

SG No. 201 $T_h^2 Pn\bar{3}$ [cubic]

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

* Wyckoff site: **2a**, site symmetry: **23**.

Table 1: Wyckoff bond: **6a@2a**

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

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

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

Table 3: Wyckoff bond: **12c@2a**

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

Table 4: Wyckoff bond: 24d@2a

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

* Wyckoff site: 4b, site symmetry: $\bar{3}$.

Table 5: Wyckoff bond: 4a@4b

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

Table 6: Wyckoff bond: 12b@4b

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

continued ...

Table 6

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

* Wyckoff site: 4c, site symmetry: $\bar{3}$.

Table 7: Wyckoff bond: 4a@4c

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

Table 8: Wyckoff bond: 12b@4c

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

* Wyckoff site: 6d, site symmetry: $222..$

Table 9: Wyckoff bond: 6a@6d

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

Table 10: Wyckoff bond: 6b@6d

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

Table 11: Wyckoff bond: 6c@6d

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

Table 12: Wyckoff bond: 12d@6d

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

continued ...

Table 12

No.	vector	center	mapping
10	$[0, X, -Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[19, -20]$
11	$[-Y, 0, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	$[21, -22]$
12	$[-Y, 0, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	$[23, -24]$

Table 13: Wyckoff bond: **12e@6d**

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

Table 14: Wyckoff bond: **12f@6d**

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

Table 15: Wyckoff bond: 24g@6d

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

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

Table 16: Wyckoff bond: 8a@8e

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

Table 17: Wyckoff bond: 24b@8e

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

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

Table 18: Wyckoff bond: 12a@12f

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

Table 19: Wyckoff bond: 12b@12f

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

Table 20: Wyckoff bond: 24c@12f

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

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

Table 21: Wyckoff bond: 12a@12g

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

Table 22: Wyckoff bond: 12b@12g

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

Table 23: Wyckoff bond: 24c@12g

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

continued ...

Table 23

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

* Wyckoff site: **24h**, site symmetry: 1

Table 24: Wyckoff bond: **24a@24h**

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

