SG No. 165 D_{3d}^4 $P\bar{3}c1$ [trigonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `2a`, site symmetry: `32.`

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

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

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

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

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

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

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

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

continued ...

Table 4

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

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

Table 7: Wyckoff bond: `4a@4c`

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

Table 8: Wyckoff bond: `12b@4c`

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]`

continued ...

Table 8

No.	vector	center	mapping
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: `4d`, site symmetry: `3..`

Table 9: Wyckoff bond: `4a@4d`

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

Table 10: Wyckoff bond: `12b@4d`

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	$[Y,\ X,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{2}-z\right]$	`[4]`
5	$[X-Y,\ -Y,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{2}-z\right]$	`[5]`
6	$[-X,\ -X+Y,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{2}-z\right]$	`[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	$[-Y,\ -X,\ Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ z+\frac{1}{2}\right]$	`[10]`
11	$[-X+Y,\ Y,\ Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ z+\frac{1}{2}\right]$	`[11]`
12	$[X,\ X-Y,\ Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ z+\frac{1}{2}\right]$	`[12]`

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

Table 11: Wyckoff bond: `6a@6e`

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: `6f`, site symmetry: `.2.`

Table 12: Wyckoff bond: `6a@6f`

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

Table 13: Wyckoff bond: `6b@6f`

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

Table 14: Wyckoff bond: `12c@6f`

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

continued ...

Table 14

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

* Wyckoff site: 12g, site symmetry: 1

Table 15: Wyckoff bond: 12a@12g

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]