

SG No. 137  $D_{4h}^{15}$   $P4_2/nmc$  [ tetragonal ]

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

\* Wyckoff site: **2a**, site symmetry:  $-4m2$

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[1, 2, -7, -8, -11, -12, 13, 14]$
2	$[0, 0, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[3, 4, -5, -6, -9, -10, 15, 16]$

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

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[1, -2, 13, -14]$
2	$[0, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[3, -4, -15, 16]$
3	$[-X, 0, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[5, -6, 9, -10]$
4	$[0, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[7, -8, -11, 12]$

Table 3: Wyckoff bond: **4c@2a**

No.	vector	center	mapping
1	$[X, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[1, -2, 7, -8]$
2	$[-X, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[3, -4, 5, -6]$
3	$[-X, -X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[9, -10, 15, -16]$
4	$[X, -X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[11, -12, 13, -14]$

Table 4: Wyckoff bond: **8d@2a**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[1, 13]$
2	$[-X, 0, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[2, 14]$
3	$[0, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[3, 16]$
4	$[0, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[4, 15]$
5	$[-X, 0, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[5, 9]$
6	$[X, 0, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[6, 10]$
7	$[0, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[7, 12]$
8	$[0, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[8, 11]$

Table 5: Wyckoff bond: **8e@2a**

No.	vector	center	mapping
1	$[X, X, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[1, -8]$
2	$[-X, -X, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[2, -7]$
3	$[-X, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[3, -6]$
4	$[X, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[4, -5]$
5	$[-X, -X, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[9, -16]$
6	$[X, X, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[10, -15]$
7	$[X, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[11, -14]$
8	$[-X, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[12, -13]$

Table 6: Wyckoff bond: **8f@2a**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[1, -2]$
2	$[-Y, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[3, -4]$
3	$[-X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[5, -6]$
4	$[Y, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[7, -8]$
5	$[-X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[9, -10]$
6	$[Y, -X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[11, -12]$
7	$[X, -Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[13, -14]$
8	$[-Y, -X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[15, -16]$

Table 7: Wyckoff bond: **16g@2a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[1]$
2	$[-X, -Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[2]$
3	$[-Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[3]$
4	$[Y, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[4]$
5	$[-X, Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[5]$
6	$[X, -Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[6]$
7	$[Y, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[7]$
8	$[-Y, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[8]$
9	$[-X, -Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[9]$
10	$[X, Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[10]$
11	$[Y, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[11]$
12	$[-Y, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[12]$
13	$[X, -Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[13]$
14	$[-X, Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[14]$
15	$[-Y, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[15]$
16	$[Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[16]$

Table 8: Wyckoff bond: 2a@2b

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, 2, -7, -8, -11, -12, 13, 14]$
2	$[0, 0, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[3, 4, -5, -6, -9, -10, 15, 16]$

Table 9: Wyckoff bond: 4b@2b

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, -2, 13, -14]$
2	$[0, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[3, -4, -15, 16]$
3	$[-X, 0, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[5, -6, 9, -10]$
4	$[0, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[7, -8, -11, 12]$

Table 10: Wyckoff bond: 4c@2b

No.	vector	center	mapping
1	$[X, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, -2, 7, -8]$
2	$[-X, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[3, -4, 5, -6]$
3	$[-X, -X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[9, -10, 15, -16]$
4	$[X, -X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[11, -12, 13, -14]$

Table 11: Wyckoff bond: 8d@2b

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, 13]$
2	$[-X, 0, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[2, 14]$
3	$[0, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[3, 16]$
4	$[0, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[4, 15]$
5	$[-X, 0, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[5, 9]$
6	$[X, 0, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[6, 10]$
7	$[0, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[7, 12]$
8	$[0, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[8, 11]$

Table 12: Wyckoff bond: **8e@2b**

No.	vector	center	mapping
1	$[X, X, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, -8]$
2	$[-X, -X, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[2, -7]$
3	$[-X, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[3, -6]$
4	$[X, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[4, -5]$
5	$[-X, -X, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[9, -16]$
6	$[X, X, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[10, -15]$
7	$[X, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[11, -14]$
8	$[-X, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[12, -13]$

Table 13: Wyckoff bond: **8f@2b**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, -2]$
2	$[-Y, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[3, -4]$
3	$[-X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[5, -6]$
4	$[Y, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[7, -8]$
5	$[-X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[9, -10]$
6	$[Y, -X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[11, -12]$
7	$[X, -Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[13, -14]$
8	$[-Y, -X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[15, -16]$

Table 14: Wyckoff bond: **16g@2b**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1]$
2	$[-X, -Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[2]$
3	$[-Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[3]$
4	$[Y, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[4]$
5	$[-X, Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[5]$
6	$[X, -Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[6]$
7	$[Y, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[7]$
8	$[-Y, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[8]$
9	$[-X, -Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[9]$
10	$[X, Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[10]$
11	$[Y, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[11]$
12	$[-Y, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[12]$
13	$[X, -Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[13]$
14	$[-X, Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[14]$
15	$[-Y, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[15]$
16	$[Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[16]$

Table 15: Wyckoff bond: 4a@4c

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{3}{4}, \frac{1}{4}, z]$	$[1, -2, 13, -14]$
2	$[0, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	$[3, -4, -15, 16]$
3	$[-X, 0, 0]$	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[5, -6, 9, -10]$
4	$[0, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	$[7, -8, -11, 12]$

Table 16: Wyckoff bond: 4b@4c

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{3}{4}, \frac{1}{4}, z]$	$[1, 2, 13, 14]$
2	$[0, 0, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	$[3, 4, 15, 16]$
3	$[0, 0, -Z]$	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[5, 6, 9, 10]$
4	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	$[7, 8, 11, 12]$

Table 17: Wyckoff bond: 8c@4c

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{3}{4}, \frac{1}{4}, z]$	$[1, 13]$
2	$[-X, 0, Z]$	$[\frac{3}{4}, \frac{1}{4}, z]$	$[2, 14]$
3	$[0, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	$[3, 16]$
4	$[0, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	$[4, 15]$
5	$[-X, 0, -Z]$	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[5, 9]$
6	$[X, 0, -Z]$	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[6, 10]$
7	$[0, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	$[7, 12]$
8	$[0, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	$[8, 11]$

Table 18: Wyckoff bond: 8d@4c

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, z]$	$[1, -2]$
2	$[-Y, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	$[3, -4]$
3	$[-X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[5, -6]$
4	$[Y, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	$[7, -8]$
5	$[-X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[9, -10]$
6	$[Y, -X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	$[11, -12]$
7	$[X, -Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, z]$	$[13, -14]$
8	$[-Y, -X, 0]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	$[15, -16]$

Table 19: Wyckoff bond: **16e@4c**

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	$[-Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[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	$[Y, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[7]
8	$[-Y, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[8]
9	$[-X, -Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, -z]$	[9]
10	$[X, Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, -z]$	[10]
11	$[Y, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[11]
12	$[-Y, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[12]
13	$[X, -Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, z]$	[13]
14	$[-X, Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, z]$	[14]
15	$[-Y, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[15]
16	$[Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[16]

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

Table 20: Wyckoff bond: **4a@4d**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[1,-2,13,-14]
2	$[0, X, 0]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[3,-4,-15,16]
3	$[-X, 0, 0]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[5,-6,9,-10]
4	$[0, X, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[7,-8,-11,12]

Table 21: Wyckoff bond: **4b@4d**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[1,2,13,14]
2	$[0, 0, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[3,4,15,16]
3	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[5,6,9,10]
4	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[7,8,11,12]

Table 22: Wyckoff bond: **8c@4d**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[1,13]

*continued ...*

Table 22

No.	vector	center	mapping
2	$[-X, 0, Z]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[2,14]
3	$[0, X, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[3,16]
4	$[0, -X, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[4,15]
5	$[-X, 0, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[5,9]
6	$[X, 0, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[6,10]
7	$[0, X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[7,12]
8	$[0, -X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[8,11]

Table 23: Wyckoff bond: **8d@4d**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[1,-2]
2	$[-Y, X, 0]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[3,-4]
3	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[5,-6]
4	$[Y, X, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[7,-8]
5	$[-X, -Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[9,-10]
6	$[Y, -X, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[11,-12]
7	$[X, -Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[13,-14]
8	$[-Y, -X, 0]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[15,-16]

Table 24: Wyckoff bond: **16e@4d**

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	$[-Y, X, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[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	$[Y, X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[7]
8	$[-Y, -X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[8]
9	$[-X, -Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[9]
10	$[X, Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[10]
11	$[Y, -X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[11]
12	$[-Y, X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[12]
13	$[X, -Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[14]
15	$[-Y, -X, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[15]
16	$[Y, X, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[16]

\* Wyckoff site: **8e**, site symmetry:  $-1$

Table 25: Wyckoff bond: **8a@8e**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1, -9]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, -10]$
3	$[-Y, X, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[3, -11]$
4	$[Y, -X, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[4, -12]$
5	$[-X, Y, -Z]$	$[0, \frac{1}{2}, 0]$	$[5, -13]$
6	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, 0]$	$[6, -14]$
7	$[Y, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[7, -15]$
8	$[-Y, -X, -Z]$	$[0, 0, \frac{1}{2}]$	$[8, -16]$

\* Wyckoff site: **8f**, site symmetry:  $\cdot \cdot 2$

Table 26: Wyckoff bond: **8a@8f**

No.	vector	center	mapping
1	$[X, X, Z]$	$[x, -x, \frac{1}{4}]$	$[1, -8]$
2	$[-X, -X, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}]$	$[2, -7]$
3	$[-X, X, Z]$	$[x + \frac{1}{2}, x, \frac{3}{4}]$	$[3, -6]$
4	$[X, -X, Z]$	$[-x, \frac{1}{2} - x, \frac{3}{4}]$	$[4, -5]$
5	$[-X, -X, -Z]$	$[-x, x, \frac{3}{4}]$	$[9, -16]$
6	$[X, X, -Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	$[10, -15]$
7	$[X, -X, -Z]$	$[\frac{1}{2} - x, -x, \frac{1}{4}]$	$[11, -14]$
8	$[-X, X, -Z]$	$[x, x + \frac{1}{2}, \frac{1}{4}]$	$[12, -13]$

Table 27: Wyckoff bond: **8b@8f**

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, -x, \frac{1}{4}]$	$[1, 8]$
2	$[-X, X, 0]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}]$	$[2, 7]$
3	$[X, X, 0]$	$[x + \frac{1}{2}, x, \frac{3}{4}]$	$[3, 6]$
4	$[-X, -X, 0]$	$[-x, \frac{1}{2} - x, \frac{3}{4}]$	$[4, 5]$
5	$[-X, X, 0]$	$[-x, x, \frac{3}{4}]$	$[9, 16]$
6	$[X, -X, 0]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	$[10, 15]$
7	$[-X, -X, 0]$	$[\frac{1}{2} - x, -x, \frac{1}{4}]$	$[11, 14]$
8	$[X, X, 0]$	$[x, x + \frac{1}{2}, \frac{1}{4}]$	$[12, 13]$

Table 28: Wyckoff bond: **16c@8f**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, -x, \frac{1}{4}]$	$[1]$

*continued ...*



Table 28

No.	vector	center	mapping
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}]$	[2]
3	$[-Y, X, Z]$	$[x + \frac{1}{2}, x, \frac{3}{4}]$	[3]
4	$[Y, -X, Z]$	$[-x, \frac{1}{2} - x, \frac{3}{4}]$	[4]
5	$[-X, Y, -Z]$	$[-x, \frac{1}{2} - x, \frac{3}{4}]$	[5]
6	$[X, -Y, -Z]$	$[x + \frac{1}{2}, x, \frac{3}{4}]$	[6]
7	$[Y, X, -Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}]$	[7]
8	$[-Y, -X, -Z]$	$[x, -x, \frac{1}{4}]$	[8]
9	$[-X, -Y, -Z]$	$[-x, x, \frac{3}{4}]$	[9]
10	$[X, Y, -Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[10]
11	$[Y, -X, -Z]$	$[\frac{1}{2} - x, -x, \frac{1}{4}]$	[11]
12	$[-Y, X, -Z]$	$[x, x + \frac{1}{2}, \frac{1}{4}]$	[12]
13	$[X, -Y, Z]$	$[x, x + \frac{1}{2}, \frac{1}{4}]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{2} - x, -x, \frac{1}{4}]$	[14]
15	$[-Y, -X, Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[15]
16	$[Y, X, Z]$	$[-x, x, \frac{3}{4}]$	[16]

\* Wyckoff site: **8g**, site symmetry: **.m**.

Table 29: Wyckoff bond: **8a@8g**

No.	vector	center	mapping
1	$[0, X, Z]$	$[\frac{1}{4}, y, z]$	[1, 14]
2	$[0, -X, Z]$	$[\frac{1}{4}, \frac{1}{2} - y, z]$	[2, 13]
3	$[-X, 0, Z]$	$[\frac{1}{2} - y, \frac{1}{4}, z + \frac{1}{2}]$	[3, 15]
4	$[X, 0, Z]$	$[y, \frac{1}{4}, z + \frac{1}{2}]$	[4, 16]
5	$[0, X, -Z]$	$[\frac{3}{4}, y + \frac{1}{2}, -z]$	[5, 10]
6	$[0, -X, -Z]$	$[\frac{3}{4}, -y, -z]$	[6, 9]
7	$[X, 0, -Z]$	$[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$	[7, 11]
8	$[-X, 0, -Z]$	$[-y, \frac{3}{4}, \frac{1}{2} - z]$	[8, 12]

Table 30: Wyckoff bond: **8b@8g**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{4}, y, z]$	[1, -14]
2	$[-X, 0, 0]$	$[\frac{1}{4}, \frac{1}{2} - y, z]$	[2, -13]
3	$[0, X, 0]$	$[\frac{1}{2} - y, \frac{1}{4}, z + \frac{1}{2}]$	[3, -15]
4	$[0, -X, 0]$	$[y, \frac{1}{4}, z + \frac{1}{2}]$	[4, -16]
5	$[-X, 0, 0]$	$[\frac{3}{4}, y + \frac{1}{2}, -z]$	[5, -10]
6	$[X, 0, 0]$	$[\frac{3}{4}, -y, -z]$	[6, -9]
7	$[0, X, 0]$	$[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$	[7, -11]
8	$[0, -X, 0]$	$[-y, \frac{3}{4}, \frac{1}{2} - z]$	[8, -12]

Table 31: Wyckoff bond: **16c@8g**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{4}, y, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{4}, \frac{1}{2} - y, z]$	[2]
3	$[-Y, X, Z]$	$[\frac{1}{2} - y, \frac{1}{4}, z + \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[y, \frac{1}{4}, z + \frac{1}{2}]$	[4]
5	$[-X, Y, -Z]$	$[\frac{3}{4}, y + \frac{1}{2}, -z]$	[5]
6	$[X, -Y, -Z]$	$[\frac{3}{4}, -y, -z]$	[6]
7	$[Y, X, -Z]$	$[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$	[7]
8	$[-Y, -X, -Z]$	$[-y, \frac{3}{4}, \frac{1}{2} - z]$	[8]
9	$[-X, -Y, -Z]$	$[\frac{3}{4}, -y, -z]$	[9]
10	$[X, Y, -Z]$	$[\frac{3}{4}, y + \frac{1}{2}, -z]$	[10]
11	$[Y, -X, -Z]$	$[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$	[11]
12	$[-Y, X, -Z]$	$[-y, \frac{3}{4}, \frac{1}{2} - z]$	[12]
13	$[X, -Y, Z]$	$[\frac{1}{4}, \frac{1}{2} - y, z]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{4}, y, z]$	[14]
15	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{4}, z + \frac{1}{2}]$	[15]
16	$[Y, X, Z]$	$[y, \frac{1}{4}, z + \frac{1}{2}]$	[16]

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

Table 32: Wyckoff bond: **16a@16h**

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	$[-Y, X, Z]$	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[4]
5	$[-X, Y, -Z]$	$[-x, y + \frac{1}{2}, -z]$	[5]
6	$[X, -Y, -Z]$	$[x + \frac{1}{2}, -y, -z]$	[6]
7	$[Y, X, -Z]$	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[7]
8	$[-Y, -X, -Z]$	$[-y, -x, \frac{1}{2} - z]$	[8]
9	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[9]
10	$[X, Y, -Z]$	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[10]
11	$[Y, -X, -Z]$	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[11]
12	$[-Y, X, -Z]$	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[12]
13	$[X, -Y, Z]$	$[x, \frac{1}{2} - y, z]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{2} - x, y, z]$	[14]
15	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[15]
16	$[Y, X, Z]$	$[y, x, z + \frac{1}{2}]$	[16]