SG No. 87 C_{4h}^{5} $I4/m$ [tetragonal]

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

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

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

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

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

Table 3: Wyckoff bond: `8c@2a`

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

* Wyckoff site: `2b`, site symmetry: `4/m..`

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,-5,-6,-7,-8]`

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

No.	vector	center	mapping
1	$[X,\ Y,\ 0]$	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[1,-2,-5,6]`
2	$[-Y,\ X,\ 0]$	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[3,-4,-7,8]`

Table 6: Wyckoff bond: `8c@2b`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[1,-5]`
2	$[-X, -Y, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[2,-6]`
3	$[-Y, X, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[3,-7]`
4	$[Y, -X, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[4,-8]`

* Wyckoff site: `4c`, site symmetry: `2/m..`

Table 7: Wyckoff bond: `4a@4c`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[0, \frac{1}{2}, 0\right]$	`[1,-2,-5,6]`
2	$[-Y, X, 0]$	$\left[\frac{1}{2}, 0, 0\right]$	`[3,-4,-7,8]`

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[1,2,-5,-6]`
2	$[0, 0, Z]$	$\left[\frac{1}{2}, 0, 0\right]$	`[3,4,-7,-8]`

Table 9: Wyckoff bond: `8c@4c`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[1,-5]`
2	$[-X, -Y, Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[2,-6]`
3	$[-Y, X, Z]$	$\left[\frac{1}{2}, 0, 0\right]$	`[3,-7]`
4	$[Y, -X, Z]$	$\left[\frac{1}{2}, 0, 0\right]$	`[4,-8]`

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

Table 10: Wyckoff bond: `4a@4d`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[1,2,-7,-8]`
2	$[0, 0, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[3,4,-5,-6]`

Table 11: Wyckoff bond: `8b@4d`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[1,-2]`
2	$[-Y, X, 0]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[3,-4]`
3	$[-X, -Y, 0]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[5,-6]`
4	$[Y, -X, 0]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[7,-8]`

Table 12: Wyckoff bond: `16c@4d`

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	$[-Y, X, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[3]`
4	$[Y, -X, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[4]`
5	$[-X, -Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[5]`
6	$[X, Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[6]`
7	$[Y, -X, -Z]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[7]`
8	$[-Y, X, -Z]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[8]`

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

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

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

Table 14: Wyckoff bond: `8b@4e`

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 15: Wyckoff bond: `16c@4e`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	`[1]`

continued ...

Table 15

No.	vector	center	mapping
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: `8f`, site symmetry: `-1`

Table 16: Wyckoff bond: `8a@8f`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,-5]`
2	$[-X, -Y, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[2,-6]`
3	$[-Y, X, Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[3,-7]`
4	$[Y, -X, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[4,-8]`

* Wyckoff site: `8g`, site symmetry: `2..`

Table 17: Wyckoff bond: `8a@8g`

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]`
3	$[-X, -Y, 0]$	$\left[0, \frac{1}{2}, -z\right]$	`[5,-6]`
4	$[Y, -X, 0]$	$\left[\frac{1}{2}, 0, -z\right]$	`[7,-8]`

Table 18: Wyckoff bond: `8b@8g`

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]`
3	$[0, 0, -Z]$	$\left[0, \frac{1}{2}, -z\right]$	`[5,6]`
4	$[0, 0, -Z]$	$\left[\frac{1}{2}, 0, -z\right]$	`[7,8]`

Table 19: Wyckoff bond: `16c@8g`

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]`
5	$[-X, -Y, -Z]$	$\left[0, \frac{1}{2}, -z\right]$	`[5]`
6	$[X, Y, -Z]$	$\left[0, \frac{1}{2}, -z\right]$	`[6]`
7	$[Y, -X, -Z]$	$\left[\frac{1}{2}, 0, -z\right]$	`[7]`
8	$[-Y, X, -Z]$	$\left[\frac{1}{2}, 0, -z\right]$	`[8]`

* Wyckoff site: `8h`, site symmetry: `m..`

Table 20: Wyckoff bond: `8a@8h`

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

Table 21: Wyckoff bond: `8b@8h`

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

Table 22: Wyckoff bond: `16c@8h`

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

* Wyckoff site: `16i`, site symmetry: `1`

Table 23: Wyckoff bond: `16a@16i`

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]`