PG No. 13 C_{4v} $4mm$ [tetragonal]

* Wyckoff site: `1a`, site symmetry: `4mm`

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

No.	vector	center	mapping
1	[0, 0, Z]	[0, 0, z]	`[1,2,3,4,5,6,7,8]`

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

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

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

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

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

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

Table 5: Wyckoff bond: `4e@1a`

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

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

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

Table 7: Wyckoff bond: `8g@1a`

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

* Wyckoff site: `4b`, site symmetry: `..m`

Table 8: Wyckoff bond: `4a@4b`

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

Table 9: Wyckoff bond: `4b@4b`

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

Table 10: Wyckoff bond: `8c@4b`

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

* Wyckoff site: `4c`, site symmetry: `.m.`

Table 11: Wyckoff bond: `4a@4c`

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

Table 12: Wyckoff bond: `4b@4c`

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

Table 13: Wyckoff bond: `8c@4c`

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

* Wyckoff site: 8d, site symmetry: 1

Table 14: Wyckoff bond: 8a@8d

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, z]$	[2]
3	$[-Y, X, Z]$	$[-y, x, z]$	[3]
4	$[Y, -X, Z]$	$[y, -x, z]$	[4]
5	$[X, -Y, Z]$	$[x, -y, z]$	[5]
6	$[-X, Y, Z]$	$[-x, y, z]$	[6]
7	$[-Y, -X, Z]$	$[-y, -x, z]$	[7]
8	$[Y, X, Z]$	$[y, x, z]$	[8]