

SG No. 207 O^1 $P432$ [cubic]

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

* Wyckoff site: **1a**, site symmetry: 432

Table 1: Wyckoff bond: **3a@1a**

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

Table 2: Wyckoff bond: **4b@1a**

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

Table 3: Wyckoff bond: **6c@1a**

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

Table 4: Wyckoff bond: **12d@1a**

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

continued ...

Table 4

No.	vector	center	mapping
11	$[X, -Y, -X]$	$[0, 0, 0]$	$[11, -18]$
12	$[-X, -Y, X]$	$[0, 0, 0]$	$[12, -17]$

Table 5: Wyckoff bond: 12e@1a

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

Table 6: Wyckoff bond: 24f@1a

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

continued ...

Table 6

No.	vector	center	mapping
21	$[Z, Y, -X]$	$[0, 0, 0]$	[21]
22	$[Z, -Y, X]$	$[0, 0, 0]$	[22]
23	$[-Z, Y, X]$	$[0, 0, 0]$	[23]
24	$[-Z, -Y, -X]$	$[0, 0, 0]$	[24]

* Wyckoff site: 1b, site symmetry: 432

Table 7: Wyckoff bond: 3a@1b

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

Table 8: Wyckoff bond: 4b@1b

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

Table 9: Wyckoff bond: 6c@1b

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

Table 10: Wyckoff bond: 12d@1b

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

continued ...

Table 10

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

Table 11: Wyckoff bond: 12e@1b

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

Table 12: Wyckoff bond: 24f@1b

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

continued ...

Table 12

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

* Wyckoff site: 3c, site symmetry: 42.2

Table 13: Wyckoff bond: 3a@3c

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

Table 14: Wyckoff bond: 6b@3c

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

Table 15: Wyckoff bond: 6c@3c

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

Table 16: Wyckoff bond: 12d@3c

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

Table 17: Wyckoff bond: 12e@3c

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

Table 18: Wyckoff bond: 12f@3c

No.	vector	center	mapping
1	[0, X, Y]	[0, 1/2, 1/2]	[1, -4]
2	[0, -X, Y]	[0, 1/2, 1/2]	[2, -3]
3	[Y, 0, X]	[1/2, 0, 1/2]	[5, -8]
4	[Y, 0, -X]	[1/2, 0, 1/2]	[6, -7]
5	[X, Y, 0]	[1/2, 1/2, 0]	[9, -12]
6	[-X, Y, 0]	[1/2, 1/2, 0]	[10, -11]
7	[X, 0, -Y]	[1/2, 0, 1/2]	[13, -16]

continued ...

Table 18

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

Table 19: Wyckoff bond: 24g@3c

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

* Wyckoff site: 3d, site symmetry: 42.2

Table 20: Wyckoff bond: 3a@3d

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

Table 21: Wyckoff bond: 6b@3d

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

Table 22: Wyckoff bond: 6c@3d

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

Table 23: Wyckoff bond: 12d@3d

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

Table 24: Wyckoff bond: 12e@3d

No.	vector	center	mapping
1	[X, Y, 0]	$[\frac{1}{2}, 0, 0]$	[1, -2]
2	[-X, Y, 0]	$[\frac{1}{2}, 0, 0]$	[3, -4]
3	[0, X, Y]	$[0, \frac{1}{2}, 0]$	[5, -6]

continued ...

Table 24

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

Table 25: Wyckoff bond: 12f@3d

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

Table 26: Wyckoff bond: 24g@3d

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

continued ...

Table 26

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

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

Table 27: Wyckoff bond: **6a@6e**

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

Table 28: Wyckoff bond: **12b@6e**

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

Table 29: Wyckoff bond: 24c@6e

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

* Wyckoff site: 6f, site symmetry: 4..

Table 30: Wyckoff bond: 6a@6f

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

Table 31: Wyckoff bond: 12b@6f

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

continued ...

Table 31

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

Table 32: Wyckoff bond: 24c@6f

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

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

Table 33: Wyckoff bond: 8a@8g

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

Table 34: Wyckoff bond: 24b@8g

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

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

Table 35: Wyckoff bond: 12a@12h

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

Table 36: Wyckoff bond: 12b@12h

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

Table 37: Wyckoff bond: 24c@12h

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

continued ...

Table 37

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

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

Table 38: Wyckoff bond: 12a@12i

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

Table 39: Wyckoff bond: 12b@12i

No.	vector	center	mapping
1	$[0, X, X]$	$[0, y, y]$	[1,18]
2	$[0, -X, X]$	$[0, -y, y]$	[2,20]
3	$[0, X, -X]$	$[0, y, -y]$	[3,17]
4	$[0, -X, -X]$	$[0, -y, -y]$	[4,19]
5	$[X, 0, X]$	$[y, 0, y]$	[5,15]

continued ...

Table 39

No.	vector	center	mapping
6	$[X, 0, -X]$	$[y, 0, -y]$	[6,13]
7	$[-X, 0, X]$	$[-y, 0, y]$	[7,16]
8	$[-X, 0, -X]$	$[-y, 0, -y]$	[8,14]
9	$[X, X, 0]$	$[y, y, 0]$	[9,21]
10	$[-X, X, 0]$	$[-y, y, 0]$	[10,23]
11	$[X, -X, 0]$	$[y, -y, 0]$	[11,22]
12	$[-X, -X, 0]$	$[-y, -y, 0]$	[12,24]

Table 40: Wyckoff bond: 24c@12i

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

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

Table 41: Wyckoff bond: 12a@12j

No.	vector	center	mapping
1	$[Y, X, -X]$	$[\frac{1}{2}, y, y]$	[1,-18]

continued ...

Table 41

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

Table 42: Wyckoff bond: 12b@12j

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

Table 43: Wyckoff bond: 24c@12j

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

continued ...

Table 43

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

* Wyckoff site: 24k, site symmetry: 1

Table 44: Wyckoff bond: 24a@24k

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