SG No. 88 C_{4h}^{6} $I4_1/a$ [tetragonal]

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

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

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

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

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

Table 3: Wyckoff bond: `16c@4a`

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

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

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

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

Table 5: Wyckoff bond: `8b@4b`

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

Table 6: Wyckoff bond: `16c@4b`

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

* Wyckoff site: `8c`, site symmetry: `-1`

Table 7: Wyckoff bond: `8a@8c`

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

* Wyckoff site: `8d`, site symmetry: `-1`

Table 8: Wyckoff bond: `8a@8d`

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

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

Table 9: Wyckoff bond: `8a@8e`

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

Table 10: Wyckoff bond: `8b@8e`

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

Table 11: Wyckoff bond: `16c@8e`

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

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

Table 12: Wyckoff bond: `16a@16f`

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