

SG No. 86  $C_{4h}^4$   $P4_2/n$  [ tetragonal ]

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

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

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

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

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

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

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

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

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

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

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

Table 5: Wyckoff bond: 4b@2b

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

Table 6: Wyckoff bond: 8c@2b

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

\* Wyckoff site: 4c, site symmetry:  $-1$

Table 7: Wyckoff bond: 4a@4c

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

\* Wyckoff site: 4d, site symmetry:  $-1$

Table 8: Wyckoff bond: 4a@4d

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

\* Wyckoff site: 4e, site symmetry:  $2..$

Table 9: Wyckoff bond: **4a@4e**

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

Table 10: Wyckoff bond: **4b@4e**

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

Table 11: Wyckoff bond: **8c@4e**

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

\* Wyckoff site: **4f**, site symmetry:  $2..$

Table 12: Wyckoff bond: **4a@4f**

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

Table 13: Wyckoff bond: **4b@4f**

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

Table 14: Wyckoff bond: **8c@4f**

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

\* Wyckoff site: **8g**, site symmetry: 1

Table 15: Wyckoff bond: **8a@8g**

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