SG No. 82 S_4^2 $I\bar{4}$ [tetragonal]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$
* Wyckoff site: `2a`, site symmetry: `-4..`

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

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

Table 2: Wyckoff bond: `4b@2a`

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: `8c@2a`

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: `2b`, site symmetry: `-4..`

Table 4: Wyckoff bond: `2a@2b`

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

Table 5: Wyckoff bond: `4b@2b`

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: `8c@2b`

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: `2c`, site symmetry: `-4..`

Table 7: Wyckoff bond: `2a@2c`

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

Table 8: Wyckoff bond: `4b@2c`

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

Table 9: Wyckoff bond: `8c@2c`

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

* Wyckoff site: `2d`, site symmetry: `-4..`

Table 10: Wyckoff bond: `2a@2d`

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

Table 11: Wyckoff bond: `4b@2d`

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

Table 12: Wyckoff bond: `8c@2d`

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

* Wyckoff site: `4e`, site symmetry: `2..`

Table 13: Wyckoff bond: `4a@4e`

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: `4b@4e`

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: `8c@4e`

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: `4f`, site symmetry: `2..`

Table 16: Wyckoff bond: `4a@4f`

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 17: Wyckoff bond: `4b@4f`

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 18: Wyckoff bond: `8c@4f`

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: `8g`, site symmetry: `1`

Table 19: Wyckoff bond: `8a@8g`

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]`