PG No. 37 $D_{3h}(1)$ $\bar{6}m2$ (-62m setting) [hexagonal]

* 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	[X, 0, $-Z$]	[0, 0, $-z$]	`[4,8]`
5	[0, X, $-Z$]	[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, $2X$, 0]	[0, 0, z]	`[1,-11]`
2	[$-2X$, $-X$, 0]	[0, 0, z]	`[2,-10]`
3	[X, $-X$, 0]	[0, 0, z]	`[3,-12]`
4	[X, $2X$, 0]	[0, 0, $-z$]	`[4,-8]`
5	[$-2X$, $-X$, 0]	[0, 0, $-z$]	`[5,-7]`
6	[X, $-X$, 0]	[0, 0, $-z$]	`[6,-9]`

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	[X, Y, $-Z$]	[0, 0, $-z$]	`[4]`
5	[$-Y$, $X-Y$, $-Z$]	[0, 0, $-z$]	`[5]`
6	[$-X+Y$, $-X$, $-Z$]	[0, 0, $-z$]	`[6]`
7	[Y, X, $-Z$]	[0, 0, $-z$]	`[7]`
8	[$X-Y$, $-Y$, $-Z$]	[0, 0, $-z$]	`[8]`
9	[$-X$, $-X+Y$, $-Z$]	[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: `3b`, site symmetry: `m2m`

Table 5: Wyckoff bond: `3a@3b`

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

Table 6: Wyckoff bond: `3b@3b`

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

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

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

Table 8: Wyckoff bond: `6d@3b`

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

Table 9: Wyckoff bond: `6e@3b`

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

Table 10: Wyckoff bond: `6f@3b`

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

Table 11: Wyckoff bond: `12g@3b`

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

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

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

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, z]$	`[1,11]`

continued ...

Table 12

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

Table 13: 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	$[X, 2X, 0]$	$[x, 0, -z]$	`[4,-8]`
5	$[-2X, -X, 0]$	$[0, x, -z]$	`[5,-7]`
6	$[X, -X, 0]$	$[-x, -x, -z]$	`[6,-9]`

Table 14: 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	$[X, Y, -Z]$	$[x, 0, -z]$	`[4]`
5	$[-Y, X-Y, -Z]$	$[0, x, -z]$	`[5]`
6	$[-X+Y, -X, -Z]$	$[-x, -x, -z]$	`[6]`
7	$[Y, X, -Z]$	$[0, x, -z]$	`[7]`
8	$[X-Y, -Y, -Z]$	$[x, 0, -z]$	`[8]`
9	$[-X, -X+Y, -Z]$	$[-x, -x, -z]$	`[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: `6d`, site symmetry: `m..`

Table 15: Wyckoff bond: `6a@6d`

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

continued ...

Table 15

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

Table 16: Wyckoff bond: `6b@6d`

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

Table 17: Wyckoff bond: `12c@6d`

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

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

Table 18: Wyckoff bond: `12a@12e`

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	$[X, Y, -Z]$	$[x, y, -z]$	`[4]`
5	$[-Y, X-Y, -Z]$	$[-y, x-y, -z]$	`[5]`

continued ...

Table 18

No.	vector	center	mapping
6	$[-X+Y,\ -X,\ -Z]$	$[-x+y,\ -x,\ -z]$	[6]
7	$[Y,\ X,\ -Z]$	$[y,\ x,\ -z]$	[7]
8	$[X-Y,\ -Y,\ -Z]$	$[x-y,\ -y,\ -z]$	[8]
9	$[-X,\ -X+Y,\ -Z]$	$[-x,\ -x+y,\ -z]$	[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]