

SG No. 141 D_{4h}^{19} $I4_1/AMD$ [tetragonal]

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

* Wyckoff site: 4a, site symmetry: -4m2

Table 1: Wyckoff bond: 4a@4a

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

Table 2: Wyckoff bond: 8b@4a

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

Table 3: Wyckoff bond: 8c@4a

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

Table 4: Wyckoff bond: 16d@4a

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

Table 5: Wyckoff bond: 16e@4a

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

Table 6: Wyckoff bond: 16f@4a

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

Table 7: Wyckoff bond: 32g@4a

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

* Wyckoff site: **4b**, site symmetry: **-4m2**

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

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

Table 9: Wyckoff bond: **8b@4b**

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

Table 10: Wyckoff bond: **8c@4b**

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

Table 11: Wyckoff bond: **16d@4b**

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

Table 12: Wyckoff bond: 16e@4b

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

Table 13: Wyckoff bond: 16f@4b

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

Table 14: Wyckoff bond: 32g@4b

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

* Wyckoff site: 8c, site symmetry: .2/m.

Table 15: Wyckoff bond: 8a@8c

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

Table 16: Wyckoff bond: 8b@8c

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

Table 17: Wyckoff bond: 16c@8c

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

* Wyckoff site: 8d, site symmetry: .2/m.

Table 18: Wyckoff bond: 8a@8d

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

Table 19: Wyckoff bond: 8b@8d

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

Table 20: Wyckoff bond: 16c@8d

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

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

Table 21: Wyckoff bond: 8a@8e

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

Table 22: Wyckoff bond: 8b@8e

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

Table 23: Wyckoff bond: 16c@8e

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

Table 24: Wyckoff bond: 16d@8e

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

Table 25: Wyckoff bond: 32e@8e

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

* Wyckoff site: 16f, site symmetry: .2.

Table 26: Wyckoff bond: 16a@16f

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

Table 27: Wyckoff bond: 16b@16f

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

Table 28: Wyckoff bond: 32c@16f

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

continued ...

Table 28

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

* Wyckoff site: 16g, site symmetry: ..2

Table 29: Wyckoff bond: 16a@16g

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

Table 30: Wyckoff bond: 16b@16g

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

Table 31: Wyckoff bond: 32c@16g

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

continued ...

Table 31

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

* Wyckoff site: 16h, site symmetry: .m.

Table 32: Wyckoff bond: 16a@16h

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

Table 33: Wyckoff bond: 16b@16h

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

Table 34: Wyckoff bond: 32c@16h

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	[2]
3	$[-Y, X, Z]$	$[\frac{1}{4} - y, \frac{3}{4}, z + \frac{1}{4}]$	[3]

continued ...

Table 34

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

* Wyckoff site: 32i, site symmetry: 1

Table 35: Wyckoff bond: 32a@32i

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