SG No. 94 D_4^6 $P4_22_12$ [tetragonal]

* plus set: $+[0, 0, 0]$

* Wyckoff site: 2a, site symmetry: 2.22

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 2b@2a

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

Table 3: Wyckoff bond: 2c@2a

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

Table 4: Wyckoff bond: 4d@2a

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

Table 5: Wyckoff bond: 4e@2a

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

Table 6: Wyckoff bond: 4f@2a

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

Table 7: Wyckoff bond: 8g@2a

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

* Wyckoff site: 2b, site symmetry: 2.22

Table 8: Wyckoff bond: 2a@2b

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

Table 9: Wyckoff bond: 2b@2b

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

Table 10: Wyckoff bond: 2c@2b

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

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

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

Table 12: Wyckoff bond: `4e@2b`

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

Table 13: Wyckoff bond: `4f@2b`

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

Table 14: Wyckoff bond: `8g@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	$[-Y, X, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[3]
4	$[Y, -X, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[4]
5	$[-X, Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[5]
6	$[X, -Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[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: `2..`

Table 15: Wyckoff bond: `4a@4c`

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

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

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

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

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

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

Table 18: Wyckoff bond: `4a@4d`

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

Table 19: Wyckoff bond: `4b@4d`

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

Table 20: Wyckoff bond: `8c@4d`

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	$[-Y, X, Z]$	$\left[0, \frac{1}{2}, z + \frac{1}{2}\right]$	[3]
4	$[Y, -X, Z]$	$\left[0, \frac{1}{2}, z + \frac{1}{2}\right]$	[4]
5	$[-X, Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$	[5]
6	$[X, -Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$	[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: `4e`, site symmetry: `..2`

Table 21: Wyckoff bond: `4a@4e`

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

Table 22: Wyckoff bond: `4b@4e`

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

Table 23: Wyckoff bond: `8c@4e`

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

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

Table 24: Wyckoff bond: `4a@4f`

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

Table 25: Wyckoff bond: `4b@4f`

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

Table 26: Wyckoff bond: `8c@4f`

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

* Wyckoff site: 8g, site symmetry: 1

Table 27: 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	$[-Y,\,X,\,Z]$	$\left[\frac{1}{2}-y,\,x+\frac{1}{2},\,z+\frac{1}{2}\right]$	[3]
4	$[Y,\,-X,\,Z]$	$\left[y+\frac{1}{2},\,\frac{1}{2}-x,\,z+\frac{1}{2}\right]$	[4]
5	$[-X,\,Y,\,-Z]$	$\left[\frac{1}{2}-x,\,y+\frac{1}{2},\,\frac{1}{2}-z\right]$	[5]
6	$[X,\,-Y,\,-Z]$	$\left[x+\frac{1}{2},\,\frac{1}{2}-y,\,\frac{1}{2}-z\right]$	[6]
7	$[Y,\,X,\,-Z]$	$[y,\,x,\,-z]$	[7]
8	$[-Y,\,-X,\,-Z]$	$[-y,\,-x,\,-z]$	[8]