PG No. 36 $D_{3d}(1)$ $\bar{3}m$ (-31m setting) [trigonal]

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

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

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

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

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

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

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

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]`

continued ...

Table 4

No.	vector	center	mapping
11	$[X-Y, -Y, Z]$	$[0, 0, z]$	`[11]`
12	$[-X, -X+Y, Z]$	$[0, 0, z]$	`[12]`

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

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

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

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

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

Table 7: Wyckoff bond: `12c@6b`

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

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

Table 8: Wyckoff bond: `6a@6c`

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

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

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

Table 10: Wyckoff bond: `12c@6c`

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]`
7	$[-X, -Y, -Z]$	$[-x, 0, -z]$	`[7]`
8	$[Y, -X+Y, -Z]$	$[0, -x, -z]$	`[8]`
9	$[X-Y, X, -Z]$	$[x, x, -z]$	`[9]`
10	$[Y, X, Z]$	$[0, x, z]$	`[10]`
11	$[X-Y, -Y, Z]$	$[x, 0, z]$	`[11]`
12	$[-X, -X+Y, Z]$	$[-x, -x, z]$	`[12]`

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

Table 11: Wyckoff bond: `12a@12d`

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]`