SG No. 98 D_4^{10} $I4_122$ [tetragonal]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$
* Wyckoff site: `4a`, site symmetry: `2.22`

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

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

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

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

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

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

Table 4: Wyckoff bond: `8d@4a`

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

Table 5: Wyckoff bond: `8e@4a`

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

Table 6: Wyckoff bond: `8f@4a`

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

Table 7: Wyckoff bond: `16g@4a`

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

* Wyckoff site: `4b`, site symmetry: `2.22`

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

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

Table 9: Wyckoff bond: `4b@4b`

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

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

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

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

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

Table 12: Wyckoff bond: `8e@4b`

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

Table 13: Wyckoff bond: `8f@4b`

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

Table 14: Wyckoff bond: `16g@4b`

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

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

Table 15: Wyckoff bond: `8a@8c`

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

Table 16: Wyckoff bond: `8b@8c`

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

Table 17: Wyckoff bond: `16c@8c`

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

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

Table 18: Wyckoff bond: `8a@8d`

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

Table 19: Wyckoff bond: `8b@8d`

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

Table 20: Wyckoff bond: `16c@8d`

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

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

Table 21: Wyckoff bond: `8a@8e`

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

Table 22: Wyckoff bond: `8b@8e`

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

Table 23: Wyckoff bond: `16c@8e`

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

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

Table 24: Wyckoff bond: `8a@8f`

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

Table 25: Wyckoff bond: `8b@8f`

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

Table 26: Wyckoff bond: `16c@8f`

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

* Wyckoff site: 16g, site symmetry: 1

Table 27: Wyckoff bond: 16a@16g

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