

SG No. 192 D_{6h}^2 $P6/mcc$ [hexagonal]

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

* Wyckoff site: **2a**, site symmetry: **622**

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, \frac{1}{4}]$	$[1, 2, 3, 4, 5, 6, -7, -8, -9, -10, -11, -12]$
2	$[0, 0, -Z]$	$[0, 0, \frac{3}{4}]$	$[13, 14, 15, 16, 17, 18, -19, -20, -21, -22, -23, -24]$

Table 2: Wyckoff bond: **6b@2a**

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[0, 0, \frac{1}{4}]$	$[1, -4, -8, 11]$
2	$[-2X, -X, 0]$	$[0, 0, \frac{1}{4}]$	$[2, -5, -7, 10]$
3	$[X, -X, 0]$	$[0, 0, \frac{1}{4}]$	$[3, -6, -9, 12]$
4	$[-X, -2X, 0]$	$[0, 0, \frac{3}{4}]$	$[13, -16, -20, 23]$
5	$[2X, X, 0]$	$[0, 0, \frac{3}{4}]$	$[14, -17, -19, 22]$
6	$[-X, X, 0]$	$[0, 0, \frac{3}{4}]$	$[15, -18, -21, 24]$

Table 3: Wyckoff bond: **6c@2a**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, \frac{1}{4}]$	$[1, -4, 8, -11]$
2	$[0, X, 0]$	$[0, 0, \frac{1}{4}]$	$[2, -5, 7, -10]$
3	$[-X, -X, 0]$	$[0, 0, \frac{1}{4}]$	$[3, -6, 9, -12]$
4	$[-X, 0, 0]$	$[0, 0, \frac{3}{4}]$	$[13, -16, 20, -23]$
5	$[0, -X, 0]$	$[0, 0, \frac{3}{4}]$	$[14, -17, 19, -22]$
6	$[X, X, 0]$	$[0, 0, \frac{3}{4}]$	$[15, -18, 21, -24]$

Table 4: Wyckoff bond: **12d@2a**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, \frac{1}{4}]$	$[1, -4]$
2	$[-Y, X - Y, 0]$	$[0, 0, \frac{1}{4}]$	$[2, -5]$
3	$[-X + Y, -X, 0]$	$[0, 0, \frac{1}{4}]$	$[3, -6]$
4	$[Y, X, 0]$	$[0, 0, \frac{1}{4}]$	$[7, -10]$
5	$[X - Y, -Y, 0]$	$[0, 0, \frac{1}{4}]$	$[8, -11]$
6	$[-X, -X + Y, 0]$	$[0, 0, \frac{1}{4}]$	$[9, -12]$
7	$[-X, -Y, 0]$	$[0, 0, \frac{3}{4}]$	$[13, -16]$
8	$[Y, -X + Y, 0]$	$[0, 0, \frac{3}{4}]$	$[14, -17]$
9	$[X - Y, X, 0]$	$[0, 0, \frac{3}{4}]$	$[15, -18]$

continued ...

Table 4

No.	vector	center	mapping
10	$[-Y, -X, 0]$	$[0, 0, \frac{3}{4}]$	$[19, -22]$
11	$[-X + Y, Y, 0]$	$[0, 0, \frac{3}{4}]$	$[20, -23]$
12	$[X, X - Y, 0]$	$[0, 0, \frac{3}{4}]$	$[21, -24]$

Table 5: Wyckoff bond: 12e@2a

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[0, 0, \frac{1}{4}]$	$[1, -8]$
2	$[-2X, -X, Z]$	$[0, 0, \frac{1}{4}]$	$[2, -7]$
3	$[X, -X, Z]$	$[0, 0, \frac{1}{4}]$	$[3, -9]$
4	$[-X, -2X, Z]$	$[0, 0, \frac{1}{4}]$	$[4, -11]$
5	$[2X, X, Z]$	$[0, 0, \frac{1}{4}]$	$[5, -10]$
6	$[-X, X, Z]$	$[0, 0, \frac{1}{4}]$	$[6, -12]$
7	$[-X, -2X, -Z]$	$[0, 0, \frac{3}{4}]$	$[13, -20]$
8	$[2X, X, -Z]$	$[0, 0, \frac{3}{4}]$	$[14, -19]$
9	$[-X, X, -Z]$	$[0, 0, \frac{3}{4}]$	$[15, -21]$
10	$[X, 2X, -Z]$	$[0, 0, \frac{3}{4}]$	$[16, -23]$
11	$[-2X, -X, -Z]$	$[0, 0, \frac{3}{4}]$	$[17, -22]$
12	$[X, -X, -Z]$	$[0, 0, \frac{3}{4}]$	$[18, -24]$

Table 6: Wyckoff bond: 12f@2a

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, \frac{1}{4}]$	$[1, -11]$
2	$[0, X, Z]$	$[0, 0, \frac{1}{4}]$	$[2, -10]$
3	$[-X, -X, Z]$	$[0, 0, \frac{1}{4}]$	$[3, -12]$
4	$[-X, 0, Z]$	$[0, 0, \frac{1}{4}]$	$[4, -8]$
5	$[0, -X, Z]$	$[0, 0, \frac{1}{4}]$	$[5, -7]$
6	$[X, X, Z]$	$[0, 0, \frac{1}{4}]$	$[6, -9]$
7	$[-X, 0, -Z]$	$[0, 0, \frac{3}{4}]$	$[13, -23]$
8	$[0, -X, -Z]$	$[0, 0, \frac{3}{4}]$	$[14, -22]$
9	$[X, X, -Z]$	$[0, 0, \frac{3}{4}]$	$[15, -24]$
10	$[X, 0, -Z]$	$[0, 0, \frac{3}{4}]$	$[16, -20]$
11	$[0, X, -Z]$	$[0, 0, \frac{3}{4}]$	$[17, -19]$
12	$[-X, -X, -Z]$	$[0, 0, \frac{3}{4}]$	$[18, -21]$

Table 7: Wyckoff bond: 24g@2a

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, \frac{1}{4}]$	[1]
2	$[-Y, X - Y, Z]$	$[0, 0, \frac{1}{4}]$	[2]
3	$[-X + Y, -X, Z]$	$[0, 0, \frac{1}{4}]$	[3]
4	$[-X, -Y, Z]$	$[0, 0, \frac{1}{4}]$	[4]
5	$[Y, -X + Y, Z]$	$[0, 0, \frac{1}{4}]$	[5]
6	$[X - Y, X, Z]$	$[0, 0, \frac{1}{4}]$	[6]
7	$[Y, X, -Z]$	$[0, 0, \frac{1}{4}]$	[7]
8	$[X - Y, -Y, -Z]$	$[0, 0, \frac{1}{4}]$	[8]
9	$[-X, -X + Y, -Z]$	$[0, 0, \frac{1}{4}]$	[9]
10	$[-Y, -X, -Z]$	$[0, 0, \frac{1}{4}]$	[10]
11	$[-X + Y, Y, -Z]$	$[0, 0, \frac{1}{4}]$	[11]
12	$[X, X - Y, -Z]$	$[0, 0, \frac{1}{4}]$	[12]
13	$[-X, -Y, -Z]$	$[0, 0, \frac{3}{4}]$	[13]
14	$[Y, -X + Y, -Z]$	$[0, 0, \frac{3}{4}]$	[14]
15	$[X - Y, X, -Z]$	$[0, 0, \frac{3}{4}]$	[15]
16	$[X, Y, -Z]$	$[0, 0, \frac{3}{4}]$	[16]
17	$[-Y, X - Y, -Z]$	$[0, 0, \frac{3}{4}]$	[17]
18	$[-X + Y, -X, -Z]$	$[0, 0, \frac{3}{4}]$	[18]
19	$[-Y, -X, Z]$	$[0, 0, \frac{3}{4}]$	[19]
20	$[-X + Y, Y, Z]$	$[0, 0, \frac{3}{4}]$	[20]
21	$[X, X - Y, Z]$	$[0, 0, \frac{3}{4}]$	[21]
22	$[Y, X, Z]$	$[0, 0, \frac{3}{4}]$	[22]
23	$[X - Y, -Y, Z]$	$[0, 0, \frac{3}{4}]$	[23]
24	$[-X, -X + Y, Z]$	$[0, 0, \frac{3}{4}]$	[24]

* Wyckoff site: 2b, site symmetry: $6/m..$

Table 8: Wyckoff bond: 2a@2b

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, -13, -14, -15, -16, -17, -18]$
2	$[0, 0, -Z]$	$[0, 0, \frac{1}{2}]$	$[7, 8, 9, 10, 11, 12, -19, -20, -21, -22, -23, -24]$

Table 9: Wyckoff bond: 6b@2b

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, 0]$	$[1, -4, -13, 16]$
2	$[-Y, X - Y, 0]$	$[0, 0, 0]$	$[2, -5, -14, 17]$
3	$[-X + Y, -X, 0]$	$[0, 0, 0]$	$[3, -6, -15, 18]$
4	$[Y, X, 0]$	$[0, 0, \frac{1}{2}]$	$[7, -10, -19, 22]$
5	$[X - Y, -Y, 0]$	$[0, 0, \frac{1}{2}]$	$[8, -11, -20, 23]$
6	$[-X, -X + Y, 0]$	$[0, 0, \frac{1}{2}]$	$[9, -12, -21, 24]$

Table 10: Wyckoff bond: 12c@2b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1, -13]$
2	$[-Y, X - Y, Z]$	$[0, 0, 0]$	$[2, -14]$
3	$[-X + Y, -X, Z]$	$[0, 0, 0]$	$[3, -15]$
4	$[-X, -Y, Z]$	$[0, 0, 0]$	$[4, -16]$
5	$[Y, -X + Y, Z]$	$[0, 0, 0]$	$[5, -17]$
6	$[X - Y, X, Z]$	$[0, 0, 0]$	$[6, -18]$
7	$[Y, X, -Z]$	$[0, 0, \frac{1}{2}]$	$[7, -19]$
8	$[X - Y, -Y, -Z]$	$[0, 0, \frac{1}{2}]$	$[8, -20]$
9	$[-X, -X + Y, -Z]$	$[0, 0, \frac{1}{2}]$	$[9, -21]$
10	$[-Y, -X, -Z]$	$[0, 0, \frac{1}{2}]$	$[10, -22]$
11	$[-X + Y, Y, -Z]$	$[0, 0, \frac{1}{2}]$	$[11, -23]$
12	$[X, X - Y, -Z]$	$[0, 0, \frac{1}{2}]$	$[12, -24]$

* Wyckoff site: 4c, site symmetry: 3.2

Table 11: Wyckoff bond: 4a@4c

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[1, 2, 3, -10, -11, -12]$
2	$[0, 0, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[4, 5, 6, -7, -8, -9]$
3	$[0, 0, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[13, 14, 15, -22, -23, -24]$
4	$[0, 0, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[16, 17, 18, -19, -20, -21]$

Table 12: Wyckoff bond: 12b@4c

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[1, -11]$
2	$[0, X, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[2, -10]$
3	$[-X, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[3, -12]$
4	$[-X, 0, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[4, -8]$
5	$[0, -X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[5, -7]$
6	$[X, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[6, -9]$
7	$[-X, 0, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[13, -23]$
8	$[0, -X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[14, -22]$
9	$[X, X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[15, -24]$
10	$[X, 0, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[16, -20]$
11	$[0, X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[17, -19]$
12	$[-X, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[18, -21]$

Table 13: Wyckoff bond: 12c@4c

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[1, 11]$
2	$[-2X, -X, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[2, 10]$
3	$[X, -X, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[3, 12]$
4	$[-X, -2X, 0]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[4, 8]$
5	$[2X, X, 0]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[5, 7]$
6	$[-X, X, 0]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[6, 9]$
7	$[-X, -2X, 0]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[13, 23]$
8	$[2X, X, 0]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[14, 22]$
9	$[-X, X, 0]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[15, 24]$
10	$[X, 2X, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[16, 20]$
11	$[-2X, -X, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[17, 19]$
12	$[X, -X, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[18, 21]$

Table 14: Wyckoff bond: 24d@4c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	[1]
2	$[-Y, X - Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	[2]
3	$[-X + Y, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	[3]
4	$[-X, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	[4]
5	$[Y, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	[5]
6	$[X - Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	[6]
7	$[Y, X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	[7]
8	$[X - Y, -Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	[8]
9	$[-X, -X + Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	[9]
10	$[-Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	[10]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	[11]
12	$[X, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	[12]
13	$[-X, -Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	[13]
14	$[Y, -X + Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	[14]
15	$[X - Y, X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	[15]
16	$[X, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	[16]
17	$[-Y, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	[17]
18	$[-X + Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	[18]
19	$[-Y, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	[19]
20	$[-X + Y, Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	[20]
21	$[X, X - Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	[21]
22	$[Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	[22]
23	$[X - Y, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	[23]
24	$[-X, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	[24]

* Wyckoff site: 4d, site symmetry: $-6..$

Table 15: Wyckoff bond: 4a@4d

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 2, 3, -16, -17, -18]$
2	$[0, 0, Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[4, 5, 6, -13, -14, -15]$
3	$[0, 0, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[7, 8, 9, -22, -23, -24]$
4	$[0, 0, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[10, 11, 12, -19, -20, -21]$

Table 16: Wyckoff bond: 12b@4d

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 16]$
2	$[-Y, X - Y, 0]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[2, 17]$
3	$[-X + Y, -X, 0]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[3, 18]$
4	$[-X, -Y, 0]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[4, 13]$
5	$[Y, -X + Y, 0]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[5, 14]$
6	$[X - Y, X, 0]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[6, 15]$
7	$[Y, X, 0]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[7, 22]$
8	$[X - Y, -Y, 0]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[8, 23]$
9	$[-X, -X + Y, 0]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[9, 24]$
10	$[-Y, -X, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[10, 19]$
11	$[-X + Y, Y, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[11, 20]$
12	$[X, X - Y, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[12, 21]$

Table 17: Wyckoff bond: 24c@4d

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1]$
2	$[-Y, X - Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[2]$
3	$[-X + Y, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[3]$
4	$[-X, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[4]$
5	$[Y, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[5]$
6	$[X - Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[6]$
7	$[Y, X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[7]$
8	$[X - Y, -Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[8]$
9	$[-X, -X + Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[9]$
10	$[-Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[10]$
11	$[-X + Y, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[11]$
12	$[X, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[12]$
13	$[-X, -Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[13]$
14	$[Y, -X + Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[14]$
15	$[X - Y, X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[15]$
16	$[X, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[16]$
17	$[-Y, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[17]$

continued ...

Table 17

No.	vector	center	mapping
18	$[-X + Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	[18]
19	$[-Y, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	[19]
20	$[-X + Y, Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	[20]
21	$[X, X - Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	[21]
22	$[Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	[22]
23	$[X - Y, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	[23]
24	$[-X, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	[24]

* Wyckoff site: **4e**, site symmetry: $6..$

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	[1,2,3,4,5,6]
2	$[0, 0, -Z]$	$[0, 0, \frac{1}{2} - z]$	[7,8,9,10,11,12]
3	$[0, 0, -Z]$	$[0, 0, -z]$	[13,14,15,16,17,18]
4	$[0, 0, Z]$	$[0, 0, z + \frac{1}{2}]$	[19,20,21,22,23,24]

Table 19: Wyckoff bond: **12b@4e**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	[1,-4]
2	$[-Y, X - Y, 0]$	$[0, 0, z]$	[2,-5]
3	$[-X + Y, -X, 0]$	$[0, 0, z]$	[3,-6]
4	$[Y, X, 0]$	$[0, 0, \frac{1}{2} - z]$	[7,-10]
5	$[X - Y, -Y, 0]$	$[0, 0, \frac{1}{2} - z]$	[8,-11]
6	$[-X, -X + Y, 0]$	$[0, 0, \frac{1}{2} - z]$	[9,-12]
7	$[-X, -Y, 0]$	$[0, 0, -z]$	[13,-16]
8	$[Y, -X + Y, 0]$	$[0, 0, -z]$	[14,-17]
9	$[X - Y, X, 0]$	$[0, 0, -z]$	[15,-18]
10	$[-Y, -X, 0]$	$[0, 0, z + \frac{1}{2}]$	[19,-22]
11	$[-X + Y, Y, 0]$	$[0, 0, z + \frac{1}{2}]$	[20,-23]
12	$[X, X - Y, 0]$	$[0, 0, z + \frac{1}{2}]$	[21,-24]

Table 20: Wyckoff bond: **24c@4e**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	[1]
2	$[-Y, X - Y, Z]$	$[0, 0, z]$	[2]
3	$[-X + Y, -X, Z]$	$[0, 0, z]$	[3]

continued ...

Table 20

No.	vector	center	mapping
4	$[-X, -Y, Z]$	$[0, 0, z]$	[4]
5	$[Y, -X + Y, Z]$	$[0, 0, z]$	[5]
6	$[X - Y, X, Z]$	$[0, 0, z]$	[6]
7	$[Y, X, -Z]$	$[0, 0, \frac{1}{2} - z]$	[7]
8	$[X - Y, -Y, -Z]$	$[0, 0, \frac{1}{2} - z]$	[8]
9	$[-X, -X + Y, -Z]$	$[0, 0, \frac{1}{2} - z]$	[9]
10	$[-Y, -X, -Z]$	$[0, 0, \frac{1}{2} - z]$	[10]
11	$[-X + Y, Y, -Z]$	$[0, 0, \frac{1}{2} - z]$	[11]
12	$[X, X - Y, -Z]$	$[0, 0, \frac{1}{2} - z]$	[12]
13	$[-X, -Y, -Z]$	$[0, 0, -z]$	[13]
14	$[Y, -X + Y, -Z]$	$[0, 0, -z]$	[14]
15	$[X - Y, X, -Z]$	$[0, 0, -z]$	[15]
16	$[X, Y, -Z]$	$[0, 0, -z]$	[16]
17	$[-Y, X - Y, -Z]$	$[0, 0, -z]$	[17]
18	$[-X + Y, -X, -Z]$	$[0, 0, -z]$	[18]
19	$[-Y, -X, Z]$	$[0, 0, z + \frac{1}{2}]$	[19]
20	$[-X + Y, Y, Z]$	$[0, 0, z + \frac{1}{2}]$	[20]
21	$[X, X - Y, Z]$	$[0, 0, z + \frac{1}{2}]$	[21]
22	$[Y, X, Z]$	$[0, 0, z + \frac{1}{2}]$	[22]
23	$[X - Y, -Y, Z]$	$[0, 0, z + \frac{1}{2}]$	[23]
24	$[-X, -X + Y, Z]$	$[0, 0, z + \frac{1}{2}]$	[24]

* Wyckoff site: **6f**, site symmetry: **222**

Table 21: Wyckoff bond: **6a@6f**

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[1,-4,-8,11]
2	$[-2X, -X, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[2,-5,-7,10]
3	$[X, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[3,-6,-9,12]
4	$[-X, -2X, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[13,-16,-20,23]
5	$[2X, X, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[14,-17,-19,22]
6	$[-X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[15,-18,-21,24]

Table 22: Wyckoff bond: **6b@6f**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[1,-4,8,-11]
2	$[0, X, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[2,-5,7,-10]
3	$[-X, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[3,-6,9,-12]
4	$[-X, 0, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[13,-16,20,-23]
5	$[0, -X, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[14,-17,19,-22]

continued ...

Table 22

No.	vector	center	mapping
6	$[X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[15, -18, 21, -24]$

Table 23: Wyckoff bond: 6c@6f

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[1, 4, -8, -11]$
2	$[0, 0, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[2, 5, -7, -10]$
3	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[3, 6, -9, -12]$
4	$[0, 0, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[13, 16, -20, -23]$
5	$[0, 0, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[14, 17, -19, -22]$
6	$[0, 0, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[15, 18, -21, -24]$

Table 24: Wyckoff bond: 12d@6f

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[1, -4]$
2	$[-Y, X - Y, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[2, -5]$
3	$[-X + Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[3, -6]$
4	$[Y, X, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[7, -10]$
5	$[X - Y, -Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[8, -11]$
6	$[-X, -X + Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[9, -12]$
7	$[-X, -Y, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[13, -16]$
8	$[Y, -X + Y, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[14, -17]$
9	$[X - Y, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[15, -18]$
10	$[-Y, -X, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[19, -22]$
11	$[-X + Y, Y, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[20, -23]$
12	$[X, X - Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[21, -24]$

Table 25: Wyckoff bond: 12e@6f

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[1, -8]$
2	$[-2X, -X, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[2, -7]$
3	$[X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[3, -9]$
4	$[-X, -2X, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[4, -11]$
5	$[2X, X, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[5, -10]$
6	$[-X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[6, -12]$
7	$[-X, -2X, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[13, -20]$
8	$[2X, X, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[14, -19]$

continued ...

Table 25

No.	vector	center	mapping
9	$[-X, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[15,-21]
10	$[X, 2X, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[16,-23]
11	$[-2X, -X, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[17,-22]
12	$[X, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[18,-24]

Table 26: Wyckoff bond: **12f@6f**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[1,-11]
2	$[0, X, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[2,-10]
3	$[-X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[3,-12]
4	$[-X, 0, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[4,-8]
5	$[0, -X, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[5,-7]
6	$[X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[6,-9]
7	$[-X, 0, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[13,-23]
8	$[0, -X, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[14,-22]
9	$[X, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[15,-24]
10	$[X, 0, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[16,-20]
11	$[0, X, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[17,-19]
12	$[-X, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[18,-21]

Table 27: Wyckoff bond: **24g@6f**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[1]
2	$[-Y, X - Y, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[2]
3	$[-X + Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[3]
4	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[4]
5	$[Y, -X + Y, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[5]
6	$[X - Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[6]
7	$[Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[7]
8	$[X - Y, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[8]
9	$[-X, -X + Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[9]
10	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[10]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[11]
12	$[X, X - Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[12]
13	$[-X, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[13]
14	$[Y, -X + Y, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[14]
15	$[X - Y, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[15]
16	$[X, Y, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[16]
17	$[-Y, X - Y, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[17]
18	$[-X + Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[18]

continued ...

Table 27

No.	vector	center	mapping
19	$[-Y, -X, Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[19]
20	$[-X + Y, Y, Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[20]
21	$[X, X - Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[21]
22	$[Y, X, Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[22]
23	$[X - Y, -Y, Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[23]
24	$[-X, -X + Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[24]

* Wyckoff site: **6g**, site symmetry: $2/m..$

Table 28: Wyckoff bond: **6a@6g**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, 0, 0]$	[1,-4,-13,16]
2	$[-Y, X - Y, 0]$	$[0, \frac{1}{2}, 0]$	[2,-5,-14,17]
3	$[-X + Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[3,-6,-15,18]
4	$[Y, X, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[7,-10,-19,22]
5	$[X - Y, -Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[8,-11,-20,23]
6	$[-X, -X + Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9,-12,-21,24]

Table 29: Wyckoff bond: **6b@6g**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, 0]$	[1,4,-13,-16]
2	$[0, 0, Z]$	$[0, \frac{1}{2}, 0]$	[2,5,-14,-17]
3	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[3,6,-15,-18]
4	$[0, 0, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[7,10,-19,-22]
5	$[0, 0, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[8,11,-20,-23]
6	$[0, 0, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9,12,-21,-24]

Table 30: Wyckoff bond: **12c@6g**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, 0, 0]$	[1,-13]
2	$[-Y, X - Y, Z]$	$[0, \frac{1}{2}, 0]$	[2,-14]
3	$[-X + Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[3,-15]
4	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, 0]$	[4,-16]
5	$[Y, -X + Y, Z]$	$[0, \frac{1}{2}, 0]$	[5,-17]
6	$[X - Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[6,-18]
7	$[Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[7,-19]
8	$[X - Y, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[8,-20]

continued ...

Table 30

No.	vector	center	mapping
9	$[-X, -X + Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9,-21]
10	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[10,-22]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[11,-23]
12	$[X, X - Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[12,-24]

* Wyckoff site: 8h, site symmetry: 3..

Table 31: Wyckoff bond: 8a@8h

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[1,2,3]
2	$[0, 0, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[4,5,6]
3	$[0, 0, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	[7,8,9]
4	$[0, 0, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[10,11,12]
5	$[0, 0, -Z]$	$[\frac{2}{3}, \frac{1}{3}, -z]$	[13,14,15]
6	$[0, 0, -Z]$	$[\frac{1}{3}, \frac{2}{3}, -z]$	[16,17,18]
7	$[0, 0, Z]$	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	[19,20,21]
8	$[0, 0, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[22,23,24]

Table 32: Wyckoff bond: 24b@8h

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[1]
2	$[-Y, X - Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[2]
3	$[-X + Y, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[3]
4	$[-X, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[4]
5	$[Y, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[5]
6	$[X - Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[6]
7	$[Y, X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	[7]
8	$[X - Y, -Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	[8]
9	$[-X, -X + Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	[9]
10	$[-Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[10]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[11]
12	$[X, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[12]
13	$[-X, -Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, -z]$	[13]
14	$[Y, -X + Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, -z]$	[14]
15	$[X - Y, X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, -z]$	[15]
16	$[X, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, -z]$	[16]
17	$[-Y, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, -z]$	[17]
18	$[-X + Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, -z]$	[18]
19	$[-Y, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	[19]
20	$[-X + Y, Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	[20]

continued ...

Table 32

No.	vector	center	mapping
21	$[X, X - Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	[21]
22	$[Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[22]
23	$[X - Y, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[23]
24	$[-X, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[24]

* Wyckoff site: 12i, site symmetry: 2..

Table 33: Wyckoff bond: 12a@12i

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, 0, z]$	[1,-4]
2	$[-Y, X - Y, 0]$	$[0, \frac{1}{2}, z]$	[2,-5]
3	$[-X + Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[3,-6]
4	$[Y, X, 0]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[7,-10]
5	$[X - Y, -Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[8,-11]
6	$[-X, -X + Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[9,-12]
7	$[-X, -Y, 0]$	$[\frac{1}{2}, 0, -z]$	[13,-16]
8	$[Y, -X + Y, 0]$	$[0, \frac{1}{2}, -z]$	[14,-17]
9	$[X - Y, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	[15,-18]
10	$[-Y, -X, 0]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[19,-22]
11	$[-X + Y, Y, 0]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[20,-23]
12	$[X, X - Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[21,-24]

Table 34: Wyckoff bond: 12b@12i

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, z]$	[1,4]
2	$[0, 0, Z]$	$[0, \frac{1}{2}, z]$	[2,5]
3	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[3,6]
4	$[0, 0, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[7,10]
5	$[0, 0, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[8,11]
6	$[0, 0, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[9,12]
7	$[0, 0, -Z]$	$[\frac{1}{2}, 0, -z]$	[13,16]
8	$[0, 0, -Z]$	$[0, \frac{1}{2}, -z]$	[14,17]
9	$[0, 0, -Z]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	[15,18]
10	$[0, 0, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[19,22]
11	$[0, 0, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[20,23]
12	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[21,24]

Table 35: Wyckoff bond: 24c@12i

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, 0, z]$	[1]
2	$[-Y, X - Y, Z]$	$[0, \frac{1}{2}, z]$	[2]
3	$[-X + Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[3]
4	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, z]$	[4]
5	$[Y, -X + Y, Z]$	$[0, \frac{1}{2}, z]$	[5]
6	$[X - Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[6]
7	$[Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[7]
8	$[X - Y, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[8]
9	$[-X, -X + Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[9]
10	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[10]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[11]
12	$[X, X - Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[12]
13	$[-X, -Y, -Z]$	$[\frac{1}{2}, 0, -z]$	[13]
14	$[Y, -X + Y, -Z]$	$[0, \frac{1}{2}, -z]$	[14]
15	$[X - Y, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	[15]
16	$[X, Y, -Z]$	$[\frac{1}{2}, 0, -z]$	[16]
17	$[-Y, X - Y, -Z]$	$[0, \frac{1}{2}, -z]$	[17]
18	$[-X + Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	[18]
19	$[-Y, -X, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[19]
20	$[-X + Y, Y, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[20]
21	$[X, X - Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[21]
22	$[Y, X, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[22]
23	$[X - Y, -Y, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[23]
24	$[-X, -X + Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[24]

* Wyckoff site: 12j, site symmetry: .2.

Table 36: Wyckoff bond: 12a@12j

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[x, 0, \frac{1}{4}]$	[1, -8]
2	$[-2X, -X, Z]$	$[0, x, \frac{1}{4}]$	[2, -7]
3	$[X, -X, Z]$	$[-x, -x, \frac{1}{4}]$	[3, -9]
4	$[-X, -2X, Z]$	$[-x, 0, \frac{1}{4}]$	[4, -11]
5	$[2X, X, Z]$	$[0, -x, \frac{1}{4}]$	[5, -10]
6	$[-X, X, Z]$	$[x, x, \frac{1}{4}]$	[6, -12]
7	$[-X, -2X, -Z]$	$[-x, 0, \frac{3}{4}]$	[13, -20]
8	$[2X, X, -Z]$	$[0, -x, \frac{3}{4}]$	[14, -19]
9	$[-X, X, -Z]$	$[x, x, \frac{3}{4}]$	[15, -21]
10	$[X, 2X, -Z]$	$[x, 0, \frac{3}{4}]$	[16, -23]
11	$[-2X, -X, -Z]$	$[0, x, \frac{3}{4}]$	[17, -22]
12	$[X, -X, -Z]$	$[-x, -x, \frac{3}{4}]$	[18, -24]

Table 37: Wyckoff bond: 12b@12j

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, \frac{1}{4}]$	[1,8]
2	$[0, X, 0]$	$[0, x, \frac{1}{4}]$	[2,7]
3	$[-X, -X, 0]$	$[-x, -x, \frac{1}{4}]$	[3,9]
4	$[-X, 0, 0]$	$[-x, 0, \frac{1}{4}]$	[4,11]
5	$[0, -X, 0]$	$[0, -x, \frac{1}{4}]$	[5,10]
6	$[X, X, 0]$	$[x, x, \frac{1}{4}]$	[6,12]
7	$[-X, 0, 0]$	$[-x, 0, \frac{3}{4}]$	[13,20]
8	$[0, -X, 0]$	$[0, -x, \frac{3}{4}]$	[14,19]
9	$[X, X, 0]$	$[x, x, \frac{3}{4}]$	[15,21]
10	$[X, 0, 0]$	$[x, 0, \frac{3}{4}]$	[16,23]
11	$[0, X, 0]$	$[0, x, \frac{3}{4}]$	[17,22]
12	$[-X, -X, 0]$	$[-x, -x, \frac{3}{4}]$	[18,24]

Table 38: Wyckoff bond: 24c@12j

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, \frac{1}{4}]$	[1]
2	$[-Y, X - Y, Z]$	$[0, x, \frac{1}{4}]$	[2]
3	$[-X + Y, -X, Z]$	$[-x, -x, \frac{1}{4}]$	[3]
4	$[-X, -Y, Z]$	$[-x, 0, \frac{1}{4}]$	[4]
5	$[Y, -X + Y, Z]$	$[0, -x, \frac{1}{4}]$	[5]
6	$[X - Y, X, Z]$	$[x, x, \frac{1}{4}]$	[6]
7	$[Y, X, -Z]$	$[0, x, \frac{1}{4}]$	[7]
8	$[X - Y, -Y, -Z]$	$[x, 0, \frac{1}{4}]$	[8]
9	$[-X, -X + Y, -Z]$	$[-x, -x, \frac{1}{4}]$	[9]
10	$[-Y, -X, -Z]$	$[0, -x, \frac{1}{4}]$	[10]
11	$[-X + Y, Y, -Z]$	$[-x, 0, \frac{1}{4}]$	[11]
12	$[X, X - Y, -Z]$	$[x, x, \frac{1}{4}]$	[12]
13	$[-X, -Y, -Z]$	$[-x, 0, \frac{3}{4}]$	[13]
14	$[Y, -X + Y, -Z]$	$[0, -x, \frac{3}{4}]$	[14]
15	$[X - Y, X, -Z]$	$[x, x, \frac{3}{4}]$	[15]
16	$[X, Y, -Z]$	$[x, 0, \frac{3}{4}]$	[16]
17	$[-Y, X - Y, -Z]$	$[0, x, \frac{3}{4}]$	[17]
18	$[-X + Y, -X, -Z]$	$[-x, -x, \frac{3}{4}]$	[18]
19	$[-Y, -X, Z]$	$[0, -x, \frac{3}{4}]$	[19]
20	$[-X + Y, Y, Z]$	$[-x, 0, \frac{3}{4}]$	[20]
21	$[X, X - Y, Z]$	$[x, x, \frac{3}{4}]$	[21]
22	$[Y, X, Z]$	$[0, x, \frac{3}{4}]$	[22]
23	$[X - Y, -Y, Z]$	$[x, 0, \frac{3}{4}]$	[23]
24	$[-X, -X + Y, Z]$	$[-x, -x, \frac{3}{4}]$	[24]

* Wyckoff site: 12k, site symmetry: $\dots 2$

Table 39: Wyckoff bond: 12a@12k

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 2x, \frac{1}{4}]$	$[1, -11]$
2	$[0, X, Z]$	$[-2x, -x, \frac{1}{4}]$	$[2, -10]$
3	$[-X, -X, Z]$	$[x, -x, \frac{1}{4}]$	$[3, -12]$
4	$[-X, 0, Z]$	$[-x, -2x, \frac{1}{4}]$	$[4, -8]$
5	$[0, -X, Z]$	$[2x, x, \frac{1}{4}]$	$[5, -7]$
6	$[X, X, Z]$	$[-x, x, \frac{1}{4}]$	$[6, -9]$
7	$[-X, 0, -Z]$	$[-x, -2x, \frac{3}{4}]$	$[13, -23]$
8	$[0, -X, -Z]$	$[2x, x, \frac{3}{4}]$	$[14, -22]$
9	$[X, X, -Z]$	$[-x, x, \frac{3}{4}]$	$[15, -24]$
10	$[X, 0, -Z]$	$[x, 2x, \frac{3}{4}]$	$[16, -20]$
11	$[0, X, -Z]$	$[-2x, -x, \frac{3}{4}]$	$[17, -19]$
12	$[-X, -X, -Z]$	$[x, -x, \frac{3}{4}]$	$[18, -21]$

Table 40: Wyckoff bond: 12b@12k

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[x, 2x, \frac{1}{4}]$	$[1, 11]$
2	$[-2X, -X, 0]$	$[-2x, -x, \frac{1}{4}]$	$[2, 10]$
3	$[X, -X, 0]$	$[x, -x, \frac{1}{4}]$	$[3, 12]$
4	$[-X, -2X, 0]$	$[-x, -2x, \frac{1}{4}]$	$[4, 8]$
5	$[2X, X, 0]$	$[2x, x, \frac{1}{4}]$	$[5, 7]$
6	$[-X, X, 0]$	$[-x, x, \frac{1}{4}]$	$[6, 9]$
7	$[-X, -2X, 0]$	$[-x, -2x, \frac{3}{4}]$	$[13, 23]$
8	$[2X, X, 0]$	$[2x, x, \frac{3}{4}]$	$[14, 22]$
9	$[-X, X, 0]$	$[-x, x, \frac{3}{4}]$	$[15, 24]$
10	$[X, 2X, 0]$	$[x, 2x, \frac{3}{4}]$	$[16, 20]$
11	$[-2X, -X, 0]$	$[-2x, -x, \frac{3}{4}]$	$[17, 19]$
12	$[X, -X, 0]$	$[x, -x, \frac{3}{4}]$	$[18, 21]$

Table 41: Wyckoff bond: 24c@12k

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

continued ...

Table 41

No.	vector	center	mapping
10	$[-Y, -X, -Z]$	$[-2x, -x, \frac{1}{4}]$	[10]
11	$[-X + Y, Y, -Z]$	$[x, 2x, \frac{1}{4}]$	[11]
12	$[X, X - Y, -Z]$	$[x, -x, \frac{1}{4}]$	[12]
13	$[-X, -Y, -Z]$	$[-x, -2x, \frac{3}{4}]$	[13]
14	$[Y, -X + Y, -Z]$	$[2x, x, \frac{3}{4}]$	[14]
15	$[X - Y, X, -Z]$	$[-x, x, \frac{3}{4}]$	[15]
16	$[X, Y, -Z]$	$[x, 2x, \frac{3}{4}]$	[16]
17	$[-Y, X - Y, -Z]$	$[-2x, -x, \frac{3}{4}]$	[17]
18	$[-X + Y, -X, -Z]$	$[x, -x, \frac{3}{4}]$	[18]
19	$[-Y, -X, Z]$	$[-2x, -x, \frac{3}{4}]$	[19]
20	$[-X + Y, Y, Z]$	$[x, 2x, \frac{3}{4}]$	[20]
21	$[X, X - Y, Z]$	$[x, -x, \frac{3}{4}]$	[21]
22	$[Y, X, Z]$	$[2x, x, \frac{3}{4}]$	[22]
23	$[X - Y, -Y, Z]$	$[-x, -2x, \frac{3}{4}]$	[23]
24	$[-X, -X + Y, Z]$	$[-x, x, \frac{3}{4}]$	[24]

* Wyckoff site: 12l, site symmetry: $m..$

Table 42: Wyckoff bond: 12a@12l

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, y, 0]$	[1,16]
2	$[-Y, X - Y, 0]$	$[-y, x - y, 0]$	[2,17]
3	$[-X + Y, -X, 0]$	$[-x + y, -x, 0]$	[3,18]
4	$[-X, -Y, 0]$	$[-x, -y, 0]$	[4,13]
5	$[Y, -X + Y, 0]$	$[y, -x + y, 0]$	[5,14]
6	$[X - Y, X, 0]$	$[x - y, x, 0]$	[6,15]
7	$[Y, X, 0]$	$[y, x, \frac{1}{2}]$	[7,22]
8	$[X - Y, -Y, 0]$	$[x - y, -y, \frac{1}{2}]$	[8,23]
9	$[-X, -X + Y, 0]$	$[-x, -x + y, \frac{1}{2}]$	[9,24]
10	$[-Y, -X, 0]$	$[-y, -x, \frac{1}{2}]$	[10,19]
11	$[-X + Y, Y, 0]$	$[-x + y, y, \frac{1}{2}]$	[11,20]
12	$[X, X - Y, 0]$	$[x, x - y, \frac{1}{2}]$	[12,21]

Table 43: Wyckoff bond: 12b@12l

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, y, 0]$	[1,-16]
2	$[0, 0, Z]$	$[-y, x - y, 0]$	[2,-17]
3	$[0, 0, Z]$	$[-x + y, -x, 0]$	[3,-18]
4	$[0, 0, Z]$	$[-x, -y, 0]$	[4,-13]
5	$[0, 0, Z]$	$[y, -x + y, 0]$	[5,-14]

continued ...

Table 43

No.	vector	center	mapping
6	$[0, 0, Z]$	$[x - y, x, 0]$	$[6, -15]$
7	$[0, 0, -Z]$	$[y, x, \frac{1}{2}]$	$[7, -22]$
8	$[0, 0, -Z]$	$[x - y, -y, \frac{1}{2}]$	$[8, -23]$
9	$[0, 0, -Z]$	$[-x, -x + y, \frac{1}{2}]$	$[9, -24]$
10	$[0, 0, -Z]$	$[-y, -x, \frac{1}{2}]$	$[10, -19]$
11	$[0, 0, -Z]$	$[-x + y, y, \frac{1}{2}]$	$[11, -20]$
12	$[0, 0, -Z]$	$[x, x - y, \frac{1}{2}]$	$[12, -21]$

Table 44: Wyckoff bond: 24c@121

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, 0]$	[1]
2	$[-Y, X - Y, Z]$	$[-y, x - y, 0]$	[2]
3	$[-X + Y, -X, Z]$	$[-x + y, -x, 0]$	[3]
4	$[-X, -Y, Z]$	$[-x, -y, 0]$	[4]
5	$[Y, -X + Y, Z]$	$[y, -x + y, 0]$	[5]
6	$[X - Y, X, Z]$	$[x - y, x, 0]$	[6]
7	$[Y, X, -Z]$	$[y, x, \frac{1}{2}]$	[7]
8	$[X - Y, -Y, -Z]$	$[x - y, -y, \frac{1}{2}]$	[8]
9	$[-X, -X + Y, -Z]$	$[-x, -x + y, \frac{1}{2}]$	[9]
10	$[-Y, -X, -Z]$	$[-y, -x, \frac{1}{2}]$	[10]
11	$[-X + Y, Y, -Z]$	$[-x + y, y, \frac{1}{2}]$	[11]
12	$[X, X - Y, -Z]$	$[x, x - y, \frac{1}{2}]$	[12]
13	$[-X, -Y, -Z]$	$[-x, -y, 0]$	[13]
14	$[Y, -X + Y, -Z]$	$[y, -x + y, 0]$	[14]
15	$[X - Y, X, -Z]$	$[x - y, x, 0]$	[15]
16	$[X, Y, -Z]$	$[x, y, 0]$	[16]
17	$[-Y, X - Y, -Z]$	$[-y, x - y, 0]$	[17]
18	$[-X + Y, -X, -Z]$	$[-x + y, -x, 0]$	[18]
19	$[-Y, -X, Z]$	$[-y, -x, \frac{1}{2}]$	[19]
20	$[-X + Y, Y, Z]$	$[-x + y, y, \frac{1}{2}]$	[20]
21	$[X, X - Y, Z]$	$[x, x - y, \frac{1}{2}]$	[21]
22	$[Y, X, Z]$	$[y, x, \frac{1}{2}]$	[22]
23	$[X - Y, -Y, Z]$	$[x - y, -y, \frac{1}{2}]$	[23]
24	$[-X, -X + Y, Z]$	$[-x, -x + y, \frac{1}{2}]$	[24]

* Wyckoff site: 24m, site symmetry: 1

Table 45: Wyckoff bond: 24a@24m

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]

continued ...

Table 45

No.	vector	center	mapping
2	$[-Y, X - Y, Z]$	$[-y, x - y, z]$	[2]
3	$[-X + Y, -X, Z]$	$[-x + y, -x, z]$	[3]
4	$[-X, -Y, Z]$	$[-x, -y, z]$	[4]
5	$[Y, -X + Y, Z]$	$[y, -x + y, z]$	[5]
6	$[X - Y, X, Z]$	$[x - y, x, z]$	[6]
7	$[Y, X, -Z]$	$[y, x, \frac{1}{2} - z]$	[7]
8	$[X - Y, -Y, -Z]$	$[x - y, -y, \frac{1}{2} - z]$	[8]
9	$[-X, -X + Y, -Z]$	$[-x, -x + y, \frac{1}{2} - z]$	[9]
10	$[-Y, -X, -Z]$	$[-y, -x, \frac{1}{2} - z]$	[10]
11	$[-X + Y, Y, -Z]$	$[-x + y, y, \frac{1}{2} - z]$	[11]
12	$[X, X - Y, -Z]$	$[x, x - y, \frac{1}{2} - z]$	[12]
13	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[13]
14	$[Y, -X + Y, -Z]$	$[y, -x + y, -z]$	[14]
15	$[X - Y, X, -Z]$	$[x - y, x, -z]$	[15]
16	$[X, Y, -Z]$	$[x, y, -z]$	[16]
17	$[-Y, X - Y, -Z]$	$[-y, x - y, -z]$	[17]
18	$[-X + Y, -X, -Z]$	$[-x + y, -x, -z]$	[18]
19	$[-Y, -X, Z]$	$[-y, -x, z + \frac{1}{2}]$	[19]
20	$[-X + Y, Y, Z]$	$[-x + y, y, z + \frac{1}{2}]$	[20]
21	$[X, X - Y, Z]$	$[x, x - y, z + \frac{1}{2}]$	[21]
22	$[Y, X, Z]$	$[y, x, z + \frac{1}{2}]$	[22]
23	$[X - Y, -Y, Z]$	$[x - y, -y, z + \frac{1}{2}]$	[23]
24	$[-X, -X + Y, Z]$	$[-x, -x + y, z + \frac{1}{2}]$	[24]