

SG No. 122  $D_{2d}^{12}$   $I\bar{4}2d$  [ tetragonal ]

\* plus set:  $+[0, 0, 0]$ ,  $+[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

\* Wyckoff site: 4a, site symmetry: -4..

Table 1: Wyckoff bond: 4a@4a

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

Table 2: Wyckoff bond: 8b@4a

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

Table 3: Wyckoff bond: 16c@4a

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

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

Table 4: Wyckoff bond: 4a@4b

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

Table 5: Wyckoff bond: 8b@4b

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

Table 6: Wyckoff bond: 16c@4b

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

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

Table 7: Wyckoff bond: 8a@8c

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

Table 8: Wyckoff bond: 8b@8c

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

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

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

Table 10: Wyckoff bond: 8a@8d

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

Table 11: Wyckoff bond: 8b@8d

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

Table 12: Wyckoff bond: 16c@8d

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

\* Wyckoff site: **16e**, site symmetry: **1**

Table 13: Wyckoff bond: **16a@16e**

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