PG No. 14 D_{2d} $\bar{4}2m$ (-42m setting) [tetragonal]

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

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

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

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

Table 3: Wyckoff bond: `4c@2a`

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

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 5: Wyckoff bond: `8e@2a`

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]`

continued ...

Table 5

No.	vector	center	mapping
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: `.2.`

Table 6: Wyckoff bond: `4a@4b`

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

Table 7: Wyckoff bond: `4b@4b`

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

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

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

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

Table 9: Wyckoff bond: `4a@4c`

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

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 11: Wyckoff bond: `8c@4c`

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: `8d`, site symmetry: `1`

Table 12: 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]`