SG No. 167 D_{3d}^{6} $R\bar{3}c$ [trigonal]

* plus set: $+[0,\,0,\,0]$, $+\left[\frac{2}{3},\,\frac{1}{3},\,\frac{1}{3}\right]$, $+\left[\frac{1}{3},\,\frac{2}{3},\,\frac{2}{3}\right]$
* Wyckoff site: `6a`, site symmetry: `32`

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

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: `18b@6a`

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

Table 3: Wyckoff bond: `18c@6a`

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

Table 4: Wyckoff bond: `36d@6a`

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: `6b`, site symmetry: `-3.`

Table 5: Wyckoff bond: `6a@6b`

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: `18b@6b`

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: `12c`, site symmetry: `3.`

Table 7: Wyckoff bond: `12a@12c`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	`[1,2,3]`
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 8: Wyckoff bond: `36b@12c`

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: `18d`, site symmetry: `-1`

Table 9: Wyckoff bond: `18a@18d`

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: `18e`, site symmetry: `.2`

Table 10: Wyckoff bond: `18a@18e`

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 11: Wyckoff bond: `18b@18e`

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]`

continued ...

Table 11

No.	vector	center	mapping
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 12: Wyckoff bond: `36c@18e`

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]`
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: `36f`, site symmetry: `1`

Table 13: Wyckoff bond: `36a@36f`

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]`