

SG No. 138  $D_{4h}^{16}$   $P4_2/nm$  [ tetragonal ]

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

\* Wyckoff site: **4a**, site symmetry: 2.22

Table 1: Wyckoff bond: **4a@4a**

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

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

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

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

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

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

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

Table 5: Wyckoff bond: **8e@4a**

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

Table 6: Wyckoff bond: **8f@4a**

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

Table 7: Wyckoff bond: **16g@4a**

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

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

Table 8: Wyckoff bond: 4a@4b

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

Table 9: Wyckoff bond: 8b@4b

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	$[-X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[5, -6]$
4	$[Y, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[7, -8]$
5	$[-X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[9, -10]$
6	$[Y, -X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[11, -12]$
7	$[X, -Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[13, -14]$
8	$[-Y, -X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[15, -16]$

Table 10: Wyckoff bond: 16c@4b

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	$[-X, Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[5]$
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	$[-X, -Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[9]$
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	$[X, -Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[13]$
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	$[Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[16]$

\* Wyckoff site: 4c, site symmetry:  $..2/m$

Table 11: Wyckoff bond: **4a@4c**

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

Table 12: Wyckoff bond: **4b@4c**

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

Table 13: Wyckoff bond: **8c@4c**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -9]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, -10]$
3	$[-Y, X, Z]$	$[\frac{1}{2}, 0, 0]$	$[3, -11]$
4	$[Y, -X, Z]$	$[0, \frac{1}{2}, 0]$	$[4, -12]$
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: **4d**, site symmetry:  $\dots 2/m$

Table 14: Wyckoff bond: **4a@4d**

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

Table 15: Wyckoff bond: **4b@4d**

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

Table 16: Wyckoff bond: **8c@4d**

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	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[5, -13]$
6	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6, -14]$
7	$[Y, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[7, -15]$
8	$[-Y, -X, -Z]$	$[0, 0, 0]$	$[8, -16]$

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

Table 17: Wyckoff bond: **4a@4e**

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

Table 18: Wyckoff bond: **4b@4e**

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

Table 19: Wyckoff bond: **8c@4e**

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

Table 20: Wyckoff bond: **8d@4e**

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	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	$[5, -6]$
4	$[Y, X, 0]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	$[7, -8]$
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	$[X, -Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	$[13, -14]$
8	$[-Y, -X, 0]$	$[\frac{1}{4}, \frac{1}{4}, z]$	$[15, -16]$

Table 21: Wyckoff bond: **16e@4e**

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

Table 22: Wyckoff bond: 8a@8f

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	$[-X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	$[5, -6]$
4	$[Y, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, -z]$	$[7, -8]$
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	$[X, -Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	$[13, -14]$
8	$[-Y, -X, 0]$	$[\frac{1}{4}, \frac{3}{4}, z]$	$[15, -16]$

Table 23: Wyckoff bond: 8b@8f

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

Table 24: Wyckoff bond: 16c@8f

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	$[-X, Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	$[5]$
6	$[X, -Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	$[6]$
7	$[Y, X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, -z]$	$[7]$
8	$[-Y, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, -z]$	$[8]$
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	$[X, -Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	$[13]$
14	$[-X, Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	$[14]$
15	$[-Y, -X, Z]$	$[\frac{1}{4}, \frac{3}{4}, z]$	$[15]$

continued ...

Table 24

No.	vector	center	mapping
16	$[Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, z]$	[16]

\* Wyckoff site: 8g, site symmetry:  $\dots$

Table 25: Wyckoff bond: 8a@8g

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

Table 26: Wyckoff bond: 8b@8g

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

Table 27: Wyckoff bond: 16c@8g

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, -x, \frac{1}{2}]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]$	[2]
3	$[-Y, X, Z]$	$[x + \frac{1}{2}, x, 0]$	[3]
4	$[Y, -X, Z]$	$[-x, \frac{1}{2} - x, 0]$	[4]
5	$[-X, Y, -Z]$	$[-x, \frac{1}{2} - x, 0]$	[5]
6	$[X, -Y, -Z]$	$[x + \frac{1}{2}, x, 0]$	[6]
7	$[Y, X, -Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]$	[7]
8	$[-Y, -X, -Z]$	$[x, -x, \frac{1}{2}]$	[8]
9	$[-X, -Y, -Z]$	$[-x, x, \frac{1}{2}]$	[9]

*continued ...*



Table 27

No.	vector	center	mapping
10	$[X, Y, -Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[10]
11	$[Y, -X, -Z]$	$[\frac{1}{2} - x, -x, 0]$	[11]
12	$[-Y, X, -Z]$	$[x, x + \frac{1}{2}, 0]$	[12]
13	$[X, -Y, Z]$	$[x, x + \frac{1}{2}, 0]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{2} - x, -x, 0]$	[14]
15	$[-Y, -X, Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[15]
16	$[Y, X, Z]$	$[-x, x, \frac{1}{2}]$	[16]

\* Wyckoff site: **8h**, site symmetry:  $\dots 2$

Table 28: Wyckoff bond: **8a@8h**

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

Table 29: Wyckoff bond: **8b@8h**

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

Table 30: Wyckoff bond: **16c@8h**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, -x, 0]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, 0]$	[2]
3	$[-Y, X, Z]$	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[3]

*continued ...*

Table 30

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

\* Wyckoff site: **8i**, site symmetry:  $\bar{3}m$

Table 31: Wyckoff bond: **8a@8i**

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

Table 32: Wyckoff bond: **8b@8i**

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

Table 33: Wyckoff bond: **16c@8i**

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

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

Table 34: Wyckoff bond: **16a@16j**

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	$[-X, Y, -Z]$	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[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	$[-Y, -X, -Z]$	$[-y, -x, -z]$	[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	$[X, -Y, Z]$	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[14]
15	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[15]
16	$[Y, X, Z]$	$[y, x, z]$	[16]