

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: .3m

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: . . 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]