

SG No. 135 D_{4h}^{13} $P4_2/mbc$ [tetragonal]

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

* Wyckoff site: 4a, site symmetry: 2/m..

Table 1: Wyckoff bond: 4a@4a

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

Table 2: Wyckoff bond: 4b@4a

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

Table 3: Wyckoff bond: 8c@4a

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

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

Table 4: Wyckoff bond: 4a@4b

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

Table 5: Wyckoff bond: 8b@4b

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

Table 6: Wyckoff bond: 16c@4b

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

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

Table 7: Wyckoff bond: 4a@4c

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

Table 8: Wyckoff bond: 4b@4c

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

Table 9: Wyckoff bond: 8c@4c

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

* Wyckoff site: 4d, site symmetry: 2.22

Table 10: Wyckoff bond: 4a@4d

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

Table 11: Wyckoff bond: 4b@4d

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

Table 12: Wyckoff bond: 4c@4d

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

Table 13: Wyckoff bond: 8d@4d

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

Table 14: Wyckoff bond: 8e@4d

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

Table 15: Wyckoff bond: 8f@4d

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

continued ...

Table 15

No.	vector	center	mapping
8	$[-Y, -X, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[15, -16]$

Table 16: Wyckoff bond: 16g@4d

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

* Wyckoff site: 8e, site symmetry: 2..

Table 17: Wyckoff bond: 8a@8e

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

Table 18: Wyckoff bond: 8b@8e

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	$[1, 2]$

continued ...

Table 18

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

Table 19: Wyckoff bond: 16c@8e

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

* Wyckoff site: 8f, site symmetry: 2..

Table 20: Wyckoff bond: 8a@8f

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

Table 21: Wyckoff bond: 8b@8f

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

Table 22: Wyckoff bond: 16c@8f

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	$[-Y, X, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[4]
5	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, -z]$	[5]
6	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, -z]$	[6]
7	$[Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[7]
8	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[8]
9	$[-X, -Y, -Z]$	$[0, \frac{1}{2}, -z]$	[9]
10	$[X, Y, -Z]$	$[0, \frac{1}{2}, -z]$	[10]
11	$[Y, -X, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[11]
12	$[-Y, X, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[12]
13	$[X, -Y, Z]$	$[\frac{1}{2}, 0, z]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{2}, 0, z]$	[14]
15	$[-Y, -X, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[15]
16	$[Y, X, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[16]

* Wyckoff site: 8g, site symmetry: ..2

Table 23: Wyckoff bond: 8a@8g

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

Table 24: Wyckoff bond: 8b@8g

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

Table 25: Wyckoff bond: 16c@8g

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

* Wyckoff site: 8h, site symmetry: m..

Table 26: Wyckoff bond: 8a@8h

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

continued ...

Table 26

No.	vector	center	mapping
7	$[Y, X, 0]$	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[7, 16]
8	$[-Y, -X, 0]$	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2}]$	[8, 15]

Table 27: Wyckoff bond: 8b@8h

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

Table 28: Wyckoff bond: 16c@8h

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

* Wyckoff site: 16i, site symmetry: 1

Table 29: Wyckoff bond: 16a@16i

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