SG No. 120 D_{2d}^{10} $I\bar{4}c2$ [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	$[X,\ X,\ 0]$	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[1,-2,7,-8]`
2	$[X,\ -X,\ 0]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[3,-4,5,-6]`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff bond: `16c@4b`

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

continued ...

Table 10

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

Table 11: Wyckoff bond: `4a@4c`

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

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

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

Table 13: Wyckoff bond: `16c@4c`

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

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

Table 14: Wyckoff bond: `4a@4d`

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

Table 15: Wyckoff bond: `4b@4d`

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

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

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

Table 17: Wyckoff bond: `8d@4d`

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

Table 18: Wyckoff bond: `8e@4d`

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

Table 19: Wyckoff bond: `8f@4d`

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

Table 20: Wyckoff bond: `16g@4d`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 27: 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	$[X, -Y, 0]$	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	[5,-6]
4	$[Y, X, 0]$	$\left[\frac{1}{2}, 0, \frac{1}{2}-z\right]$	[7,-8]

Table 28: 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	$[0, 0, Z]$	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	[5,6]
4	$[0, 0, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{2}-z\right]$	[7,8]

Table 29: 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	$[X, -Y, Z]$	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	[5]
6	$[-X, Y, Z]$	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	[6]
7	$[Y, X, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{2}-z\right]$	[7]
8	$[-Y, -X, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{2}-z\right]$	[8]

* Wyckoff site: 8h, site symmetry: ..2

Table 30: Wyckoff bond: 8a@8h

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

Table 31: Wyckoff bond: `8b@8h`

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

Table 32: Wyckoff bond: `16c@8h`

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

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

Table 33: 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	$[X,\ -Y,\ Z]$	$\left[x,\ -y,\ z+\frac{1}{2}\right]$	`[5]`
6	$[-X,\ Y,\ Z]$	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	`[6]`
7	$[Y,\ X,\ -Z]$	$\left[y,\ x,\ \frac{1}{2}-z\right]$	`[7]`
8	$[-Y,\ -X,\ -Z]$	$\left[-y,\ -x,\ \frac{1}{2}-z\right]$	`[8]`