

SG No. 193 D_{6h}^3 $P6_3/mcm$ [hexagonal]

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

* Wyckoff site: **2a**, site symmetry: $-62m$

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

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

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

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

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

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

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

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

continued ...

Table 4

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

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	$[-X, -2X, Z]$	$[0, 0, \frac{3}{4}]$	$[4, -11]$
5	$[2X, X, Z]$	$[0, 0, \frac{3}{4}]$	$[5, -10]$
6	$[-X, X, Z]$	$[0, 0, \frac{3}{4}]$	$[6, -12]$
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	$[X, 2X, -Z]$	$[0, 0, \frac{1}{4}]$	$[16, -23]$
11	$[-2X, -X, -Z]$	$[0, 0, \frac{1}{4}]$	$[17, -22]$
12	$[X, -X, -Z]$	$[0, 0, \frac{1}{4}]$	$[18, -24]$

Table 6: Wyckoff bond: 12f@2a

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

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	$[-X, -Y, Z]$	$[0, 0, \frac{3}{4}]$	[4]
5	$[Y, -X + Y, Z]$	$[0, 0, \frac{3}{4}]$	[5]
6	$[X - Y, X, Z]$	$[0, 0, \frac{3}{4}]$	[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	$[-Y, -X, -Z]$	$[0, 0, \frac{3}{4}]$	[10]
11	$[-X + Y, Y, -Z]$	$[0, 0, \frac{3}{4}]$	[11]
12	$[X, X - Y, -Z]$	$[0, 0, \frac{3}{4}]$	[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	$[X, Y, -Z]$	$[0, 0, \frac{1}{4}]$	[16]
17	$[-Y, X - Y, -Z]$	$[0, 0, \frac{1}{4}]$	[17]
18	$[-X + Y, -X, -Z]$	$[0, 0, \frac{1}{4}]$	[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	$[Y, X, Z]$	$[0, 0, \frac{1}{4}]$	[22]
23	$[X - Y, -Y, Z]$	$[0, 0, \frac{1}{4}]$	[23]
24	$[-X, -X + Y, Z]$	$[0, 0, \frac{1}{4}]$	[24]

* Wyckoff site: **2b**, site symmetry: **-3.m**

Table 8: Wyckoff bond: **2a@2b**

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

Table 9: Wyckoff bond: **6b@2b**

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

Table 10: Wyckoff bond: 6c@2b

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

Table 11: Wyckoff bond: 12d@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	$[-X, -Y, Z]$	$[0, 0, \frac{1}{2}]$	$[4, -16]$
5	$[Y, -X + Y, Z]$	$[0, 0, \frac{1}{2}]$	$[5, -17]$
6	$[X - Y, X, Z]$	$[0, 0, \frac{1}{2}]$	$[6, -18]$
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	$[-Y, -X, -Z]$	$[0, 0, 0]$	$[10, -22]$
11	$[-X + Y, Y, -Z]$	$[0, 0, 0]$	$[11, -23]$
12	$[X, X - Y, -Z]$	$[0, 0, 0]$	$[12, -24]$

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

Table 12: Wyckoff bond: 4a@4c

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

Table 13: Wyckoff bond: 12b@4c

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[1, 16]$
2	$[-Y, X - Y, 0]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[2, 17]$

continued ...

Table 13

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

Table 14: Wyckoff bond: 24c@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	$[-X, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	[4]
5	$[Y, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	[5]
6	$[X - Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	[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	$[-Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	[10]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	[11]
12	$[X, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	[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	$[X, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	[16]
17	$[-Y, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	[17]
18	$[-X + Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	[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	$[Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	[22]
23	$[X - Y, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	[23]
24	$[-X, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	[24]

* Wyckoff site: 4d, site symmetry: 3.2

Table 15: Wyckoff bond: 4a@4d

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

Table 16: Wyckoff bond: 12b@4d

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

Table 17: Wyckoff bond: 12c@4d

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

Table 18: Wyckoff bond: **24d@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	$[-X, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	[4]
5	$[Y, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	[5]
6	$[X - Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	[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	$[-Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	[10]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	[11]
12	$[X, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	[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	$[X, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	[16]
17	$[-Y, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	[17]
18	$[-X + Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	[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	$[Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	[22]
23	$[X - Y, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	[23]
24	$[-X, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, 0]$	[24]

* Wyckoff site: **4e**, site symmetry: **3.m**

Table 19: Wyckoff bond: **4a@4e**

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

Table 20: Wyckoff bond: **12b@4e**

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

continued ...

Table 20

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

Table 21: Wyckoff bond: 12c@4e

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

Table 22: Wyckoff bond: 24d@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]
4	$[-X, -Y, Z]$	$[0, 0, z + \frac{1}{2}]$	[4]
5	$[Y, -X + Y, Z]$	$[0, 0, z + \frac{1}{2}]$	[5]
6	$[X - Y, X, Z]$	$[0, 0, z + \frac{1}{2}]$	[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	$[-Y, -X, -Z]$	$[0, 0, -z]$	[10]
11	$[-X + Y, Y, -Z]$	$[0, 0, -z]$	[11]
12	$[X, X - Y, -Z]$	$[0, 0, -z]$	[12]
13	$[-X, -Y, -Z]$	$[0, 0, -z]$	[13]
14	$[Y, -X + Y, -Z]$	$[0, 0, -z]$	[14]

continued ...

Table 22

No.	vector	center	mapping
15	$[X - Y, X, -Z]$	$[0, 0, -z]$	[15]
16	$[X, Y, -Z]$	$[0, 0, \frac{1}{2} - z]$	[16]
17	$[-Y, X - Y, -Z]$	$[0, 0, \frac{1}{2} - z]$	[17]
18	$[-X + Y, -X, -Z]$	$[0, 0, \frac{1}{2} - z]$	[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	$[Y, X, Z]$	$[0, 0, z]$	[22]
23	$[X - Y, -Y, Z]$	$[0, 0, z]$	[23]
24	$[-X, -X + Y, Z]$	$[0, 0, z]$	[24]

* Wyckoff site: 6f, site symmetry: $\dots 2/m$

Table 23: Wyckoff bond: 6a@6f

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

Table 24: Wyckoff bond: 6b@6f

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

Table 25: Wyckoff bond: 12c@6f

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	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[4, -16]

continued ...

Table 25

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

* Wyckoff site: **6g**, site symmetry: **m2m**

Table 26: Wyckoff bond: **6a@6g**

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

Table 27: Wyckoff bond: **6b@6g**

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

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

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

Table 29: Wyckoff bond: 12d06g

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

Table 30: Wyckoff bond: 12e06g

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	$[-X, -2X, Z]$	$[-x, 0, \frac{3}{4}]$	$[4, -11]$
5	$[2X, X, Z]$	$[0, -x, \frac{3}{4}]$	$[5, -10]$
6	$[-X, X, Z]$	$[x, x, \frac{3}{4}]$	$[6, -12]$
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	$[X, 2X, -Z]$	$[x, 0, \frac{1}{4}]$	$[16, -23]$
11	$[-2X, -X, -Z]$	$[0, x, \frac{1}{4}]$	$[17, -22]$
12	$[X, -X, -Z]$	$[-x, -x, \frac{1}{4}]$	$[18, -24]$

Table 31: Wyckoff bond: 12f06g

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, \frac{1}{4}]$	$[1, 23]$
2	$[0, X, Z]$	$[0, x, \frac{1}{4}]$	$[2, 22]$
3	$[-X, -X, Z]$	$[-x, -x, \frac{1}{4}]$	$[3, 24]$
4	$[-X, 0, Z]$	$[-x, 0, \frac{3}{4}]$	$[4, 20]$
5	$[0, -X, Z]$	$[0, -x, \frac{3}{4}]$	$[5, 19]$
6	$[X, X, Z]$	$[x, x, \frac{3}{4}]$	$[6, 21]$
7	$[0, X, -Z]$	$[0, x, \frac{1}{4}]$	$[7, 17]$

continued ...

Table 31

No.	vector	center	mapping
8	$[X, 0, -Z]$	$[x, 0, \frac{1}{4}]$	[8,16]
9	$[-X, -X, -Z]$	$[-x, -x, \frac{1}{4}]$	[9,18]
10	$[0, -X, -Z]$	$[0, -x, \frac{3}{4}]$	[10,14]
11	$[-X, 0, -Z]$	$[-x, 0, \frac{3}{4}]$	[11,13]
12	$[X, X, -Z]$	$[x, x, \frac{3}{4}]$	[12,15]

Table 32: Wyckoff bond: **24g@6g**

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	$[-X, -Y, Z]$	$[-x, 0, \frac{3}{4}]$	[4]
5	$[Y, -X + Y, Z]$	$[0, -x, \frac{3}{4}]$	[5]
6	$[X - Y, X, Z]$	$[x, x, \frac{3}{4}]$	[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	$[-Y, -X, -Z]$	$[0, -x, \frac{3}{4}]$	[10]
11	$[-X + Y, Y, -Z]$	$[-x, 0, \frac{3}{4}]$	[11]
12	$[X, X - Y, -Z]$	$[x, x, \frac{3}{4}]$	[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	$[X, Y, -Z]$	$[x, 0, \frac{1}{4}]$	[16]
17	$[-Y, X - Y, -Z]$	$[0, x, \frac{1}{4}]$	[17]
18	$[-X + Y, -X, -Z]$	$[-x, -x, \frac{1}{4}]$	[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	$[Y, X, Z]$	$[0, x, \frac{1}{4}]$	[22]
23	$[X - Y, -Y, Z]$	$[x, 0, \frac{1}{4}]$	[23]
24	$[-X, -X + Y, Z]$	$[-x, -x, \frac{1}{4}]$	[24]

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

Table 33: Wyckoff bond: **8a@8h**

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

continued ...

Table 33

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

Table 34: 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	$[-X, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[4]
5	$[Y, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[5]
6	$[X - Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[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	$[-Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, -z]$	[10]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, -z]$	[11]
12	$[X, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, -z]$	[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	$[X, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[16]
17	$[-Y, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[17]
18	$[-X + Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[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]
21	$[X, X - Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	[21]
22	$[Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[22]
23	$[X - Y, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[23]
24	$[-X, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[24]

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

Table 35: Wyckoff bond: **12a@12i**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 2x, 0]$	$[1, -11]$
2	$[0, X, Z]$	$[-2x, -x, 0]$	$[2, -10]$
3	$[-X, -X, Z]$	$[x, -x, 0]$	$[3, -12]$

continued ...

Table 35

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

Table 36: Wyckoff bond: 12b@12i

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

Table 37: Wyckoff bond: 24c@12i

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

continued ...

Table 37

No.	vector	center	mapping
14	$[Y, -X + Y, -Z]$	$[2x, x, 0]$	[14]
15	$[X - Y, X, -Z]$	$[-x, x, 0]$	[15]
16	$[X, Y, -Z]$	$[x, 2x, \frac{1}{2}]$	[16]
17	$[-Y, X - Y, -Z]$	$[-2x, -x, \frac{1}{2}]$	[17]
18	$[-X + Y, -X, -Z]$	$[x, -x, \frac{1}{2}]$	[18]
19	$[-Y, -X, Z]$	$[-2x, -x, \frac{1}{2}]$	[19]
20	$[-X + Y, Y, Z]$	$[x, 2x, \frac{1}{2}]$	[20]
21	$[X, X - Y, Z]$	$[x, -x, \frac{1}{2}]$	[21]
22	$[Y, X, Z]$	$[2x, x, 0]$	[22]
23	$[X - Y, -Y, Z]$	$[-x, -2x, 0]$	[23]
24	$[-X, -X + Y, Z]$	$[-x, x, 0]$	[24]

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

Table 38: Wyckoff bond: 12a@12j

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

Table 39: Wyckoff bond: 12b@12j

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

continued ...

Table 39

No.	vector	center	mapping
10	$[0, 0, -Z]$	$[-y, -x, \frac{3}{4}]$	[10,-19]
11	$[0, 0, -Z]$	$[-x + y, y, \frac{3}{4}]$	[11,-20]
12	$[0, 0, -Z]$	$[x, x - y, \frac{3}{4}]$	[12,-21]

Table 40: Wyckoff bond: 24c@12j

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

* Wyckoff site: 12k, site symmetry: $\bar{6}m$

Table 41: Wyckoff bond: 12a@12k

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, z]$	[1,23]
2	$[0, X, Z]$	$[0, x, z]$	[2,22]
3	$[-X, -X, Z]$	$[-x, -x, z]$	[3,24]
4	$[-X, 0, Z]$	$[-x, 0, z + \frac{1}{2}]$	[4,20]
5	$[0, -X, Z]$	$[0, -x, z + \frac{1}{2}]$	[5,19]

continued ...

Table 41

No.	vector	center	mapping
6	$[X, X, Z]$	$[x, x, z + \frac{1}{2}]$	[6,21]
7	$[0, X, -Z]$	$[0, x, \frac{1}{2} - z]$	[7,17]
8	$[X, 0, -Z]$	$[x, 0, \frac{1}{2} - z]$	[8,16]
9	$[-X, -X, -Z]$	$[-x, -x, \frac{1}{2} - z]$	[9,18]
10	$[0, -X, -Z]$	$[0, -x, -z]$	[10,14]
11	$[-X, 0, -Z]$	$[-x, 0, -z]$	[11,13]
12	$[X, X, -Z]$	$[x, x, -z]$	[12,15]

Table 42: Wyckoff bond: 12b@12k

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

Table 43: Wyckoff bond: 24c@12k

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

continued ...

Table 43

No.	vector	center	mapping
16	$[X, Y, -Z]$	$[x, 0, \frac{1}{2} - z]$	[16]
17	$[-Y, X - Y, -Z]$	$[0, x, \frac{1}{2} - z]$	[17]
18	$[-X + Y, -X, -Z]$	$[-x, -x, \frac{1}{2} - z]$	[18]
19	$[-Y, -X, Z]$	$[0, -x, z + \frac{1}{2}]$	[19]
20	$[-X + Y, Y, Z]$	$[-x, 0, z + \frac{1}{2}]$	[20]
21	$[X, X - Y, Z]$	$[x, x, z + \frac{1}{2}]$	[21]
22	$[Y, X, Z]$	$[0, x, z]$	[22]
23	$[X - Y, -Y, Z]$	$[x, 0, z]$	[23]
24	$[-X, -X + Y, Z]$	$[-x, -x, z]$	[24]

* Wyckoff site: 241, site symmetry: 1

Table 44: Wyckoff bond: 24a@241

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