X+Y,\ Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[12]`

* Wyckoff site: `2b`, site symmetry: `-3..`

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

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

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

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	$[-Y,\ -X,\ -Z]$	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[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: `3.2`

Table 7: Wyckoff bond: `2a@2c`

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	$[0,\ 0,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	`[7,8,9,-10,-11,-12]`

Table 8: Wyckoff bond: `6b@2c`

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

continued ...

Table 8

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

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

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

Table 10: Wyckoff bond: `12d@2c`

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

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

Table 11: Wyckoff bond: `2a@2d`

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

Table 12: Wyckoff bond: `6b@2d`

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

Table 13: Wyckoff bond: `6c@2d`

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

Table 14: Wyckoff bond: `12d@2d`

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

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

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	`[1,2,3]`

continued ...

Table 15

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

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

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

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

Table 17: Wyckoff bond: `4a@4f`

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	$[0,\ 0,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ -z\right]$	`[7,8,9]`
4	$[0,\ 0,\ Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ z+\frac{1}{2}\right]$	`[10,11,12]`

Table 18: Wyckoff bond: `12b@4f`

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	$[-Y,\ -X,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}-z\right]$	`[4]`
5	$[-X+Y,\ Y,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}-z\right]$	`[5]`
6	$[X,\ X-Y,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}-z\right]$	`[6]`
7	$[-X,\ -Y,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ -z\right]$	`[7]`

continued ...

Table 18

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

* Wyckoff site: `6g`, site symmetry: `-1`

Table 19: Wyckoff bond: `6a@6g`

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

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

Table 20: Wyckoff bond: `6a@6h`

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

Table 21: Wyckoff bond: `6b@6h`

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

Table 22: Wyckoff bond: `12c@6h`

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

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

Table 23: Wyckoff bond: `12a@12i`

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