

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]