PG No. 27 D_{6h} $6/mmm$ [hexagonal]

* Wyckoff site: `2a`, site symmetry: `6mm`

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	`[1,2,3,4,5,6,19,20,21,22,23,24]`
2	$[0, 0, -Z]$	$[0, 0, -z]$	`[7,8,9,10,11,12,13,14,15,16,17,18]`

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

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[0, 0, z]$	`[1,-4,20,-23]`
2	$[-2X, -X, 0]$	$[0, 0, z]$	`[2,-5,19,-22]`
3	$[X, -X, 0]$	$[0, 0, z]$	`[3,-6,21,-24]`
4	$[2X, X, 0]$	$[0, 0, -z]$	`[7,-10,14,-17]`
5	$[-X, -2X, 0]$	$[0, 0, -z]$	`[8,-11,13,-16]`
6	$[-X, X, 0]$	$[0, 0, -z]$	`[9,-12,15,-18]`

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

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, z]$	`[1,-4,-20,23]`
2	$[0, X, 0]$	$[0, 0, z]$	`[2,-5,-19,22]`
3	$[-X, -X, 0]$	$[0, 0, z]$	`[3,-6,-21,24]`
4	$[0, X, 0]$	$[0, 0, -z]$	`[7,-10,-14,17]`
5	$[X, 0, 0]$	$[0, 0, -z]$	`[8,-11,-13,16]`
6	$[-X, -X, 0]$	$[0, 0, -z]$	`[9,-12,-15,18]`

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

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	`[1,-4]`
2	$[-Y, X-Y, 0]$	$[0, 0, z]$	`[2,-5]`
3	$[-X+Y, -X, 0]$	$[0, 0, z]$	`[3,-6]`
4	$[Y, X, 0]$	$[0, 0, -z]$	`[7,-10]`
5	$[X-Y, -Y, 0]$	$[0, 0, -z]$	`[8,-11]`
6	$[-X, -X+Y, 0]$	$[0, 0, -z]$	`[9,-12]`
7	$[-X, -Y, 0]$	$[0, 0, -z]$	`[13,-16]`
8	$[Y, -X+Y, 0]$	$[0, 0, -z]$	`[14,-17]`
9	$[X-Y, X, 0]$	$[0, 0, -z]$	`[15,-18]`
10	$[-Y, -X, 0]$	$[0, 0, z]$	`[19,-22]`

continued ...

Table 4

No.	vector	center	mapping
11	$[-X+Y,\ Y,\ 0]$	$[0,\ 0,\ z]$	`[20,-23]`
12	$[X,\ X-Y,\ 0]$	$[0,\ 0,\ z]$	`[21,-24]`

Table 5: Wyckoff bond: `12e@2a`

No.	vector	center	mapping
1	$[X,\ 2X,\ Z]$	$[0,\ 0,\ z]$	`[1,20]`
2	$[-2X,\ -X,\ Z]$	$[0,\ 0,\ z]$	`[2,19]`
3	$[X,\ -X,\ Z]$	$[0,\ 0,\ z]$	`[3,21]`
4	$[-X,\ -2X,\ Z]$	$[0,\ 0,\ z]$	`[4,23]`
5	$[2X,\ X,\ Z]$	$[0,\ 0,\ z]$	`[5,22]`
6	$[-X,\ X,\ Z]$	$[0,\ 0,\ z]$	`[6,24]`
7	$[2X,\ X,\ -Z]$	$[0,\ 0,\ -z]$	`[7,14]`
8	$[-X,\ -2X,\ -Z]$	$[0,\ 0,\ -z]$	`[8,13]`
9	$[-X,\ X,\ -Z]$	$[0,\ 0,\ -z]$	`[9,15]`
10	$[-2X,\ -X,\ -Z]$	$[0,\ 0,\ -z]$	`[10,17]`
11	$[X,\ 2X,\ -Z]$	$[0,\ 0,\ -z]$	`[11,16]`
12	$[X,\ -X,\ -Z]$	$[0,\ 0,\ -z]$	`[12,18]`

Table 6: Wyckoff bond: `12f@2a`

No.	vector	center	mapping
1	$[X,\ 0,\ Z]$	$[0,\ 0,\ z]$	`[1,23]`
2	$[0,\ X,\ Z]$	$[0,\ 0,\ z]$	`[2,22]`
3	$[-X,\ -X,\ Z]$	$[0,\ 0,\ z]$	`[3,24]`
4	$[-X,\ 0,\ Z]$	$[0,\ 0,\ z]$	`[4,20]`
5	$[0,\ -X,\ Z]$	$[0,\ 0,\ z]$	`[5,19]`
6	$[X,\ X,\ Z]$	$[0,\ 0,\ z]$	`[6,21]`
7	$[0,\ X,\ -Z]$	$[0,\ 0,\ -z]$	`[7,17]`
8	$[X,\ 0,\ -Z]$	$[0,\ 0,\ -z]$	`[8,16]`
9	$[-X,\ -X,\ -Z]$	$[0,\ 0,\ -z]$	`[9,18]`
10	$[0,\ -X,\ -Z]$	$[0,\ 0,\ -z]$	`[10,14]`
11	$[-X,\ 0,\ -Z]$	$[0,\ 0,\ -z]$	`[11,13]`
12	$[X,\ X,\ -Z]$	$[0,\ 0,\ -z]$	`[12,15]`

Table 7: Wyckoff bond: `24g@2a`

No.	vector	center	mapping
1	$[X,\ Y,\ Z]$	$[0,\ 0,\ z]$	`[1]`

continued ...

Table 7

No.	vector	center	mapping
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]`
11	$[-X+Y, Y, -Z]$	$[0, 0, -z]$	`[11]`
12	$[X, X-Y, -Z]$	$[0, 0, -z]$	`[12]`
13	$[-X, -Y, -Z]$	$[0, 0, -z]$	`[13]`
14	$[Y, -X+Y, -Z]$	$[0, 0, -z]$	`[14]`
15	$[X-Y, X, -Z]$	$[0, 0, -z]$	`[15]`
16	$[X, Y, -Z]$	$[0, 0, -z]$	`[16]`
17	$[-Y, X-Y, -Z]$	$[0, 0, -z]$	`[17]`
18	$[-X+Y, -X, -Z]$	$[0, 0, -z]$	`[18]`
19	$[-Y, -X, Z]$	$[0, 0, z]$	`[19]`
20	$[-X+Y, Y, Z]$	$[0, 0, z]$	`[20]`
21	$[X, X-Y, Z]$	$[0, 0, z]$	`[21]`
22	$[Y, X, Z]$	$[0, 0, z]$	`[22]`
23	$[X-Y, -Y, Z]$	$[0, 0, z]$	`[23]`
24	$[-X, -X+Y, Z]$	$[0, 0, z]$	`[24]`

* Wyckoff site: `6b`, site symmetry: `m2m`

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

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[x, 0, 0]$	`[1,-8,16,-23]`
2	$[-2X, -X, 0]$	$[0, x, 0]$	`[2,-7,17,-22]`
3	$[X, -X, 0]$	$[-x, -x, 0]$	`[3,-9,18,-24]`
4	$[-X, -2X, 0]$	$[-x, 0, 0]$	`[4,-11,13,-20]`
5	$[2X, X, 0]$	$[0, -x, 0]$	`[5,-10,14,-19]`
6	$[-X, X, 0]$	$[x, x, 0]$	`[6,-12,15,-21]`

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

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	`[1,8,16,23]`
2	$[0, X, 0]$	$[0, x, 0]$	`[2,7,17,22]`
3	$[-X, -X, 0]$	$[-x, -x, 0]$	`[3,9,18,24]`

continued ...

Table 9

No.	vector	center	mapping
4	$[-X, 0, 0]$	$[-x, 0, 0]$	`[4,11,13,20]`
5	$[0, -X, 0]$	$[0, -x, 0]$	`[5,10,14,19]`
6	$[X, X, 0]$	$[x, x, 0]$	`[6,12,15,21]`

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, 0, 0]$	`[1,-8,-16,23]`
2	$[0, 0, Z]$	$[0, x, 0]$	`[2,-7,-17,22]`
3	$[0, 0, Z]$	$[-x, -x, 0]$	`[3,-9,-18,24]`
4	$[0, 0, Z]$	$[-x, 0, 0]$	`[4,-11,-13,20]`
5	$[0, 0, Z]$	$[0, -x, 0]$	`[5,-10,-14,19]`
6	$[0, 0, Z]$	$[x, x, 0]$	`[6,-12,-15,21]`

Table 11: Wyckoff bond: `12d@6b`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, 0, 0]$	`[1,16]`
2	$[-Y, X-Y, 0]$	$[0, x, 0]$	`[2,17]`
3	$[-X+Y, -X, 0]$	$[-x, -x, 0]$	`[3,18]`
4	$[-X, -Y, 0]$	$[-x, 0, 0]$	`[4,13]`
5	$[Y, -X+Y, 0]$	$[0, -x, 0]$	`[5,14]`
6	$[X-Y, X, 0]$	$[x, x, 0]$	`[6,15]`
7	$[Y, X, 0]$	$[0, x, 0]$	`[7,22]`
8	$[X-Y, -Y, 0]$	$[x, 0, 0]$	`[8,23]`
9	$[-X, -X+Y, 0]$	$[-x, -x, 0]$	`[9,24]`
10	$[-Y, -X, 0]$	$[0, -x, 0]$	`[10,19]`
11	$[-X+Y, Y, 0]$	$[-x, 0, 0]$	`[11,20]`
12	$[X, X-Y, 0]$	$[x, x, 0]$	`[12,21]`

Table 12: Wyckoff bond: `12e@6b`

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]`

continued ...

Table 12

No.	vector	center	mapping
7	$[-X, -2X, -Z]$	$[-x, 0, 0]$	`[13,-20]`
8	$[2X, X, -Z]$	$[0, -x, 0]$	`[14,-19]`
9	$[-X, X, -Z]$	$[x, x, 0]$	`[15,-21]`
10	$[X, 2X, -Z]$	$[x, 0, 0]$	`[16,-23]`
11	$[-2X, -X, -Z]$	$[0, x, 0]$	`[17,-22]`
12	$[X, -X, -Z]$	$[-x, -x, 0]$	`[18,-24]`

Table 13: Wyckoff bond: `12f@6b`

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, 0]$	`[1,23]`
2	$[0, X, Z]$	$[0, x, 0]$	`[2,22]`
3	$[-X, -X, Z]$	$[-x, -x, 0]$	`[3,24]`
4	$[-X, 0, Z]$	$[-x, 0, 0]$	`[4,20]`
5	$[0, -X, Z]$	$[0, -x, 0]$	`[5,19]`
6	$[X, X, Z]$	$[x, x, 0]$	`[6,21]`
7	$[0, X, -Z]$	$[0, x, 0]$	`[7,17]`
8	$[X, 0, -Z]$	$[x, 0, 0]$	`[8,16]`
9	$[-X, -X, -Z]$	$[-x, -x, 0]$	`[9,18]`
10	$[0, -X, -Z]$	$[0, -x, 0]$	`[10,14]`
11	$[-X, 0, -Z]$	$[-x, 0, 0]$	`[11,13]`
12	$[X, X, -Z]$	$[x, x, 0]$	`[12,15]`

Table 14: Wyckoff bond: `24g@6b`

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]`
13	$[-X, -Y, -Z]$	$[-x, 0, 0]$	`[13]`
14	$[Y, -X+Y, -Z]$	$[0, -x, 0]$	`[14]`
15	$[X-Y, X, -Z]$	$[x, x, 0]$	`[15]`
16	$[X, Y, -Z]$	$[x, 0, 0]$	`[16]`

continued ...

Table 14

No.	vector	center	mapping
17	$[-Y, X-Y, -Z]$	$[0, x, 0]$	`[17]`
18	$[-X+Y, -X, -Z]$	$[-x, -x, 0]$	`[18]`
19	$[-Y, -X, Z]$	$[0, -x, 0]$	`[19]`
20	$[-X+Y, Y, Z]$	$[-x, 0, 0]$	`[20]`
21	$[X, X-Y, Z]$	$[x, x, 0]$	`[21]`
22	$[Y, X, Z]$	$[0, x, 0]$	`[22]`
23	$[X-Y, -Y, Z]$	$[x, 0, 0]$	`[23]`
24	$[-X, -X+Y, Z]$	$[-x, -x, 0]$	`[24]`

* Wyckoff site: `6c`, site symmetry: `mm2`

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

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[x, 2x, 0]$	`[1,11,16,20]`
2	$[-2X, -X, 0]$	$[-2x, -x, 0]$	`[2,10,17,19]`
3	$[X, -X, 0]$	$[x, -x, 0]$	`[3,12,18,21]`
4	$[-X, -2X, 0]$	$[-x, -2x, 0]$	`[4,8,13,23]`
5	$[2X, X, 0]$	$[2x, x, 0]$	`[5,7,14,22]`
6	$[-X, X, 0]$	$[-x, x, 0]$	`[6,9,15,24]`

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

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 2x, 0]$	`[1,-11,16,-20]`
2	$[0, X, 0]$	$[-2x, -x, 0]$	`[2,-10,17,-19]`
3	$[-X, -X, 0]$	$[x, -x, 0]$	`[3,-12,18,-21]`
4	$[-X, 0, 0]$	$[-x, -2x, 0]$	`[4,-8,13,-23]`
5	$[0, -X, 0]$	$[2x, x, 0]$	`[5,-7,14,-22]`
6	$[X, X, 0]$	$[-x, x, 0]$	`[6,-9,15,-24]`

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, 2x, 0]$	`[1,-11,-16,20]`
2	$[0, 0, Z]$	$[-2x, -x, 0]$	`[2,-10,-17,19]`
3	$[0, 0, Z]$	$[x, -x, 0]$	`[3,-12,-18,21]`
4	$[0, 0, Z]$	$[-x, -2x, 0]$	`[4,-8,-13,23]`
5	$[0, 0, Z]$	$[2x, x, 0]$	`[5,-7,-14,22]`
6	$[0, 0, Z]$	$[-x, x, 0]$	`[6,-9,-15,24]`

Table 18: Wyckoff bond: `12d@6c`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, 2x, 0]$	`[1,16]`
2	$[-Y, X-Y, 0]$	$[-2x, -x, 0]$	`[2,17]`
3	$[-X+Y, -X, 0]$	$[x, -x, 0]$	`[3,18]`
4	$[-X, -Y, 0]$	$[-x, -2x, 0]$	`[4,13]`
5	$[Y, -X+Y, 0]$	$[2x, x, 0]$	`[5,14]`
6	$[X-Y, X, 0]$	$[-x, x, 0]$	`[6,15]`
7	$[Y, X, 0]$	$[2x, x, 0]$	`[7,22]`
8	$[X-Y, -Y, 0]$	$[-x, -2x, 0]$	`[8,23]`
9	$[-X, -X+Y, 0]$	$[-x, x, 0]$	`[9,24]`
10	$[-Y, -X, 0]$	$[-2x, -x, 0]$	`[10,19]`
11	$[-X+Y, Y, 0]$	$[x, 2x, 0]$	`[11,20]`
12	$[X, X-Y, 0]$	$[x, -x, 0]$	`[12,21]`

Table 19: Wyckoff bond: `12e@6c`

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[x, 2x, 0]$	`[1,20]`
2	$[-2X, -X, Z]$	$[-2x, -x, 0]$	`[2,19]`
3	$[X, -X, Z]$	$[x, -x, 0]$	`[3,21]`
4	$[-X, -2X, Z]$	$[-x, -2x, 0]$	`[4,23]`
5	$[2X, X, Z]$	$[2x, x, 0]$	`[5,22]`
6	$[-X, X, Z]$	$[-x, x, 0]$	`[6,24]`
7	$[2X, X, -Z]$	$[2x, x, 0]$	`[7,14]`
8	$[-X, -2X, -Z]$	$[-x, -2x, 0]$	`[8,13]`
9	$[-X, X, -Z]$	$[-x, x, 0]$	`[9,15]`
10	$[-2X, -X, -Z]$	$[-2x, -x, 0]$	`[10,17]`
11	$[X, 2X, -Z]$	$[x, 2x, 0]$	`[11,16]`
12	$[X, -X, -Z]$	$[x, -x, 0]$	`[12,18]`

Table 20: Wyckoff bond: `12f@6c`

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 2x, 0]$	`[1,-11]`
2	$[0, X, Z]$	$[-2x, -x, 0]$	`[2,-10]`
3	$[-X, -X, Z]$	$[x, -x, 0]$	`[3,-12]`
4	$[-X, 0, Z]$	$[-x, -2x, 0]$	`[4,-8]`
5	$[0, -X, Z]$	$[2x, x, 0]$	`[5,-7]`
6	$[X, X, Z]$	$[-x, x, 0]$	`[6,-9]`
7	$[-X, 0, -Z]$	$[-x, -2x, 0]$	`[13,-23]`

continued ...

Table 20

No.	vector	center	mapping
8	$[0, -X, -Z]$	$[2x, x, 0]$	`[14,-22]`
9	$[X, X, -Z]$	$[-x, x, 0]$	`[15,-24]`
10	$[X, 0, -Z]$	$[x, 2x, 0]$	`[16,-20]`
11	$[0, X, -Z]$	$[-2x, -x, 0]$	`[17,-19]`
12	$[-X, -X, -Z]$	$[x, -x, 0]$	`[18,-21]`

Table 21: Wyckoff bond: `24g@6c`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 2x, 0]$	`[1]`
2	$[-Y, X-Y, Z]$	$[-2x, -x, 0]$	`[2]`
3	$[-X+Y, -X, Z]$	$[x, -x, 0]$	`[3]`
4	$[-X, -Y, Z]$	$[-x, -2x, 0]$	`[4]`
5	$[Y, -X+Y, Z]$	$[2x, x, 0]$	`[5]`
6	$[X-Y, X, Z]$	$[-x, x, 0]$	`[6]`
7	$[Y, X, -Z]$	$[2x, x, 0]$	`[7]`
8	$[X-Y, -Y, -Z]$	$[-x, -2x, 0]$	`[8]`
9	$[-X, -X+Y, -Z]$	$[-x, x, 0]$	`[9]`
10	$[-Y, -X, -Z]$	$[-2x, -x, 0]$	`[10]`
11	$[-X+Y, Y, -Z]$	$[x, 2x, 0]$	`[11]`
12	$[X, X-Y, -Z]$	$[x, -x, 0]$	`[12]`
13	$[-X, -Y, -Z]$	$[-x, -2x, 0]$	`[13]`
14	$[Y, -X+Y, -Z]$	$[2x, x, 0]$	`[14]`
15	$[X-Y, X, -Z]$	$[-x, x, 0]$	`[15]`
16	$[X, Y, -Z]$	$[x, 2x, 0]$	`[16]`
17	$[-Y, X-Y, -Z]$	$[-2x, -x, 0]$	`[17]`
18	$[-X+Y, -X, -Z]$	$[x, -x, 0]$	`[18]`
19	$[-Y, -X, Z]$	$[-2x, -x, 0]$	`[19]`
20	$[-X+Y, Y, Z]$	$[x, 2x, 0]$	`[20]`
21	$[X, X-Y, Z]$	$[x, -x, 0]$	`[21]`
22	$[Y, X, Z]$	$[2x, x, 0]$	`[22]`
23	$[X-Y, -Y, Z]$	$[-x, -2x, 0]$	`[23]`
24	$[-X, -X+Y, Z]$	$[-x, x, 0]$	`[24]`

* Wyckoff site: `12d`, site symmetry: `..m`

Table 22: Wyckoff bond: `12a@12d`

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, z]$	`[1,23]`
2	$[0, X, Z]$	$[0, x, z]$	`[2,22]`
3	$[-X, -X, Z]$	$[-x, -x, z]$	`[3,24]`

continued ...

Table 22

No.	vector	center	mapping
4	$[-X, 0, Z]$	$[-x, 0, z]$	[4,20]
5	$[0, -X, Z]$	$[0, -x, z]$	[5,19]
6	$[X, X, Z]$	$[x, x, z]$	[6,21]
7	$[0, X, -Z]$	$[0, x, -z]$	[7,17]
8	$[X, 0, -Z]$	$[x, 0, -z]$	[8,16]
9	$[-X, -X, -Z]$	$[-x, -x, -z]$	[9,18]
10	$[0, -X, -Z]$	$[0, -x, -z]$	[10,14]
11	$[-X, 0, -Z]$	$[-x, 0, -z]$	[11,13]
12	$[X, X, -Z]$	$[x, x, -z]$	[12,15]

Table 23: Wyckoff bond: 12b@12d

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[x, 0, z]$	[1,-23]
2	$[-2X, -X, 0]$	$[0, x, z]$	[2,-22]
3	$[X, -X, 0]$	$[-x, -x, z]$	[3,-24]
4	$[-X, -2X, 0]$	$[-x, 0, z]$	[4,-20]
5	$[2X, X, 0]$	$[0, -x, z]$	[5,-19]
6	$[-X, X, 0]$	$[x, x, z]$	[6,-21]
7	$[2X, X, 0]$	$[0, x, -z]$	[7,-17]
8	$[-X, -2X, 0]$	$[x, 0, -z]$	[8,-16]
9	$[-X, X, 0]$	$[-x, -x, -z]$	[9,-18]
10	$[-2X, -X, 0]$	$[0, -x, -z]$	[10,-14]
11	$[X, 2X, 0]$	$[-x, 0, -z]$	[11,-13]
12	$[X, -X, 0]$	$[x, x, -z]$	[12,-15]

Table 24: Wyckoff bond: 24c@12d

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]
13	$[-X, -Y, -Z]$	$[-x, 0, -z]$	[13]

continued ...

Table 24

No.	vector	center	mapping
14	$[Y, -X+Y, -Z]$	$[0, -x, -z]$	[14]
15	$[X-Y, X, -Z]$	$[x, x, -z]$	[15]
16	$[X, Y, -Z]$	$[x, 0, -z]$	[16]
17	$[-Y, X-Y, -Z]$	$[0, x, -z]$	[17]
18	$[-X+Y, -X, -Z]$	$[-x, -x, -z]$	[18]
19	$[-Y, -X, Z]$	$[0, -x, z]$	[19]
20	$[-X+Y, Y, Z]$	$[-x, 0, z]$	[20]
21	$[X, X-Y, Z]$	$[x, x, z]$	[21]
22	$[Y, X, Z]$	$[0, x, z]$	[22]
23	$[X-Y, -Y, Z]$	$[x, 0, z]$	[23]
24	$[-X, -X+Y, Z]$	$[-x, -x, z]$	[24]

* Wyckoff site: 12e, site symmetry: .m.

Table 25: Wyckoff bond: 12a@12e

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[x, 2x, z]$	[1,20]
2	$[-2X, -X, Z]$	$[-2x, -x, z]$	[2,19]
3	$[X, -X, Z]$	$[x, -x, z]$	[3,21]
4	$[-X, -2X, Z]$	$[-x, -2x, z]$	[4,23]
5	$[2X, X, Z]$	$[2x, x, z]$	[5,22]
6	$[-X, X, Z]$	$[-x, x, z]$	[6,24]
7	$[2X, X, -Z]$	$[2x, x, -z]$	[7,14]
8	$[-X, -2X, -Z]$	$[-x, -2x, -z]$	[8,13]
9	$[-X, X, -Z]$	$[-x, x, -z]$	[9,15]
10	$[-2X, -X, -Z]$	$[-2x, -x, -z]$	[10,17]
11	$[X, 2X, -Z]$	$[x, 2x, -z]$	[11,16]
12	$[X, -X, -Z]$	$[x, -x, -z]$	[12,18]

Table 26: Wyckoff bond: 12b@12e

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 2x, z]$	[1,-20]
2	$[0, X, 0]$	$[-2x, -x, z]$	[2,-19]
3	$[-X, -X, 0]$	$[x, -x, z]$	[3,-21]
4	$[-X, 0, 0]$	$[-x, -2x, z]$	[4,-23]
5	$[0, -X, 0]$	$[2x, x, z]$	[5,-22]
6	$[X, X, 0]$	$[-x, x, z]$	[6,-24]
7	$[0, X, 0]$	$[2x, x, -z]$	[7,-14]
8	$[X, 0, 0]$	$[-x, -2x, -z]$	[8,-13]
9	$[-X, -X, 0]$	$[-x, x, -z]$	[9,-15]

continued ...

Table 26

No.	vector	center	mapping
10	$[0, -X, 0]$	$[-2x, -x, -z]$	`[10,-17]`
11	$[-X, 0, 0]$	$[x, 2x, -z]$	`[11,-16]`
12	$[X, X, 0]$	$[x, -x, -z]$	`[12,-18]`

Table 27: Wyckoff bond: `24c@12e`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 2x, z]$	`[1]`
2	$[-Y, X-Y, Z]$	$[-2x, -x, z]$	`[2]`
3	$[-X+Y, -X, Z]$	$[x, -x, z]$	`[3]`
4	$[-X, -Y, Z]$	$[-x, -2x, z]$	`[4]`
5	$[Y, -X+Y, Z]$	$[2x, x, z]$	`[5]`
6	$[X-Y, X, Z]$	$[-x, x, z]$	`[6]`
7	$[Y, X, -Z]$	$[2x, x, -z]$	`[7]`
8	$[X-Y, -Y, -Z]$	$[-x, -2x, -z]$	`[8]`
9	$[-X, -X+Y, -Z]$	$[-x, x, -z]$	`[9]`
10	$[-Y, -X, -Z]$	$[-2x, -x, -z]$	`[10]`
11	$[-X+Y, Y, -Z]$	$[x, 2x, -z]$	`[11]`
12	$[X, X-Y, -Z]$	$[x, -x, -z]$	`[12]`
13	$[-X, -Y, -Z]$	$[-x, -2x, -z]$	`[13]`
14	$[Y, -X+Y, -Z]$	$[2x, x, -z]$	`[14]`
15	$[X-Y, X, -Z]$	$[-x, x, -z]$	`[15]`
16	$[X, Y, -Z]$	$[x, 2x, -z]$	`[16]`
17	$[-Y, X-Y, -Z]$	$[-2x, -x, -z]$	`[17]`
18	$[-X+Y, -X, -Z]$	$[x, -x, -z]$	`[18]`
19	$[-Y, -X, Z]$	$[-2x, -x, z]$	`[19]`
20	$[-X+Y, Y, Z]$	$[x, 2x, z]$	`[20]`
21	$[X, X-Y, Z]$	$[x, -x, z]$	`[21]`
22	$[Y, X, Z]$	$[2x, x, z]$	`[22]`
23	$[X-Y, -Y, Z]$	$[-x, -2x, z]$	`[23]`
24	$[-X, -X+Y, Z]$	$[-x, x, z]$	`[24]`

* Wyckoff site: `12f`, site symmetry: `m..`

Table 28: Wyckoff bond: `12a@12f`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, y, 0]$	`[1,16]`
2	$[-Y, X-Y, 0]$	$[-y, x-y, 0]$	`[2,17]`
3	$[-X+Y, -X, 0]$	$[-x+y, -x, 0]$	`[3,18]`
4	$[-X, -Y, 0]$	$[-x, -y, 0]$	`[4,13]`
5	$[Y, -X+Y, 0]$	$[y, -x+y, 0]$	`[5,14]`

continued ...

Table 28

No.	vector	center	mapping
6	$[X-Y,\ X,\ 0]$	$[x-y,\ x,\ 0]$	`[6,15]`
7	$[Y,\ X,\ 0]$	$[y,\ x,\ 0]$	`[7,22]`
8	$[X-Y,\ -Y,\ 0]$	$[x-y,\ -y,\ 0]$	`[8,23]`
9	$[-X,\ -X+Y,\ 0]$	$[-x,\ -x+y,\ 0]$	`[9,24]`
10	$[-Y,\ -X,\ 0]$	$[-y,\ -x,\ 0]$	`[10,19]`
11	$[-X+Y,\ Y,\ 0]$	$[-x+y,\ y,\ 0]$	`[11,20]`
12	$[X,\ X-Y,\ 0]$	$[x,\ x-y,\ 0]$	`[12,21]`

Table 29: Wyckoff bond: `12b@12f`

No.	vector	center	mapping
1	$[0,\ 0,\ Z]$	$[x,\ y,\ 0]$	`[1,-16]`
2	$[0,\ 0,\ Z]$	$[-y,\ x-y,\ 0]$	`[2,-17]`
3	$[0,\ 0,\ Z]$	$[-x+y,\ -x,\ 0]$	`[3,-18]`
4	$[0,\ 0,\ Z]$	$[-x,\ -y,\ 0]$	`[4,-13]`
5	$[0,\ 0,\ Z]$	$[y,\ -x+y,\ 0]$	`[5,-14]`
6	$[0,\ 0,\ Z]$	$[x-y,\ x,\ 0]$	`[6,-15]`
7	$[0,\ 0,\ -Z]$	$[y,\ x,\ 0]$	`[7,-22]`
8	$[0,\ 0,\ -Z]$	$[x-y,\ -y,\ 0]$	`[8,-23]`
9	$[0,\ 0,\ -Z]$	$[-x,\ -x+y,\ 0]$	`[9,-24]`
10	$[0,\ 0,\ -Z]$	$[-y,\ -x,\ 0]$	`[10,-19]`
11	$[0,\ 0,\ -Z]$	$[-x+y,\ y,\ 0]$	`[11,-20]`
12	$[0,\ 0,\ -Z]$	$[x,\ x-y,\ 0]$	`[12,-21]`

Table 30: Wyckoff bond: `24c@12f`

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]`
13	$[-X,\ -Y,\ -Z]$	$[-x,\ -y,\ 0]$	`[13]`
14	$[Y,\ -X+Y,\ -Z]$	$[y,\ -x+y,\ 0]$	`[14]`
15	$[X-Y,\ X,\ -Z]$	$[x-y,\ x,\ 0]$	`[15]`

continued ...

Table 30

No.	vector	center	mapping
16	$[X, Y, -Z]$	$[x, y, 0]$	[16]
17	$[-Y, X-Y, -Z]$	$[-y, x-y, 0]$	[17]
18	$[-X+Y, -X, -Z]$	$[-x+y, -x, 0]$	[18]
19	$[-Y, -X, Z]$	$[-y, -x, 0]$	[19]
20	$[-X+Y, Y, Z]$	$[-x+y, y, 0]$	[20]
21	$[X, X-Y, Z]$	$[x, x-y, 0]$	[21]
22	$[Y, X, Z]$	$[y, x, 0]$	[22]
23	$[X-Y, -Y, Z]$	$[x-y, -y, 0]$	[23]
24	$[-X, -X+Y, Z]$	$[-x, -x+y, 0]$	[24]

* Wyckoff site: 24g, site symmetry: 1

Table 31: Wyckoff bond: 24a@24g

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]
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]
13	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[13]
14	$[Y, -X+Y, -Z]$	$[y, -x+y, -z]$	[14]
15	$[X-Y, X, -Z]$	$[x-y, x, -z]$	[15]
16	$[X, Y, -Z]$	$[x, y, -z]$	[16]
17	$[-Y, X-Y, -Z]$	$[-y, x-y, -z]$	[17]
18	$[-X+Y, -X, -Z]$	$[-x+y, -x, -z]$	[18]
19	$[-Y, -X, Z]$	$[-y, -x, z]$	[19]
20	$[-X+Y, Y, Z]$	$[-x+y, y, z]$	[20]
21	$[X, X-Y, Z]$	$[x, x-y, z]$	[21]
22	$[Y, X, Z]$	$[y, x, z]$	[22]
23	$[X-Y, -Y, Z]$	$[x-y, -y, z]$	[23]
24	$[-X, -X+Y, Z]$	$[-x, -x+y, z]$	[24]