

SG No. 229 O_h^9 $Im\bar{3}m$ [cubic]

* plus set: $+ [0, 0, 0]$, $+ [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

* Wyckoff site: 2a, site symmetry: m-3m

Table 1: Wyckoff bond: 6a@2a

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

Table 2: Wyckoff bond: 8b@2a

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

Table 3: Wyckoff bond: 12c@2a

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

Table 4: Wyckoff bond: 24d@2a

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

continued ...

Table 4

No.	vector	center	mapping
11	$[X, -Y, -X]$	$[0, 0, 0]$	$[11, -18, -35, 42]$
12	$[-X, -Y, X]$	$[0, 0, 0]$	$[12, -17, -36, 41]$

Table 5: Wyckoff bond: 24e@2a

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

Table 6: Wyckoff bond: 48f@2a

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

continued ...

Table 6

No.	vector	center	mapping
21	$[Z, Y, -X]$	$[0, 0, 0]$	$[21, -45]$
22	$[Z, -Y, X]$	$[0, 0, 0]$	$[22, -46]$
23	$[-Z, Y, X]$	$[0, 0, 0]$	$[23, -47]$
24	$[-Z, -Y, -X]$	$[0, 0, 0]$	$[24, -48]$

* Wyckoff site: 6b, site symmetry: 4/mmm.m

Table 7: Wyckoff bond: 6a@6b

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

Table 8: Wyckoff bond: 12b@6b

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

Table 9: Wyckoff bond: 12c@6b

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

Table 10: Wyckoff bond: 24d@6b

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

Table 11: Wyckoff bond: 24e@6b

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

Table 12: Wyckoff bond: 24f@6b

No.	vector	center	mapping
1	[0, X, Y]	[0, $\frac{1}{2}$, $\frac{1}{2}$]	[1, -4, -25, 28]
2	[0, -X, Y]	[0, $\frac{1}{2}$, $\frac{1}{2}$]	[2, -3, -26, 27]
3	[Y, 0, X]	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[5, -8, -29, 32]
4	[Y, 0, -X]	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[6, -7, -30, 31]
5	[X, Y, 0]	[$\frac{1}{2}$, $\frac{1}{2}$, 0]	[9, -12, -33, 36]
6	[-X, Y, 0]	[$\frac{1}{2}$, $\frac{1}{2}$, 0]	[10, -11, -34, 35]
7	[X, 0, -Y]	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[13, -16, -37, 40]
8	[-X, 0, -Y]	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[14, -15, -38, 39]
9	[0, Y, -X]	[0, $\frac{1}{2}$, $\frac{1}{2}$]	[17, -20, -41, 44]

continued ...

Table 12

No.	vector	center	mapping
10	$[0, Y, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[18, -19, -42, 43]$
11	$[Y, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[21, -24, -45, 48]$
12	$[Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[22, -23, -46, 47]$

Table 13: Wyckoff bond: 48g@6b

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

* Wyckoff site: 8c, site symmetry: .-3m

Table 14: Wyckoff bond: 8a@8c

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

Table 15: Wyckoff bond: 24b@8c

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

Table 16: Wyckoff bond: 24c@8c

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

Table 17: Wyckoff bond: 48d@8c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, -25]$
2	$[-X, -Y, Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	$[2, -26]$
3	$[-X, Y, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[3, -27]$
4	$[X, -Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[4, -28]$
5	$[Z, X, Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[5, -29]$
6	$[Z, -X, -Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[6, -30]$
7	$[-Z, -X, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	$[7, -31]$
8	$[-Z, X, -Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[8, -32]$
9	$[Y, Z, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[9, -33]$

continued ...

Table 17

No.	vector	center	mapping
10	$[-Y, Z, -X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[10, -34]
11	$[Y, -Z, -X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[11, -35]
12	$[-Y, -Z, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[12, -36]
13	$[Y, X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[13, -37]
14	$[-Y, -X, -Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[14, -38]
15	$[Y, -X, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[15, -39]
16	$[-Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[16, -40]
17	$[X, Z, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[17, -41]
18	$[-X, Z, Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[18, -42]
19	$[-X, -Z, -Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[19, -43]
20	$[X, -Z, Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[20, -44]
21	$[Z, Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[21, -45]
22	$[Z, -Y, X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[22, -46]
23	$[-Z, Y, X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[23, -47]
24	$[-Z, -Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[24, -48]

* Wyckoff site: 12d, site symmetry: -4m.2

Table 18: Wyckoff bond: 12a@12d

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

Table 19: Wyckoff bond: 24b@12d

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

continued ...

Table 19

No.	vector	center	mapping
12	$[X, -X, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[34, -35, -46, 47]$

Table 20: Wyckoff bond: 24c@12d

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

Table 21: Wyckoff bond: 48d@12d

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

continued ...

Table 21

No.	vector	center	mapping
22	$[X, -X, Y]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[34, -46]
23	$[-X, X, Y]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[35, -47]
24	$[X, X, -Y]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[36, -45]

Table 22: Wyckoff bond: 48e@12d

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

Table 23: Wyckoff bond: 48f@12d

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

continued ...

Table 23

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

Table 24: Wyckoff bond: 96g@12d

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

continued ...

Table 24

No.	vector	center	mapping
24	$[-Z, -Y, -X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[24]
25	$[-X, -Y, -Z]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[27]
28	$[-X, Y, Z]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[28]
29	$[-Z, -X, -Y]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[29]
30	$[-Z, X, Y]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[30]
31	$[Z, X, -Y]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[31]
32	$[Z, -X, Y]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[32]
33	$[-Y, -Z, -X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[33]
34	$[Y, -Z, X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[34]
35	$[-Y, Z, X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[35]
36	$[Y, Z, -X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[37]
38	$[Y, X, Z]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[39]
40	$[Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[42]
43	$[X, Z, Y]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[44]
45	$[-Z, -Y, X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[45]
46	$[-Z, Y, -X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[46]
47	$[Z, -Y, -X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[47]
48	$[Z, Y, X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[48]

* Wyckoff site: 12e, site symmetry: 4m.m

Table 25: Wyckoff bond: 12a@12e

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 26: Wyckoff bond: 24b@12e

No.	vector	center	mapping
1	$[0, X, X]$	$[x, 0, 0]$	[1,-4,-42,43]

continued ...

Table 26

No.	vector	center	mapping
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 27: Wyckoff bond: 24c@12e

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 28: Wyckoff bond: 48d@12e

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	$[X, -X, -Y]$	$[0, 0, -x]$	$[11, 47]$

continued ...

Table 28

No.	vector	center	mapping
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 29: Wyckoff bond: 48e@12e

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]
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 30: Wyckoff bond: 48f@12e

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 31: Wyckoff bond: 96g@12e

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]

continued ...

Table 31

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

* Wyckoff site: 16f, site symmetry: .3m

Table 32: Wyckoff bond: 16a@16f

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]

continued ...

Table 32

No.	vector	center	mapping
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 33: Wyckoff bond: 48b@16f

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	$[Y, -X, X]$	$[x, -x, x]$	$[22, 32]$
23	$[-Y, X, X]$	$[-x, x, x]$	$[23, 30]$
24	$[-Y, -X, -X]$	$[-x, -x, -x]$	$[24, 29]$

Table 34: Wyckoff bond: 48c@16f

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	$[0, X, X]$	$[-x, x, -x]$	$[8, -46]$

continued ...

Table 34

No.	vector	center	mapping
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 35: Wyckoff bond: 96d@16f

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]

continued ...

Table 35

No.	vector	center	mapping
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: 24g, site symmetry: `mm2..`

Table 36: Wyckoff bond: 24a@24g

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

Table 37: Wyckoff bond: 24b@24g

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

Table 38: Wyckoff bond: 48c@24g

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

Table 39: Wyckoff bond: 48d@24g

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

Table 40: Wyckoff bond: 96e@24g

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

continued ...

Table 40

No.	vector	center	mapping
16	$[-Y, X, Z]$	$[0, x, \frac{1}{2}]$	[16]
17	$[X, Z, -Y]$	$[x, \frac{1}{2}, 0]$	[17]
18	$[-X, Z, Y]$	$[-x, \frac{1}{2}, 0]$	[18]
19	$[-X, -Z, -Y]$	$[-x, \frac{1}{2}, 0]$	[19]
20	$[X, -Z, Y]$	$[x, \frac{1}{2}, 0]$	[20]
21	$[Z, Y, -X]$	$[\frac{1}{2}, 0, -x]$	[21]
22	$[Z, -Y, X]$	$[\frac{1}{2}, 0, x]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{2}, 0, x]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{2}, 0, -x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, 0, \frac{1}{2}]$	[25]
26	$[X, Y, -Z]$	$[x, 0, \frac{1}{2}]$	[26]
27	$[X, -Y, Z]$	$[x, 0, \frac{1}{2}]$	[27]
28	$[-X, Y, Z]$	$[-x, 0, \frac{1}{2}]$	[28]
29	$[-Z, -X, -Y]$	$[\frac{1}{2}, -x, 0]$	[29]
30	$[-Z, X, Y]$	$[\frac{1}{2}, x, 0]$	[30]
31	$[Z, X, -Y]$	$[\frac{1}{2}, x, 0]$	[31]
32	$[Z, -X, Y]$	$[\frac{1}{2}, -x, 0]$	[32]
33	$[-Y, -Z, -X]$	$[0, \frac{1}{2}, -x]$	[33]
34	$[Y, -Z, X]$	$[0, \frac{1}{2}, x]$	[34]
35	$[-Y, Z, X]$	$[0, \frac{1}{2}, x]$	[35]
36	$[Y, Z, -X]$	$[0, \frac{1}{2}, -x]$	[36]
37	$[-Y, -X, Z]$	$[0, -x, \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[0, x, \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[0, x, \frac{1}{2}]$	[39]
40	$[Y, -X, -Z]$	$[0, -x, \frac{1}{2}]$	[40]
41	$[-X, -Z, Y]$	$[-x, \frac{1}{2}, 0]$	[41]
42	$[X, -Z, -Y]$	$[x, \frac{1}{2}, 0]$	[42]
43	$[X, Z, Y]$	$[x, \frac{1}{2}, 0]$	[43]
44	$[-X, Z, -Y]$	$[-x, \frac{1}{2}, 0]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2}, 0, x]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2}, 0, -x]$	[46]
47	$[Z, -Y, -X]$	$[\frac{1}{2}, 0, -x]$	[47]
48	$[Z, Y, X]$	$[\frac{1}{2}, 0, x]$	[48]

* Wyckoff site: 24h, site symmetry: $m\cdot m2$

Table 41: Wyckoff bond: 24a@24h

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]

continued ...

Table 41

No.	vector	center	mapping
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 42: Wyckoff bond: 24b@24h

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 43: Wyckoff bond: 24c@24h

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]
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 44: Wyckoff bond: 48d@24h

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 45: Wyckoff bond: 48e@24h

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]
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]

continued ...

Table 45

No.	vector	center	mapping
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 46: Wyckoff bond: 48f@24h

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]
24	$[-Y, -X, 0]$	$[-y, -y, 0]$	[24,45]

Table 47: Wyckoff bond: 96g@24h

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]
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]

continued ...

Table 47

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

* Wyckoff site: 48i, site symmetry: ..2

Table 48: Wyckoff bond: 48a@48i

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

Table 49: Wyckoff bond: 48b@48i

No.	vector	center	mapping
1	$[0, X, -X]$	$[\frac{1}{4}, y, \frac{1}{2} - y]$	[1,19]
2	$[0, -X, -X]$	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	[2,17]
3	$[0, X, X]$	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[3,20]
4	$[0, -X, X]$	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	[4,18]
5	$[-X, 0, X]$	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[5,14]
6	$[-X, 0, -X]$	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[6,16]

continued ...

Table 49

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

Table 50: Wyckoff bond: 96c@48i

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

continued ...

Table 50

No.	vector	center	mapping
23	$[-Z, Y, X]$	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[23]
24	$[-Z, -Y, -X]$	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[24]
25	$[-X, -Y, -Z]$	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{4}, y, y + \frac{1}{2}]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{4}, -y, \frac{1}{2} - y]$	[27]
28	$[-X, Y, Z]$	$[\frac{3}{4}, y, \frac{1}{2} - y]$	[28]
29	$[-Z, -X, -Y]$	$[y + \frac{1}{2}, \frac{3}{4}, -y]$	[29]
30	$[-Z, X, Y]$	$[y + \frac{1}{2}, \frac{1}{4}, y]$	[30]
31	$[Z, X, -Y]$	$[\frac{1}{2} - y, \frac{1}{4}, -y]$	[31]
32	$[Z, -X, Y]$	$[\frac{1}{2} - y, \frac{3}{4}, y]$	[32]
33	$[-Y, -Z, -X]$	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[33]
34	$[Y, -Z, X]$	$[y, y + \frac{1}{2}, \frac{1}{4}]$	[34]
35	$[-Y, Z, X]$	$[-y, \frac{1}{2} - y, \frac{1}{4}]$	[35]
36	$[Y, Z, -X]$	$[y, \frac{1}{2} - y, \frac{3}{4}]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{4}, -y]$	[37]
38	$[Y, X, Z]$	$[y + \frac{1}{2}, \frac{3}{4}, -y]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2} - y, \frac{3}{4}, y]$	[39]
40	$[Y, -X, -Z]$	$[y + \frac{1}{2}, \frac{1}{4}, y]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{4}, y, y + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{3}{4}, y, \frac{1}{2} - y]$	[42]
43	$[X, Z, Y]$	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{4}, -y, \frac{1}{2} - y]$	[44]
45	$[-Z, -Y, X]$	$[y, \frac{1}{2} - y, \frac{3}{4}]$	[45]
46	$[-Z, Y, -X]$	$[y, y + \frac{1}{2}, \frac{1}{4}]$	[46]
47	$[Z, -Y, -X]$	$[-y, \frac{1}{2} - y, \frac{1}{4}]$	[47]
48	$[Z, Y, X]$	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[48]

* Wyckoff site: 48j, site symmetry: m..

Table 51: Wyckoff bond: 48a@48j

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]

continued ...

Table 51

No.	vector	center	mapping
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 52: Wyckoff bond: 48b@48j

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 53: Wyckoff bond: 96c@48j

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]
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]

continued ...

Table 53

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

* Wyckoff site: 48k, site symmetry: ..m

Table 54: Wyckoff bond: 48a@48k

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]
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 55: Wyckoff bond: 48b@48k

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]

continued ...

Table 55

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

Table 56: Wyckoff bond: 96c@48k

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]

continued ...

Table 56

No.	vector	center	mapping
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]
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: 961, site symmetry: 1

Table 57: Wyckoff bond: 96a@961

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]

continued ...

Table 57

No.	vector	center	mapping
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]
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]