SG No. 157 C_{3v}^{2} $P31m$ [trigonal]

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

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

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

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

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

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

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

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

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: `2b`, site symmetry: `3..`

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

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

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

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]`

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

Table 7: Wyckoff bond: `3a@3c`

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

Table 8: Wyckoff bond: `3b@3c`

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

Table 9: Wyckoff bond: `6c@3c`

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

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

Table 10: Wyckoff bond: `6a@6d`

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]`