SG No. 81 S_4^1 $P\bar{4}$ [tetragonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `1a`, site symmetry: `-4..`

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, 0]$	`[1,2,-3,-4]`

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

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, 0]$	`[1,-2]`
2	$[Y, -X, 0]$	$[0, 0, 0]$	`[3,-4]`

Table 3: Wyckoff bond: `4c@1a`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	`[1]`
2	$[-X, -Y, Z]$	$[0, 0, 0]$	`[2]`
3	$[Y, -X, -Z]$	$[0, 0, 0]$	`[3]`
4	$[-Y, X, -Z]$	$[0, 0, 0]$	`[4]`

* Wyckoff site: `1b`, site symmetry: `-4..`

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[1,2,-3,-4]`

Table 5: Wyckoff bond: `2b@1b`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[0, 0, \frac{1}{2}\right]$	`[1,-2]`
2	$[Y, -X, 0]$	$\left[0, 0, \frac{1}{2}\right]$	`[3,-4]`

Table 6: Wyckoff bond: `4c@1b`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[2]`
3	$[Y, -X, -Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[3]`
4	$[-Y, X, -Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[4]`

* Wyckoff site: `1c`, site symmetry: `-4..`

Table 7: Wyckoff bond: `1a@1c`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[1,2,-3,-4]`

Table 8: Wyckoff bond: `2b@1c`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[1,-2]`
2	$[Y, -X, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[3,-4]`

Table 9: Wyckoff bond: `4c@1c`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[2]`
3	$[Y, -X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[3]`
4	$[-Y, X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[4]`

* Wyckoff site: `1d`, site symmetry: `-4..`

Table 10: Wyckoff bond: `1a@1d`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[1,2,-3,-4]`

Table 11: Wyckoff bond: `2b@1d`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[1,-2]`
2	$[Y, -X, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[3,-4]`

Table 12: Wyckoff bond: `4c@1d`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[2]`
3	$[Y, -X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[3]`
4	$[-Y, X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[4]`

* Wyckoff site: `2e`, site symmetry: `2..`

Table 13: Wyckoff bond: `2a@2e`

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

Table 14: Wyckoff bond: `2b@2e`

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

Table 15: Wyckoff bond: `4c@2e`

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]`

* Wyckoff site: `2f`, site symmetry: `2..`

Table 16: Wyckoff bond: `2a@2f`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[1,-2]`
2	$[Y, -X, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[3,-4]`

Table 17: Wyckoff bond: `2b@2f`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[1,2]`
2	$[0, 0, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[3,4]`

Table 18: Wyckoff bond: `4c@2f`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[2]`
3	$[Y, -X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[3]`
4	$[-Y, X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[4]`

* Wyckoff site: `2g`, site symmetry: `2..`

Table 19: Wyckoff bond: `2a@2g`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[0, \frac{1}{2}, z\right]$	`[1,-2]`
2	$[Y, -X, 0]$	$\left[\frac{1}{2}, 0, -z\right]$	`[3,-4]`

Table 20: Wyckoff bond: `2b@2g`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[0, \frac{1}{2}, z\right]$	`[1,2]`
2	$[0, 0, -Z]$	$\left[\frac{1}{2}, 0, -z\right]$	`[3,4]`

Table 21: Wyckoff bond: `4c@2g`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[0, \frac{1}{2}, z\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[0, \frac{1}{2}, z\right]$	`[2]`
3	$[Y, -X, -Z]$	$\left[\frac{1}{2}, 0, -z\right]$	`[3]`
4	$[-Y, X, -Z]$	$\left[\frac{1}{2}, 0, -z\right]$	`[4]`

* Wyckoff site: `4h`, site symmetry: `1`

Table 22: Wyckoff bond: `4a@4h`

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]`