

SG No. 114 D_{2d}^4 $P\bar{4}2_1c$ [tetragonal]

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

* Wyckoff site: **2a**, site symmetry: $-4..$

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

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

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

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

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

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

* Wyckoff site: **2b**, site symmetry: $-4..$

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

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

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

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

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

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

* Wyckoff site: **4c**, site symmetry: $2..$

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

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

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

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

Table 9: 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	$[Y, -X, -Z]$	$[0, 0, -z]$	[3]
4	$[-Y, X, -Z]$	$[0, 0, -z]$	[4]
5	$[-X, Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[5]
6	$[X, -Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[6]
7	$[-Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[7]
8	$[Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[8]

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

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

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

Table 11: Wyckoff bond: **4b@4d**

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

Table 12: Wyckoff bond: **8c@4d**

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

* Wyckoff site: **8e**, site symmetry: **1**

Table 13: Wyckoff bond: **8a@8e**

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	$[-X, Y, -Z]$	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[5]
6	$[X, -Y, -Z]$	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[6]
7	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[7]
8	$[Y, X, Z]$	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[8]