

PG No. 32 O_h $m\bar{3}m$ [cubic]

* Wyckoff site: 6a, site symmetry: $4m.m$

Table 1: Wyckoff bond: 6a@6a

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	$[1, 4, 17, 20, 26, 27, 42, 43]$
2	$[-X, 0, 0]$	$[-x, 0, 0]$	$[2, 3, 18, 19, 25, 28, 41, 44]$
3	$[0, X, 0]$	$[0, x, 0]$	$[5, 8, 13, 16, 30, 31, 38, 39]$
4	$[0, -X, 0]$	$[0, -x, 0]$	$[6, 7, 14, 15, 29, 32, 37, 40]$
5	$[0, 0, X]$	$[0, 0, x]$	$[9, 12, 22, 23, 34, 35, 45, 48]$
6	$[0, 0, -X]$	$[0, 0, -x]$	$[10, 11, 21, 24, 33, 36, 46, 47]$

Table 2: Wyckoff bond: 12b@6a

No.	vector	center	mapping
1	$[0, X, X]$	$[x, 0, 0]$	$[1, -4, -42, 43]$
2	$[0, -X, X]$	$[-x, 0, 0]$	$[2, -3, 41, -44]$
3	$[X, 0, X]$	$[0, x, 0]$	$[5, -8, 38, -39]$
4	$[X, 0, -X]$	$[0, -x, 0]$	$[6, -7, -37, 40]$
5	$[X, X, 0]$	$[0, 0, x]$	$[9, -12, -45, 48]$
6	$[-X, X, 0]$	$[0, 0, -x]$	$[10, -11, 46, -47]$
7	$[X, 0, -X]$	$[0, x, 0]$	$[13, -16, -30, 31]$
8	$[-X, 0, -X]$	$[0, -x, 0]$	$[14, -15, 29, -32]$
9	$[0, X, -X]$	$[x, 0, 0]$	$[17, -20, 26, -27]$
10	$[0, X, X]$	$[-x, 0, 0]$	$[18, -19, -25, 28]$
11	$[X, X, 0]$	$[0, 0, -x]$	$[21, -24, -33, 36]$
12	$[X, -X, 0]$	$[0, 0, x]$	$[22, -23, 34, -35]$

Table 3: Wyckoff bond: 12c@6a

No.	vector	center	mapping
1	$[0, 0, X]$	$[x, 0, 0]$	$[1, -4, -26, 27]$
2	$[0, 0, -X]$	$[-x, 0, 0]$	$[2, -3, -25, 28]$
3	$[X, 0, 0]$	$[0, x, 0]$	$[5, -8, -30, 31]$
4	$[X, 0, 0]$	$[0, -x, 0]$	$[6, -7, -29, 32]$
5	$[0, X, 0]$	$[0, 0, x]$	$[9, -12, -34, 35]$
6	$[0, X, 0]$	$[0, 0, -x]$	$[10, -11, -33, 36]$
7	$[0, 0, -X]$	$[0, x, 0]$	$[13, -16, -38, 39]$
8	$[0, 0, -X]$	$[0, -x, 0]$	$[14, -15, -37, 40]$
9	$[0, X, 0]$	$[x, 0, 0]$	$[17, -20, -42, 43]$
10	$[0, X, 0]$	$[-x, 0, 0]$	$[18, -19, -41, 44]$
11	$[X, 0, 0]$	$[0, 0, -x]$	$[21, -24, -46, 47]$
12	$[X, 0, 0]$	$[0, 0, x]$	$[22, -23, -45, 48]$

Table 4: Wyckoff bond: 24d@6a

No.	vector	center	mapping
1	$[Y, X, X]$	$[x, 0, 0]$	$[1, 43]$
2	$[-Y, -X, X]$	$[-x, 0, 0]$	$[2, 41]$
3	$[-Y, X, -X]$	$[-x, 0, 0]$	$[3, 44]$
4	$[Y, -X, -X]$	$[x, 0, 0]$	$[4, 42]$
5	$[X, Y, X]$	$[0, x, 0]$	$[5, 38]$
6	$[X, -Y, -X]$	$[0, -x, 0]$	$[6, 40]$
7	$[-X, -Y, X]$	$[0, -x, 0]$	$[7, 37]$
8	$[-X, Y, -X]$	$[0, x, 0]$	$[8, 39]$
9	$[X, X, Y]$	$[0, 0, x]$	$[9, 48]$
10	$[-X, X, -Y]$	$[0, 0, -x]$	$[10, 46]$
11	$[X, -X, -Y]$	$[0, 0, -x]$	$[11, 47]$
12	$[-X, -X, Y]$	$[0, 0, x]$	$[12, 45]$
13	$[X, Y, -X]$	$[0, x, 0]$	$[13, 31]$
14	$[-X, -Y, -X]$	$[0, -x, 0]$	$[14, 29]$
15	$[X, -Y, X]$	$[0, -x, 0]$	$[15, 32]$
16	$[-X, Y, X]$	$[0, x, 0]$	$[16, 30]$
17	$[Y, X, -X]$	$[x, 0, 0]$	$[17, 26]$
18	$[-Y, X, X]$	$[-x, 0, 0]$	$[18, 28]$
19	$[-Y, -X, -X]$	$[-x, 0, 0]$	$[19, 25]$
20	$[Y, -X, X]$	$[x, 0, 0]$	$[20, 27]$
21	$[X, X, -Y]$	$[0, 0, -x]$	$[21, 36]$
22	$[X, -X, Y]$	$[0, 0, x]$	$[22, 34]$
23	$[-X, X, Y]$	$[0, 0, x]$	$[23, 35]$
24	$[-X, -X, -Y]$	$[0, 0, -x]$	$[24, 33]$

Table 5: Wyckoff bond: 24e@6a

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, 0, 0]$	$[1, 26]$
2	$[-X, -Y, 0]$	$[-x, 0, 0]$	$[2, 25]$
3	$[-X, Y, 0]$	$[-x, 0, 0]$	$[3, 28]$
4	$[X, -Y, 0]$	$[x, 0, 0]$	$[4, 27]$
5	$[0, X, Y]$	$[0, x, 0]$	$[5, 30]$
6	$[0, -X, -Y]$	$[0, -x, 0]$	$[6, 29]$
7	$[0, -X, Y]$	$[0, -x, 0]$	$[7, 32]$
8	$[0, X, -Y]$	$[0, x, 0]$	$[8, 31]$
9	$[Y, 0, X]$	$[0, 0, x]$	$[9, 34]$
10	$[-Y, 0, -X]$	$[0, 0, -x]$	$[10, 33]$
11	$[Y, 0, -X]$	$[0, 0, -x]$	$[11, 36]$
12	$[-Y, 0, X]$	$[0, 0, x]$	$[12, 35]$
13	$[Y, X, 0]$	$[0, x, 0]$	$[13, 38]$
14	$[-Y, -X, 0]$	$[0, -x, 0]$	$[14, 37]$

continued ...

Table 5

No.	vector	center	mapping
15	$[Y, -X, 0]$	$[0, -x, 0]$	$[15, 40]$
16	$[-Y, X, 0]$	$[0, x, 0]$	$[16, 39]$
17	$[X, 0, -Y]$	$[x, 0, 0]$	$[17, 42]$
18	$[-X, 0, Y]$	$[-x, 0, 0]$	$[18, 41]$
19	$[-X, 0, -Y]$	$[-x, 0, 0]$	$[19, 44]$
20	$[X, 0, Y]$	$[x, 0, 0]$	$[20, 43]$
21	$[0, Y, -X]$	$[0, 0, -x]$	$[21, 46]$
22	$[0, -Y, X]$	$[0, 0, x]$	$[22, 45]$
23	$[0, Y, X]$	$[0, 0, x]$	$[23, 48]$
24	$[0, -Y, -X]$	$[0, 0, -x]$	$[24, 47]$

Table 6: Wyckoff bond: 24f@6a

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	$[Y, -X, 0]$	$[0, 0, x]$	$[22, -23]$
13	$[0, -X, -Y]$	$[-x, 0, 0]$	$[25, -28]$
14	$[0, X, -Y]$	$[x, 0, 0]$	$[26, -27]$
15	$[-Y, 0, -X]$	$[0, -x, 0]$	$[29, -32]$
16	$[-Y, 0, X]$	$[0, x, 0]$	$[30, -31]$
17	$[-X, -Y, 0]$	$[0, 0, -x]$	$[33, -36]$
18	$[X, -Y, 0]$	$[0, 0, x]$	$[34, -35]$
19	$[-X, 0, Y]$	$[0, -x, 0]$	$[37, -40]$
20	$[X, 0, Y]$	$[0, x, 0]$	$[38, -39]$
21	$[0, -Y, X]$	$[-x, 0, 0]$	$[41, -44]$
22	$[0, -Y, -X]$	$[x, 0, 0]$	$[42, -43]$
23	$[-Y, -X, 0]$	$[0, 0, x]$	$[45, -48]$
24	$[-Y, X, 0]$	$[0, 0, -x]$	$[46, -47]$

Table 7: Wyckoff bond: 48g@6a

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]
25	$[-X, -Y, -Z]$	$[-x, 0, 0]$	[25]
26	$[X, Y, -Z]$	$[x, 0, 0]$	[26]
27	$[X, -Y, Z]$	$[x, 0, 0]$	[27]
28	$[-X, Y, Z]$	$[-x, 0, 0]$	[28]
29	$[-Z, -X, -Y]$	$[0, -x, 0]$	[29]
30	$[-Z, X, Y]$	$[0, x, 0]$	[30]
31	$[Z, X, -Y]$	$[0, x, 0]$	[31]
32	$[Z, -X, Y]$	$[0, -x, 0]$	[32]
33	$[-Y, -Z, -X]$	$[0, 0, -x]$	[33]
34	$[Y, -Z, X]$	$[0, 0, x]$	[34]
35	$[-Y, Z, X]$	$[0, 0, x]$	[35]
36	$[Y, Z, -X]$	$[0, 0, -x]$	[36]
37	$[-Y, -X, Z]$	$[0, -x, 0]$	[37]
38	$[Y, X, Z]$	$[0, x, 0]$	[38]
39	$[-Y, X, -Z]$	$[0, x, 0]$	[39]
40	$[Y, -X, -Z]$	$[0, -x, 0]$	[40]
41	$[-X, -Z, Y]$	$[-x, 0, 0]$	[41]
42	$[X, -Z, -Y]$	$[x, 0, 0]$	[42]
43	$[X, Z, Y]$	$[x, 0, 0]$	[43]
44	$[-X, Z, -Y]$	$[-x, 0, 0]$	[44]
45	$[-Z, -Y, X]$	$[0, 0, x]$	[45]
46	$[-Z, Y, -X]$	$[0, 0, -x]$	[46]

continued ...

Table 7

No.	vector	center	mapping
47	$[Z, -Y, -X]$	$[0, 0, -x]$	[47]
48	$[Z, Y, X]$	$[0, 0, x]$	[48]

* Wyckoff site: 8b, site symmetry: $.3\bar{m}$

Table 8: Wyckoff bond: 8a@8b

No.	vector	center	mapping
1	$[X, X, X]$	$[x, x, x]$	[1, 5, 9, 38, 43, 48]
2	$[-X, -X, X]$	$[-x, -x, x]$	[2, 7, 12, 37, 41, 45]
3	$[-X, X, -X]$	$[-x, x, -x]$	[3, 8, 10, 39, 44, 46]
4	$[X, -X, -X]$	$[x, -x, -x]$	[4, 6, 11, 40, 42, 47]
5	$[X, X, -X]$	$[x, x, -x]$	[13, 17, 21, 26, 31, 36]
6	$[-X, -X, -X]$	$[-x, -x, -x]$	[14, 19, 24, 25, 29, 33]
7	$[X, -X, X]$	$[x, -x, x]$	[15, 20, 22, 27, 32, 34]
8	$[-X, X, X]$	$[-x, x, x]$	[16, 18, 23, 28, 30, 35]

Table 9: Wyckoff bond: 24b@8b

No.	vector	center	mapping
1	$[X, X, Y]$	$[x, x, x]$	[1, 38]
2	$[-X, -X, Y]$	$[-x, -x, x]$	[2, 37]
3	$[-X, X, -Y]$	$[-x, x, -x]$	[3, 39]
4	$[X, -X, -Y]$	$[x, -x, -x]$	[4, 40]
5	$[Y, X, X]$	$[x, x, x]$	[5, 48]
6	$[Y, -X, -X]$	$[x, -x, -x]$	[6, 47]
7	$[-Y, -X, X]$	$[-x, -x, x]$	[7, 45]
8	$[-Y, X, -X]$	$[-x, x, -x]$	[8, 46]
9	$[X, Y, X]$	$[x, x, x]$	[9, 43]
10	$[-X, Y, -X]$	$[-x, x, -x]$	[10, 44]
11	$[X, -Y, -X]$	$[x, -x, -x]$	[11, 42]
12	$[-X, -Y, X]$	$[-x, -x, x]$	[12, 41]
13	$[X, X, -Y]$	$[x, x, -x]$	[13, 26]
14	$[-X, -X, -Y]$	$[-x, -x, -x]$	[14, 25]
15	$[X, -X, Y]$	$[x, -x, x]$	[15, 27]
16	$[-X, X, Y]$	$[-x, x, x]$	[16, 28]
17	$[X, Y, -X]$	$[x, x, -x]$	[17, 36]
18	$[-X, Y, X]$	$[-x, x, x]$	[18, 35]
19	$[-X, -Y, -X]$	$[-x, -x, -x]$	[19, 33]
20	$[X, -Y, X]$	$[x, -x, x]$	[20, 34]
21	$[Y, X, -X]$	$[x, x, -x]$	[21, 31]
22	$[Y, -X, X]$	$[x, -x, x]$	[22, 32]

continued ...

Table 9

No.	vector	center	mapping
23	$[-Y, X, X]$	$[-x, x, x]$	[23,30]
24	$[-Y, -X, -X]$	$[-x, -x, -x]$	[24,29]

Table 10: Wyckoff bond: 24c@8b

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, x, x]$	[1,-38]
2	$[-X, X, 0]$	$[-x, -x, x]$	[2,-37]
3	$[-X, -X, 0]$	$[-x, x, -x]$	[3,-39]
4	$[X, X, 0]$	$[x, -x, -x]$	[4,-40]
5	$[0, X, -X]$	$[x, x, x]$	[5,-48]
6	$[0, -X, X]$	$[x, -x, -x]$	[6,-47]
7	$[0, -X, -X]$	$[-x, -x, x]$	[7,-45]
8	$[0, X, X]$	$[-x, x, -x]$	[8,-46]
9	$[-X, 0, X]$	$[x, x, x]$	[9,-43]
10	$[X, 0, -X]$	$[-x, x, -x]$	[10,-44]
11	$[-X, 0, -X]$	$[x, -x, -x]$	[11,-42]
12	$[X, 0, X]$	$[-x, -x, x]$	[12,-41]
13	$[-X, X, 0]$	$[x, x, -x]$	[13,-26]
14	$[X, -X, 0]$	$[-x, -x, -x]$	[14,-25]
15	$[-X, -X, 0]$	$[x, -x, x]$	[15,-27]
16	$[X, X, 0]$	$[-x, x, x]$	[16,-28]
17	$[X, 0, X]$	$[x, x, -x]$	[17,-36]
18	$[-X, 0, -X]$	$[-x, x, x]$	[18,-35]
19	$[-X, 0, X]$	$[-x, -x, -x]$	[19,-33]
20	$[X, 0, -X]$	$[x, -x, x]$	[20,-34]
21	$[0, -X, -X]$	$[x, x, -x]$	[21,-31]
22	$[0, X, X]$	$[x, -x, x]$	[22,-32]
23	$[0, -X, X]$	$[-x, x, x]$	[23,-30]
24	$[0, X, -X]$	$[-x, -x, -x]$	[24,-29]

Table 11: Wyckoff bond: 48d@8b

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]

continued ...

Table 11

No.	vector	center	mapping
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]
25	$[-X, -Y, -Z]$	$[-x, -x, -x]$	[25]
26	$[X, Y, -Z]$	$[x, x, -x]$	[26]
27	$[X, -Y, Z]$	$[x, -x, x]$	[27]
28	$[-X, Y, Z]$	$[-x, x, x]$	[28]
29	$[-Z, -X, -Y]$	$[-x, -x, -x]$	[29]
30	$[-Z, X, Y]$	$[-x, x, x]$	[30]
31	$[Z, X, -Y]$	$[x, x, -x]$	[31]
32	$[Z, -X, Y]$	$[x, -x, x]$	[32]
33	$[-Y, -Z, -X]$	$[-x, -x, -x]$	[33]
34	$[Y, -Z, X]$	$[x, -x, x]$	[34]
35	$[-Y, Z, X]$	$[-x, x, x]$	[35]
36	$[Y, Z, -X]$	$[x, x, -x]$	[36]
37	$[-Y, -X, Z]$	$[-x, -x, x]$	[37]
38	$[Y, X, Z]$	$[x, x, x]$	[38]
39	$[-Y, X, -Z]$	$[-x, x, -x]$	[39]
40	$[Y, -X, -Z]$	$[x, -x, -x]$	[40]
41	$[-X, -Z, Y]$	$[-x, -x, x]$	[41]
42	$[X, -Z, -Y]$	$[x, -x, -x]$	[42]
43	$[X, Z, Y]$	$[x, x, x]$	[43]
44	$[-X, Z, -Y]$	$[-x, x, -x]$	[44]
45	$[-Z, -Y, X]$	$[-x, -x, x]$	[45]
46	$[-Z, Y, -X]$	$[-x, x, -x]$	[46]
47	$[Z, -Y, -X]$	$[x, -x, -x]$	[47]
48	$[Z, Y, X]$	$[x, x, x]$	[48]

* Wyckoff site: 12c, site symmetry: $m.m2$

Table 12: Wyckoff bond: 12a@12c

No.	vector	center	mapping
1	$[0, X, X]$	$[0, y, y]$	$[1, 18, 28, 43]$
2	$[0, -X, X]$	$[0, -y, y]$	$[2, 20, 27, 41]$
3	$[0, X, -X]$	$[0, y, -y]$	$[3, 17, 26, 44]$
4	$[0, -X, -X]$	$[0, -y, -y]$	$[4, 19, 25, 42]$
5	$[X, 0, X]$	$[y, 0, y]$	$[5, 15, 32, 38]$
6	$[X, 0, -X]$	$[y, 0, -y]$	$[6, 13, 31, 40]$
7	$[-X, 0, X]$	$[-y, 0, y]$	$[7, 16, 30, 37]$
8	$[-X, 0, -X]$	$[-y, 0, -y]$	$[8, 14, 29, 39]$
9	$[X, X, 0]$	$[y, y, 0]$	$[9, 21, 36, 48]$
10	$[-X, X, 0]$	$[-y, y, 0]$	$[10, 23, 35, 46]$
11	$[X, -X, 0]$	$[y, -y, 0]$	$[11, 22, 34, 47]$
12	$[-X, -X, 0]$	$[-y, -y, 0]$	$[12, 24, 33, 45]$

Table 13: Wyckoff bond: 12b@12c

No.	vector	center	mapping
1	$[0, X, -X]$	$[0, y, y]$	$[1, -18, 28, -43]$
2	$[0, -X, -X]$	$[0, -y, y]$	$[2, -20, 27, -41]$
3	$[0, X, X]$	$[0, y, -y]$	$[3, -17, 26, -44]$
4	$[0, -X, X]$	$[0, -y, -y]$	$[4, -19, 25, -42]$
5	$[-X, 0, X]$	$[y, 0, y]$	$[5, -15, 32, -38]$
6	$[-X, 0, -X]$	$[y, 0, -y]$	$[6, -13, 31, -40]$
7	$[X, 0, X]$	$[-y, 0, y]$	$[7, -16, 30, -37]$
8	$[X, 0, -X]$	$[-y, 0, -y]$	$[8, -14, 29, -39]$
9	$[X, -X, 0]$	$[y, y, 0]$	$[9, -21, 36, -48]$
10	$[-X, -X, 0]$	$[-y, y, 0]$	$[10, -23, 35, -46]$
11	$[X, X, 0]$	$[y, -y, 0]$	$[11, -22, 34, -47]$
12	$[-X, X, 0]$	$[-y, -y, 0]$	$[12, -24, 33, -45]$

Table 14: Wyckoff bond: 12c@12c

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, y]$	$[1, -18, -28, 43]$
2	$[-X, 0, 0]$	$[0, -y, y]$	$[2, -20, -27, 41]$
3	$[-X, 0, 0]$	$[0, y, -y]$	$[3, -17, -26, 44]$
4	$[X, 0, 0]$	$[0, -y, -y]$	$[4, -19, -25, 42]$
5	$[0, X, 0]$	$[y, 0, y]$	$[5, -15, -32, 38]$
6	$[0, -X, 0]$	$[y, 0, -y]$	$[6, -13, -31, 40]$
7	$[0, -X, 0]$	$[-y, 0, y]$	$[7, -16, -30, 37]$
8	$[0, X, 0]$	$[-y, 0, -y]$	$[8, -14, -29, 39]$
9	$[0, 0, X]$	$[y, y, 0]$	$[9, -21, -36, 48]$

continued ...

Table 14

No.	vector	center	mapping
10	$[0, 0, -X]$	$[-y, y, 0]$	$[10, -23, -35, 46]$
11	$[0, 0, -X]$	$[y, -y, 0]$	$[11, -22, -34, 47]$
12	$[0, 0, X]$	$[-y, -y, 0]$	$[12, -24, -33, 45]$

Table 15: Wyckoff bond: 24d@12c

No.	vector	center	mapping
1	$[Y, X, X]$	$[0, y, y]$	$[1, 43]$
2	$[-Y, -X, X]$	$[0, -y, y]$	$[2, 41]$
3	$[-Y, X, -X]$	$[0, y, -y]$	$[3, 44]$
4	$[Y, -X, -X]$	$[0, -y, -y]$	$[4, 42]$
5	$[X, Y, X]$	$[y, 0, y]$	$[5, 38]$
6	$[X, -Y, -X]$	$[y, 0, -y]$	$[6, 40]$
7	$[-X, -Y, X]$	$[-y, 0, y]$	$[7, 37]$
8	$[-X, Y, -X]$	$[-y, 0, -y]$	$[8, 39]$
9	$[X, X, Y]$	$[y, y, 0]$	$[9, 48]$
10	$[-X, X, -Y]$	$[-y, y, 0]$	$[10, 46]$
11	$[X, -X, -Y]$	$[y, -y, 0]$	$[11, 47]$
12	$[-X, -X, Y]$	$[-y, -y, 0]$	$[12, 45]$
13	$[X, Y, -X]$	$[y, 0, -y]$	$[13, 31]$
14	$[-X, -Y, -X]$	$[-y, 0, -y]$	$[14, 29]$
15	$[X, -Y, X]$	$[y, 0, y]$	$[15, 32]$
16	$[-X, Y, X]$	$[-y, 0, y]$	$[16, 30]$
17	$[Y, X, -X]$	$[0, y, -y]$	$[17, 26]$
18	$[-Y, X, X]$	$[0, y, y]$	$[18, 28]$
19	$[-Y, -X, -X]$	$[0, -y, -y]$	$[19, 25]$
20	$[Y, -X, X]$	$[0, -y, y]$	$[20, 27]$
21	$[X, X, -Y]$	$[y, y, 0]$	$[21, 36]$
22	$[X, -X, Y]$	$[y, -y, 0]$	$[22, 34]$
23	$[-X, X, Y]$	$[-y, y, 0]$	$[23, 35]$
24	$[-X, -X, -Y]$	$[-y, -y, 0]$	$[24, 33]$

Table 16: Wyckoff bond: 24e@12c

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	$[X, -Y, X]$	$[-y, 0, y]$	$[7, -16]$

continued ...

Table 16

No.	vector	center	mapping
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	$[-X, X, Y]$	$[-y, -y, 0]$	$[12, -24]$
13	$[-Y, -X, X]$	$[0, -y, -y]$	$[25, -42]$
14	$[Y, X, X]$	$[0, y, -y]$	$[26, -44]$
15	$[Y, -X, -X]$	$[0, -y, y]$	$[27, -41]$
16	$[-Y, X, -X]$	$[0, y, y]$	$[28, -43]$
17	$[X, -Y, -X]$	$[-y, 0, -y]$	$[29, -39]$
18	$[X, Y, X]$	$[-y, 0, y]$	$[30, -37]$
19	$[-X, Y, -X]$	$[y, 0, -y]$	$[31, -40]$
20	$[-X, -Y, X]$	$[y, 0, y]$	$[32, -38]$
21	$[-X, X, -Y]$	$[-y, -y, 0]$	$[33, -45]$
22	$[X, X, Y]$	$[y, -y, 0]$	$[34, -47]$
23	$[-X, -X, Y]$	$[-y, y, 0]$	$[35, -46]$
24	$[X, -X, -Y]$	$[y, y, 0]$	$[36, -48]$

Table 17: Wyckoff bond: $24f@12c$

No.	vector	center	mapping
1	$[0, X, Y]$	$[0, y, y]$	$[1, 28]$
2	$[0, -X, Y]$	$[0, -y, y]$	$[2, 27]$
3	$[0, X, -Y]$	$[0, y, -y]$	$[3, 26]$
4	$[0, -X, -Y]$	$[0, -y, -y]$	$[4, 25]$
5	$[Y, 0, X]$	$[y, 0, y]$	$[5, 32]$
6	$[Y, 0, -X]$	$[y, 0, -y]$	$[6, 31]$
7	$[-Y, 0, X]$	$[-y, 0, y]$	$[7, 30]$
8	$[-Y, 0, -X]$	$[-y, 0, -y]$	$[8, 29]$
9	$[X, Y, 0]$	$[y, y, 0]$	$[9, 36]$
10	$[-X, Y, 0]$	$[-y, y, 0]$	$[10, 35]$
11	$[X, -Y, 0]$	$[y, -y, 0]$	$[11, 34]$
12	$[-X, -Y, 0]$	$[-y, -y, 0]$	$[12, 33]$
13	$[X, 0, -Y]$	$[y, 0, -y]$	$[13, 40]$
14	$[-X, 0, -Y]$	$[-y, 0, -y]$	$[14, 39]$
15	$[X, 0, Y]$	$[y, 0, y]$	$[15, 38]$
16	$[-X, 0, Y]$	$[-y, 0, y]$	$[16, 37]$
17	$[0, Y, -X]$	$[0, y, -y]$	$[17, 44]$
18	$[0, Y, X]$	$[0, y, y]$	$[18, 43]$
19	$[0, -Y, -X]$	$[0, -y, -y]$	$[19, 42]$
20	$[0, -Y, X]$	$[0, -y, y]$	$[20, 41]$
21	$[Y, X, 0]$	$[y, y, 0]$	$[21, 48]$
22	$[Y, -X, 0]$	$[y, -y, 0]$	$[22, 47]$
23	$[-Y, X, 0]$	$[-y, y, 0]$	$[23, 46]$

continued ...

Table 17

No.	vector	center	mapping
24	$[-Y, -X, 0]$	$[-y, -y, 0]$	[24, 45]

Table 18: Wyckoff bond: 48g@12c

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]
25	$[-X, -Y, -Z]$	$[0, -y, -y]$	[25]
26	$[X, Y, -Z]$	$[0, y, -y]$	[26]
27	$[X, -Y, Z]$	$[0, -y, y]$	[27]
28	$[-X, Y, Z]$	$[0, y, y]$	[28]
29	$[-Z, -X, -Y]$	$[-y, 0, -y]$	[29]
30	$[-Z, X, Y]$	$[-y, 0, y]$	[30]
31	$[Z, X, -Y]$	$[y, 0, -y]$	[31]
32	$[Z, -X, Y]$	$[y, 0, y]$	[32]
33	$[-Y, -Z, -X]$	$[-y, -y, 0]$	[33]
34	$[Y, -Z, X]$	$[y, -y, 0]$	[34]
35	$[-Y, Z, X]$	$[-y, y, 0]$	[35]
36	$[Y, Z, -X]$	$[y, y, 0]$	[36]
37	$[-Y, -X, Z]$	$[-y, 0, y]$	[37]
38	$[Y, X, Z]$	$[y, 0, y]$	[38]
39	$[-Y, X, -Z]$	$[-y, 0, -y]$	[39]

continued ...

Table 18

No.	vector	center	mapping
40	$[Y, -X, -Z]$	$[y, 0, -y]$	[40]
41	$[-X, -Z, Y]$	$[0, -y, y]$	[41]
42	$[X, -Z, -Y]$	$[0, -y, -y]$	[42]
43	$[X, Z, Y]$	$[0, y, y]$	[43]
44	$[-X, Z, -Y]$	$[0, y, -y]$	[44]
45	$[-Z, -Y, X]$	$[-y, -y, 0]$	[45]
46	$[-Z, Y, -X]$	$[-y, y, 0]$	[46]
47	$[Z, -Y, -X]$	$[y, -y, 0]$	[47]
48	$[Z, Y, X]$	$[y, y, 0]$	[48]

* Wyckoff site: 24d, site symmetry: $m..$

Table 19: Wyckoff bond: 24a@24d

No.	vector	center	mapping
1	$[0, X, Y]$	$[0, y, z]$	[1,28]
2	$[0, -X, Y]$	$[0, -y, z]$	[2,27]
3	$[0, X, -Y]$	$[0, y, -z]$	[3,26]
4	$[0, -X, -Y]$	$[0, -y, -z]$	[4,25]
5	$[Y, 0, X]$	$[z, 0, y]$	[5,32]
6	$[Y, 0, -X]$	$[z, 0, -y]$	[6,31]
7	$[-Y, 0, X]$	$[-z, 0, y]$	[7,30]
8	$[-Y, 0, -X]$	$[-z, 0, -y]$	[8,29]
9	$[X, Y, 0]$	$[y, z, 0]$	[9,36]
10	$[-X, Y, 0]$	$[-y, z, 0]$	[10,35]
11	$[X, -Y, 0]$	$[y, -z, 0]$	[11,34]
12	$[-X, -Y, 0]$	$[-y, -z, 0]$	[12,33]
13	$[X, 0, -Y]$	$[y, 0, -z]$	[13,40]
14	$[-X, 0, -Y]$	$[-y, 0, -z]$	[14,39]
15	$[X, 0, Y]$	$[y, 0, z]$	[15,38]
16	$[-X, 0, Y]$	$[-y, 0, z]$	[16,37]
17	$[0, Y, -X]$	$[0, z, -y]$	[17,44]
18	$[0, Y, X]$	$[0, z, y]$	[18,43]
19	$[0, -Y, -X]$	$[0, -z, -y]$	[19,42]
20	$[0, -Y, X]$	$[0, -z, y]$	[20,41]
21	$[Y, X, 0]$	$[z, y, 0]$	[21,48]
22	$[Y, -X, 0]$	$[z, -y, 0]$	[22,47]
23	$[-Y, X, 0]$	$[-z, y, 0]$	[23,46]
24	$[-Y, -X, 0]$	$[-z, -y, 0]$	[24,45]

Table 20: Wyckoff bond: 24b@24d

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, z]$	$[1, -28]$
2	$[-X, 0, 0]$	$[0, -y, z]$	$[2, -27]$
3	$[-X, 0, 0]$	$[0, y, -z]$	$[3, -26]$
4	$[X, 0, 0]$	$[0, -y, -z]$	$[4, -25]$
5	$[0, X, 0]$	$[z, 0, y]$	$[5, -32]$
6	$[0, -X, 0]$	$[z, 0, -y]$	$[6, -31]$
7	$[0, -X, 0]$	$[-z, 0, y]$	$[7, -30]$
8	$[0, X, 0]$	$[-z, 0, -y]$	$[8, -29]$
9	$[0, 0, X]$	$[y, z, 0]$	$[9, -36]$
10	$[0, 0, -X]$	$[-y, z, 0]$	$[10, -35]$
11	$[0, 0, -X]$	$[y, -z, 0]$	$[11, -34]$
12	$[0, 0, X]$	$[-y, -z, 0]$	$[12, -33]$
13	$[0, X, 0]$	$[y, 0, -z]$	$[13, -40]$
14	$[0, -X, 0]$	$[-y, 0, -z]$	$[14, -39]$
15	$[0, -X, 0]$	$[y, 0, z]$	$[15, -38]$
16	$[0, X, 0]$	$[-y, 0, z]$	$[16, -37]$
17	$[X, 0, 0]$	$[0, z, -y]$	$[17, -44]$
18	$[-X, 0, 0]$	$[0, z, y]$	$[18, -43]$
19	$[-X, 0, 0]$	$[0, -z, -y]$	$[19, -42]$
20	$[X, 0, 0]$	$[0, -z, y]$	$[20, -41]$
21	$[0, 0, -X]$	$[z, y, 0]$	$[21, -48]$
22	$[0, 0, X]$	$[z, -y, 0]$	$[22, -47]$
23	$[0, 0, X]$	$[-z, y, 0]$	$[23, -46]$
24	$[0, 0, -X]$	$[-z, -y, 0]$	$[24, -45]$

Table 21: Wyckoff bond: 48c@24d

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

continued ...

Table 21

No.	vector	center	mapping
16	$[-Y, X, Z]$	$[-y, 0, z]$	[16]
17	$[X, Z, -Y]$	$[0, z, -y]$	[17]
18	$[-X, Z, Y]$	$[0, z, y]$	[18]
19	$[-X, -Z, -Y]$	$[0, -z, -y]$	[19]
20	$[X, -Z, Y]$	$[0, -z, y]$	[20]
21	$[Z, Y, -X]$	$[z, y, 0]$	[21]
22	$[Z, -Y, X]$	$[z, -y, 0]$	[22]
23	$[-Z, Y, X]$	$[-z, y, 0]$	[23]
24	$[-Z, -Y, -X]$	$[-z, -y, 0]$	[24]
25	$[-X, -Y, -Z]$	$[0, -y, -z]$	[25]
26	$[X, Y, -Z]$	$[0, y, -z]$	[26]
27	$[X, -Y, Z]$	$[0, -y, z]$	[27]
28	$[-X, Y, Z]$	$[0, y, z]$	[28]
29	$[-Z, -X, -Y]$	$[-z, 0, -y]$	[29]
30	$[-Z, X, Y]$	$[-z, 0, y]$	[30]
31	$[Z, X, -Y]$	$[z, 0, -y]$	[31]
32	$[Z, -X, Y]$	$[z, 0, y]$	[32]
33	$[-Y, -Z, -X]$	$[-y, -z, 0]$	[33]
34	$[Y, -Z, X]$	$[y, -z, 0]$	[34]
35	$[-Y, Z, X]$	$[-y, z, 0]$	[35]
36	$[Y, Z, -X]$	$[y, z, 0]$	[36]
37	$[-Y, -X, Z]$	$[-y, 0, z]$	[37]
38	$[Y, X, Z]$	$[y, 0, z]$	[38]
39	$[-Y, X, -Z]$	$[-y, 0, -z]$	[39]
40	$[Y, -X, -Z]$	$[y, 0, -z]$	[40]
41	$[-X, -Z, Y]$	$[0, -z, y]$	[41]
42	$[X, -Z, -Y]$	$[0, -z, -y]$	[42]
43	$[X, Z, Y]$	$[0, z, y]$	[43]
44	$[-X, Z, -Y]$	$[0, z, -y]$	[44]
45	$[-Z, -Y, X]$	$[-z, -y, 0]$	[45]
46	$[-Z, Y, -X]$	$[-z, y, 0]$	[46]
47	$[Z, -Y, -X]$	$[z, -y, 0]$	[47]
48	$[Z, Y, X]$	$[z, y, 0]$	[48]

* Wyckoff site: 24e, site symmetry: $\bar{3}m$

Table 22: Wyckoff bond: 24a@24e

No.	vector	center	mapping
1	$[X, X, Y]$	$[x, x, z]$	[1,38]
2	$[-X, -X, Y]$	$[-x, -x, z]$	[2,37]
3	$[-X, X, -Y]$	$[-x, x, -z]$	[3,39]
4	$[X, -X, -Y]$	$[x, -x, -z]$	[4,40]
5	$[Y, X, X]$	$[z, x, x]$	[5,48]
6	$[Y, -X, -X]$	$[z, -x, -x]$	[6,47]

continued ...

Table 22

No.	vector	center	mapping
7	$[-Y, -X, X]$	$[-z, -x, x]$	[7,45]
8	$[-Y, X, -X]$	$[-z, x, -x]$	[8,46]
9	$[X, Y, X]$	$[x, z, x]$	[9,43]
10	$[-X, Y, -X]$	$[-x, z, -x]$	[10,44]
11	$[X, -Y, -X]$	$[x, -z, -x]$	[11,42]
12	$[-X, -Y, X]$	$[-x, -z, x]$	[12,41]
13	$[X, X, -Y]$	$[x, x, -z]$	[13,26]
14	$[-X, -X, -Y]$	$[-x, -x, -z]$	[14,25]
15	$[X, -X, Y]$	$[x, -x, z]$	[15,27]
16	$[-X, X, Y]$	$[-x, x, z]$	[16,28]
17	$[X, Y, -X]$	$[x, z, -x]$	[17,36]
18	$[-X, Y, X]$	$[-x, z, x]$	[18,35]
19	$[-X, -Y, -X]$	$[-x, -z, -x]$	[19,33]
20	$[X, -Y, X]$	$[x, -z, x]$	[20,34]
21	$[Y, X, -X]$	$[z, x, -x]$	[21,31]
22	$[Y, -X, X]$	$[z, -x, x]$	[22,32]
23	$[-Y, X, X]$	$[-z, x, x]$	[23,30]
24	$[-Y, -X, -X]$	$[-z, -x, -x]$	[24,29]

Table 23: Wyckoff bond: 24b@24e

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, x, z]$	[1,-38]
2	$[-X, X, 0]$	$[-x, -x, z]$	[2,-37]
3	$[-X, -X, 0]$	$[-x, x, -z]$	[3,-39]
4	$[X, X, 0]$	$[x, -x, -z]$	[4,-40]
5	$[0, X, -X]$	$[z, x, x]$	[5,-48]
6	$[0, -X, X]$	$[z, -x, -x]$	[6,-47]
7	$[0, -X, -X]$	$[-z, -x, x]$	[7,-45]
8	$[0, X, X]$	$[-z, x, -x]$	[8,-46]
9	$[-X, 0, X]$	$[x, z, x]$	[9,-43]
10	$[X, 0, -X]$	$[-x, z, -x]$	[10,-44]
11	$[-X, 0, -X]$	$[x, -z, -x]$	[11,-42]
12	$[X, 0, X]$	$[-x, -z, x]$	[12,-41]
13	$[-X, X, 0]$	$[x, x, -z]$	[13,-26]
14	$[X, -X, 0]$	$[-x, -x, -z]$	[14,-25]
15	$[-X, -X, 0]$	$[x, -x, z]$	[15,-27]
16	$[X, X, 0]$	$[-x, x, z]$	[16,-28]
17	$[X, 0, X]$	$[x, z, -x]$	[17,-36]
18	$[-X, 0, -X]$	$[-x, z, x]$	[18,-35]
19	$[-X, 0, X]$	$[-x, -z, -x]$	[19,-33]
20	$[X, 0, -X]$	$[x, -z, x]$	[20,-34]
21	$[0, -X, -X]$	$[z, x, -x]$	[21,-31]
22	$[0, X, X]$	$[z, -x, x]$	[22,-32]

continued ...

Table 23

No.	vector	center	mapping
23	$[0, -X, X]$	$[-z, x, x]$	[23,-30]
24	$[0, X, -X]$	$[-z, -x, -x]$	[24,-29]

Table 24: Wyckoff bond: 48c@24e

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, z]$	[1]
2	$[-X, -Y, Z]$	$[-x, -x, z]$	[2]
3	$[-X, Y, -Z]$	$[-x, x, -z]$	[3]
4	$[X, -Y, -Z]$	$[x, -x, -z]$	[4]
5	$[Z, X, Y]$	$[z, x, x]$	[5]
6	$[Z, -X, -Y]$	$[z, -x, -x]$	[6]
7	$[-Z, -X, Y]$	$[-z, -x, x]$	[7]
8	$[-Z, X, -Y]$	$[-z, x, -x]$	[8]
9	$[Y, Z, X]$	$[x, z, x]$	[9]
10	$[-Y, Z, -X]$	$[-x, z, -x]$	[10]
11	$[Y, -Z, -X]$	$[x, -z, -x]$	[11]
12	$[-Y, -Z, X]$	$[-x, -z, x]$	[12]
13	$[Y, X, -Z]$	$[x, x, -z]$	[13]
14	$[-Y, -X, -Z]$	$[-x, -x, -z]$	[14]
15	$[Y, -X, Z]$	$[x, -x, z]$	[15]
16	$[-Y, X, Z]$	$[-x, x, z]$	[16]
17	$[X, Z, -Y]$	$[x, z, -x]$	[17]
18	$[-X, Z, Y]$	$[-x, z, x]$	[18]
19	$[-X, -Z, -Y]$	$[-x, -z, -x]$	[19]
20	$[X, -Z, Y]$	$[x, -z, x]$	[20]
21	$[Z, Y, -X]$	$[z, x, -x]$	[21]
22	$[Z, -Y, X]$	$[z, -x, x]$	[22]
23	$[-Z, Y, X]$	$[-z, x, x]$	[23]
24	$[-Z, -Y, -X]$	$[-z, -x, -x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, -x, -z]$	[25]
26	$[X, Y, -Z]$	$[x, x, -z]$	[26]
27	$[X, -Y, Z]$	$[x, -x, z]$	[27]
28	$[-X, Y, Z]$	$[-x, x, z]$	[28]
29	$[-Z, -X, -Y]$	$[-z, -x, -x]$	[29]
30	$[-Z, X, Y]$	$[-z, x, x]$	[30]
31	$[Z, X, -Y]$	$[z, x, -x]$	[31]
32	$[Z, -X, Y]$	$[z, -x, x]$	[32]
33	$[-Y, -Z, -X]$	$[-x, -z, -x]$	[33]
34	$[Y, -Z, X]$	$[x, -z, x]$	[34]
35	$[-Y, Z, X]$	$[-x, z, x]$	[35]
36	$[Y, Z, -X]$	$[x, z, -x]$	[36]
37	$[-Y, -X, Z]$	$[-x, -x, z]$	[37]
38	$[Y, X, Z]$	$[x, x, z]$	[38]

continued ...

Table 24

No.	vector	center	mapping
39	$[-Y, X, -Z]$	$[-x, x, -z]$	[39]
40	$[Y, -X, -Z]$	$[x, -x, -z]$	[40]
41	$[-X, -Z, Y]$	$[-x, -z, x]$	[41]
42	$[X, -Z, -Y]$	$[x, -z, -x]$	[42]
43	$[X, Z, Y]$	$[x, z, x]$	[43]
44	$[-X, Z, -Y]$	$[-x, z, -x]$	[44]
45	$[-Z, -Y, X]$	$[-z, -x, x]$	[45]
46	$[-Z, Y, -X]$	$[-z, x, -x]$	[46]
47	$[Z, -Y, -X]$	$[z, -x, -x]$	[47]
48	$[Z, Y, X]$	$[z, x, x]$	[48]

* Wyckoff site: **48f**, site symmetry: **1**

Table 25: Wyckoff bond: **48a@48f**

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]
25	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[25]
26	$[X, Y, -Z]$	$[x, y, -z]$	[26]
27	$[X, -Y, Z]$	$[x, -y, z]$	[27]
28	$[-X, Y, Z]$	$[-x, y, z]$	[28]
29	$[-Z, -X, -Y]$	$[-z, -x, -y]$	[29]

continued ...

Table 25

No.	vector	center	mapping
30	$[-Z, X, Y]$	$[-z, x, y]$	[30]
31	$[Z, X, -Y]$	$[z, x, -y]$	[31]
32	$[Z, -X, Y]$	$[z, -x, y]$	[32]
33	$[-Y, -Z, -X]$	$[-y, -z, -x]$	[33]
34	$[Y, -Z, X]$	$[y, -z, x]$	[34]
35	$[-Y, Z, X]$	$[-y, z, x]$	[35]
36	$[Y, Z, -X]$	$[y, z, -x]$	[36]
37	$[-Y, -X, Z]$	$[-y, -x, z]$	[37]
38	$[Y, X, Z]$	$[y, x, z]$	[38]
39	$[-Y, X, -Z]$	$[-y, x, -z]$	[39]
40	$[Y, -X, -Z]$	$[y, -x, -z]$	[40]
41	$[-X, -Z, Y]$	$[-x, -z, y]$	[41]
42	$[X, -Z, -Y]$	$[x, -z, -y]$	[42]
43	$[X, Z, Y]$	$[x, z, y]$	[43]
44	$[-X, Z, -Y]$	$[-x, z, -y]$	[44]
45	$[-Z, -Y, X]$	$[-z, -y, x]$	[45]
46	$[-Z, Y, -X]$	$[-z, y, -x]$	[46]
47	$[Z, -Y, -X]$	$[z, -y, -x]$	[47]
48	$[Z, Y, X]$	$[z, y, x]$	[48]