PG No. 20 D_{3d} $\bar{3}m$ (-3m1 setting) [trigonal]

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

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

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

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

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

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

Table 7: Wyckoff bond: `12c@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	$[Y, X, -Z]$	$[0, x, 0]$	`[4]`
5	$[X-Y, -Y, -Z]$	$[x, 0, 0]$	`[5]`
6	$[-X, -X+Y, -Z]$	$[-x, -x, 0]$	`[6]`
7	$[-X, -Y, -Z]$	$[-x, 0, 0]$	`[7]`
8	$[Y, -X+Y, -Z]$	$[0, -x, 0]$	`[8]`
9	$[X-Y, X, -Z]$	$[x, x, 0]$	`[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 8: Wyckoff bond: 6a@6c

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

Table 9: Wyckoff bond: 6b@6c

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

Table 10: Wyckoff bond: 12c@6c

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