

SG No. 221 O_h^1 $Pm\bar{3}m$ [cubic]

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

* Wyckoff site: **1a**, site symmetry: **m-3m**

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

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, 0]$	$[1, -2, -3, 4, 17, -18, -19, 20, -25, 26, 27, -28, -41, 42, 43, -44]$
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: **4b@1a**

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: **6c@1a**

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: **12d@1a**

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: 12e@1a

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: 24f@1a

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: **1b**, site symmetry: **m-3m**

Table 7: Wyckoff bond: **3a@1b**

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

Table 8: Wyckoff bond: **4b@1b**

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

Table 9: Wyckoff bond: **6c@1b**

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

Table 10: Wyckoff bond: **12d@1b**

No.	vector	center	mapping
1	$[X, X, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, -14, -25, 38]$
2	$[-X, -X, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, -13, -26, 37]$
3	$[-X, X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, -15, -27, 39]$

continued ...

Table 10

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

Table 11: Wyckoff bond: **12e@1b**

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

Table 12: Wyckoff bond: **24f@1b**

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

continued ...

Table 12

No.	vector	center	mapping
14	$[-Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[14,-38]
15	$[Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[15,-39]
16	$[-Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[16,-40]
17	$[X, Z, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[17,-41]
18	$[-X, Z, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[18,-42]
19	$[-X, -Z, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[19,-43]
20	$[X, -Z, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[20,-44]
21	$[Z, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[21,-45]
22	$[Z, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[22,-46]
23	$[-Z, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[23,-47]
24	$[-Z, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[24,-48]

* Wyckoff site: 3c, site symmetry: 4/mm.m

Table 13: Wyckoff bond: 3a@3c

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[1,-2,-3,4,17,-18,-19,20,-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 14: Wyckoff bond: 6b@3c

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 15: Wyckoff bond: 6c@3c

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 16: Wyckoff bond: 12d@3c

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 17: Wyckoff bond: 12e@3c

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 18: Wyckoff bond: 12f@3c

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	$[X, 0, -Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[13, -16, -37, 40]$

continued ...

Table 18

No.	vector	center	mapping
8	$[-X, 0, -Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[14, -15, -38, 39]$
9	$[0, Y, -X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[17, -20, -41, 44]$
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 19: Wyckoff bond: 24g@3c

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: 3d, site symmetry: $4/\text{mm.m}$

Table 20: Wyckoff bond: 3a@3d

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

Table 21: Wyckoff bond: 6b@3d

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

Table 22: Wyckoff bond: 6c@3d

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

Table 23: Wyckoff bond: 12d@3d

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

Table 24: Wyckoff bond: 12e@3d

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, 0, 0]$	$[1, -2, -25, 26]$
2	$[-X, Y, 0]$	$[\frac{1}{2}, 0, 0]$	$[3, -4, -27, 28]$
3	$[0, X, Y]$	$[0, \frac{1}{2}, 0]$	$[5, -6, -29, 30]$

continued ...

Table 24

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

Table 25: Wyckoff bond: 12f03d

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

Table 26: Wyckoff bond: 24g03d

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

continued ...

Table 26

No.	vector	center	mapping
14	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, 0]$	[14, -38]
15	$[Y, -X, Z]$	$[0, \frac{1}{2}, 0]$	[15, -39]
16	$[-Y, X, Z]$	$[0, \frac{1}{2}, 0]$	[16, -40]
17	$[X, Z, -Y]$	$[\frac{1}{2}, 0, 0]$	[17, -41]
18	$[-X, Z, Y]$	$[\frac{1}{2}, 0, 0]$	[18, -42]
19	$[-X, -Z, -Y]$	$[\frac{1}{2}, 0, 0]$	[19, -43]
20	$[X, -Z, Y]$	$[\frac{1}{2}, 0, 0]$	[20, -44]
21	$[Z, Y, -X]$	$[0, 0, \frac{1}{2}]$	[21, -45]
22	$[Z, -Y, X]$	$[0, 0, \frac{1}{2}]$	[22, -46]
23	$[-Z, Y, X]$	$[0, 0, \frac{1}{2}]$	[23, -47]
24	$[-Z, -Y, -X]$	$[0, 0, \frac{1}{2}]$	[24, -48]

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

Table 27: Wyckoff bond: 6a@6e

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 28: Wyckoff bond: 12b@6e

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 29: Wyckoff bond: 12c@6e

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 30: Wyckoff bond: 24d@6e

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 31: Wyckoff bond: 24e@6e

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 32: Wyckoff bond: 24f@6e

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, 0, 0]$	$[1, -4]$
2	$[0, -X, Y]$	$[-x, 0, 0]$	$[2, -3]$
3	$[Y, 0, X]$	$[0, x, 0]$	$[5, -8]$
4	$[Y, 0, -X]$	$[0, -x, 0]$	$[6, -7]$
5	$[X, Y, 0]$	$[0, 0, x]$	$[9, -12]$
6	$[-X, Y, 0]$	$[0, 0, -x]$	$[10, -11]$
7	$[X, 0, -Y]$	$[0, x, 0]$	$[13, -16]$
8	$[-X, 0, -Y]$	$[0, -x, 0]$	$[14, -15]$
9	$[0, Y, -X]$	$[x, 0, 0]$	$[17, -20]$
10	$[0, Y, X]$	$[-x, 0, 0]$	$[18, -19]$
11	$[Y, X, 0]$	$[0, 0, -x]$	$[21, -24]$
12	$[Y, -X, 0]$	$[0, 0, x]$	$[22, -23]$
13	$[0, -X, -Y]$	$[-x, 0, 0]$	$[25, -28]$
14	$[0, X, -Y]$	$[x, 0, 0]$	$[26, -27]$
15	$[-Y, 0, -X]$	$[0, -x, 0]$	$[29, -32]$

continued ...

Table 32

No.	vector	center	mapping
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 33: Wyckoff bond: 48g06e

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]

continued ...

Table 33

No.	vector	center	mapping
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: **6f**, site symmetry: **4m.m**

Table 34: Wyckoff bond: **6a@6f**

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

Table 35: Wyckoff bond: **12b@6f**

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

continued ...

Table 35

No.	vector	center	mapping
10	$[0, X, X]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[18, -19, -25, 28]$
11	$[X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	$[21, -24, -33, 36]$
12	$[X, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, x]$	$[22, -23, 34, -35]$

Table 36: Wyckoff bond: 12c@6f

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

Table 37: Wyckoff bond: 24d@6f

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

continued ...

Table 37

No.	vector	center	mapping
20	$[Y, -X, X]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[20, 27]$
21	$[X, X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	$[21, 36]$
22	$[X, -X, Y]$	$[\frac{1}{2}, \frac{1}{2}, x]$	$[22, 34]$
23	$[-X, X, Y]$	$[\frac{1}{2}, \frac{1}{2}, x]$	$[23, 35]$
24	$[-X, -X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	$[24, 33]$

Table 38: Wyckoff bond: **24e06f**

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

Table 39: Wyckoff bond: **24f06f**

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

continued ...

Table 39

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

Table 40: Wyckoff bond: 48g@6f

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

continued ...

Table 40

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

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

Table 41: Wyckoff bond: 8a@8g

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 42: Wyckoff bond: 24b08g

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 43: Wyckoff bond: 24c08g

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	$[-X, -X, 0]$	$[x, -x, x]$	$[15, -27]$

continued ...

Table 43

No.	vector	center	mapping
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 44: Wyckoff bond: 48d08g

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]
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]

continued ...

Table 44

No.	vector	center	mapping
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: 12h, site symmetry: mm2. .

Table 45: Wyckoff bond: 12a@12h

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

Table 46: Wyckoff bond: 12b@12h

No.	vector	center	mapping
1	$[0, 0, X]$	$[x, \frac{1}{2}, 0]$	[1, -4, -26, 27]
2	$[0, 0, X]$	$[-x, \frac{1}{2}, 0]$	[2, -3, -25, 28]
3	$[X, 0, 0]$	$[0, x, \frac{1}{2}]$	[5, -8, -30, 31]

continued ...

Table 46

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

Table 47: Wyckoff bond: 12c@12h

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

Table 48: Wyckoff bond: 24d@12h

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

continued ...

Table 48

No.	vector	center	mapping
14	$[-Y, -X, 0]$	$[\frac{1}{2}, -x, 0]$	[14,37]
15	$[Y, -X, 0]$	$[\frac{1}{2}, -x, 0]$	[15,40]
16	$[-Y, X, 0]$	$[\frac{1}{2}, x, 0]$	[16,39]
17	$[X, 0, -Y]$	$[x, 0, \frac{1}{2}]$	[17,42]
18	$[-X, 0, Y]$	$[-x, 0, \frac{1}{2}]$	[18,41]
19	$[-X, 0, -Y]$	$[-x, 0, \frac{1}{2}]$	[19,44]
20	$[X, 0, Y]$	$[x, 0, \frac{1}{2}]$	[20,43]
21	$[0, Y, -X]$	$[0, \frac{1}{2}, -x]$	[21,46]
22	$[0, -Y, X]$	$[0, \frac{1}{2}, x]$	[22,45]
23	$[0, Y, X]$	$[0, \frac{1}{2}, x]$	[23,48]
24	$[0, -Y, -X]$	$[0, \frac{1}{2}, -x]$	[24,47]

Table 49: Wyckoff bond: 24e@12h

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

Table 50: Wyckoff bond: 24f@12h

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

Table 51: Wyckoff bond: 48g@12h

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

continued ...

Table 51

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

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

Table 52: Wyckoff bond: 12a@12i

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 52

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 53: Wyckoff bond: 12b@12i

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 54: Wyckoff bond: 12c@12i

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 55: Wyckoff bond: 24d@12i

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 56: Wyckoff bond: 24e@12i

No.	vector	center	mapping
1	$[Y, X, -X]$	$[0, y, y]$	$[1, -18]$
2	$[-Y, -X, -X]$	$[0, -y, y]$	$[2, -20]$
3	$[-Y, X, X]$	$[0, y, -y]$	$[3, -17]$
4	$[Y, -X, X]$	$[0, -y, -y]$	$[4, -19]$
5	$[-X, Y, X]$	$[y, 0, y]$	$[5, -15]$
6	$[-X, -Y, -X]$	$[y, 0, -y]$	$[6, -13]$
7	$[X, -Y, X]$	$[-y, 0, y]$	$[7, -16]$
8	$[X, Y, -X]$	$[-y, 0, -y]$	$[8, -14]$
9	$[X, -X, Y]$	$[y, y, 0]$	$[9, -21]$
10	$[-X, -X, -Y]$	$[-y, y, 0]$	$[10, -23]$
11	$[X, X, -Y]$	$[y, -y, 0]$	$[11, -22]$
12	$[-X, X, Y]$	$[-y, -y, 0]$	$[12, -24]$
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 56

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 57: Wyckoff bond: 24f@12i

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 58: Wyckoff bond: 48g@12i

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, y]$	[1]
2	$[-X, -Y, Z]$	$[0, -y, y]$	[2]
3	$[-X, Y, -Z]$	$[0, y, -y]$	[3]
4	$[X, -Y, -Z]$	$[0, -y, -y]$	[4]
5	$[Z, X, Y]$	$[y, 0, y]$	[5]
6	$[Z, -X, -Y]$	$[y, 0, -y]$	[6]
7	$[-Z, -X, Y]$	$[-y, 0, y]$	[7]
8	$[-Z, X, -Y]$	$[-y, 0, -y]$	[8]
9	$[Y, Z, X]$	$[y, y, 0]$	[9]
10	$[-Y, Z, -X]$	$[-y, y, 0]$	[10]
11	$[Y, -Z, -X]$	$[y, -y, 0]$	[11]
12	$[-Y, -Z, X]$	$[-y, -y, 0]$	[12]
13	$[Y, X, -Z]$	$[y, 0, -y]$	[13]
14	$[-Y, -X, -Z]$	$[-y, 0, -y]$	[14]
15	$[Y, -X, Z]$	$[y, 0, y]$	[15]
16	$[-Y, X, Z]$	$[-y, 0, y]$	[16]
17	$[X, Z, -Y]$	$[0, y, -y]$	[17]
18	$[-X, Z, Y]$	$[0, y, y]$	[18]
19	$[-X, -Z, -Y]$	$[0, -y, -y]$	[19]
20	$[X, -Z, Y]$	$[0, -y, y]$	[20]
21	$[Z, Y, -X]$	$[y, y, 0]$	[21]
22	$[Z, -Y, X]$	$[y, -y, 0]$	[22]
23	$[-Z, Y, X]$	$[-y, y, 0]$	[23]
24	$[-Z, -Y, -X]$	$[-y, -y, 0]$	[24]
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 58

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

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

Table 59: Wyckoff bond: 12a@12j

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

Table 60: Wyckoff bond: 12b@12j

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

Table 61: Wyckoff bond: 12c@12j

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

Table 62: Wyckoff bond: 24d@12j

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

Table 63: Wyckoff bond: 24e@12j

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

Table 64: Wyckoff bond: 24f@12j

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

continued ...

Table 64

No.	vector	center	mapping
16	$[-X, 0, Y]$	$[-y, \frac{1}{2}, y]$	[16,37]
17	$[0, Y, -X]$	$[\frac{1}{2}, y, -y]$	[17,44]
18	$[0, Y, X]$	$[\frac{1}{2}, y, y]$	[18,43]
19	$[0, -Y, -X]$	$[\frac{1}{2}, -y, -y]$	[19,42]
20	$[0, -Y, X]$	$[\frac{1}{2}, -y, y]$	[20,41]
21	$[Y, X, 0]$	$[y, y, \frac{1}{2}]$	[21,48]
22	$[Y, -X, 0]$	$[y, -y, \frac{1}{2}]$	[22,47]
23	$[-Y, X, 0]$	$[-y, y, \frac{1}{2}]$	[23,46]
24	$[-Y, -X, 0]$	$[-y, -y, \frac{1}{2}]$	[24,45]

Table 65: Wyckoff bond: 48g@12j

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, y, y]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2}, -y, y]$	[2]
3	$[-X, Y, -Z]$	$[\frac{1}{2}, y, -y]$	[3]
4	$[X, -Y, -Z]$	$[\frac{1}{2}, -y, -y]$	[4]
5	$[Z, X, Y]$	$[y, \frac{1}{2}, y]$	[5]
6	$[Z, -X, -Y]$	$[y, \frac{1}{2}, -y]$	[6]
7	$[-Z, -X, Y]$	$[-y, \frac{1}{2}, y]$	[7]
8	$[-Z, X, -Y]$	$[-y, \frac{1}{2}, -y]$	[8]
9	$[Y, Z, X]$	$[y, y, \frac{1}{2}]$	[9]
10	$[-Y, Z, -X]$	$[-y, y, \frac{1}{2}]$	[10]
11	$[Y, -Z, -X]$	$[y, -y, \frac{1}{2}]$	[11]
12	$[-Y, -Z, X]$	$[-y, -y, \frac{1}{2}]$	[12]
13	$[Y, X, -Z]$	$[y, \frac{1}{2}, -y]$	[13]
14	$[-Y, -X, -Z]$	$[-y, \frac{1}{2}, -y]$	[14]
15	$[Y, -X, Z]$	$[y, \frac{1}{2}, y]$	[15]
16	$[-Y, X, Z]$	$[-y, \frac{1}{2}, y]$	[16]
17	$[X, Z, -Y]$	$[\frac{1}{2}, y, -y]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{2}, y, y]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{2}, -y, -y]$	[19]
20	$[X, -Z, Y]$	$[\frac{1}{2}, -y, y]$	[20]
21	$[Z, Y, -X]$	$[y, y, \frac{1}{2}]$	[21]
22	$[Z, -Y, X]$	$[y, -y, \frac{1}{2}]$	[22]
23	$[-Z, Y, X]$	$[-y, y, \frac{1}{2}]$	[23]
24	$[-Z, -Y, -X]$	$[-y, -y, \frac{1}{2}]$	[24]
25	$[-X, -Y, -Z]$	$[\frac{1}{2}, -y, -y]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{2}, y, -y]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{2}, -y, y]$	[27]
28	$[-X, Y, Z]$	$[\frac{1}{2}, y, y]$	[28]
29	$[-Z, -X, -Y]$	$[-y, \frac{1}{2}, -y]$	[29]
30	$[-Z, X, Y]$	$[-y, \frac{1}{2}, y]$	[30]
31	$[Z, X, -Y]$	$[y, \frac{1}{2}, -y]$	[31]

continued ...

Table 65

No.	vector	center	mapping
32	$[Z, -X, Y]$	$[y, \frac{1}{2}, y]$	[32]
33	$[-Y, -Z, -X]$	$[-y, -y, \frac{1}{2}]$	[33]
34	$[Y, -Z, X]$	$[y, -y, \frac{1}{2}]$	[34]
35	$[-Y, Z, X]$	$[-y, y, \frac{1}{2}]$	[35]
36	$[Y, Z, -X]$	$[y, y, \frac{1}{2}]$	[36]
37	$[-Y, -X, Z]$	$[-y, \frac{1}{2}, y]$	[37]
38	$[Y, X, Z]$	$[y, \frac{1}{2}, y]$	[38]
39	$[-Y, X, -Z]$	$[-y, \frac{1}{2}, -y]$	[39]
40	$[Y, -X, -Z]$	$[y, \frac{1}{2}, -y]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2}, -y, y]$	[41]
42	$[X, -Z, -Y]$	$[\frac{1}{2}, -y, -y]$	[42]
43	$[X, Z, Y]$	$[\frac{1}{2}, y, y]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2}, y, -y]$	[44]
45	$[-Z, -Y, X]$	$[-y, -y, \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[-y, y, \frac{1}{2}]$	[46]
47	$[Z, -Y, -X]$	$[y, -y, \frac{1}{2}]$	[47]
48	$[Z, Y, X]$	$[y, y, \frac{1}{2}]$	[48]

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

Table 66: Wyckoff bond: 24a@24k

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]

continued ...

Table 66

No.	vector	center	mapping
23	$[-Y, X, 0]$	$[-z, y, 0]$	[23, 46]
24	$[-Y, -X, 0]$	$[-z, -y, 0]$	[24, 45]

Table 67: Wyckoff bond: 24b@24k

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 68: Wyckoff bond: 48c@24k

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]

continued ...

Table 68

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

* Wyckoff site: 24l, site symmetry: $m\bar{1}$.

Table 69: Wyckoff bond: 24a@241

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

Table 70: Wyckoff bond: 24b@241

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

continued ...

Table 70

No.	vector	center	mapping
16	$[0, X, 0]$	$[-y, \frac{1}{2}, z]$	[16,-37]
17	$[X, 0, 0]$	$[\frac{1}{2}, z, -y]$	[17,-44]
18	$[-X, 0, 0]$	$[\frac{1}{2}, z, y]$	[18,-43]
19	$[-X, 0, 0]$	$[\frac{1}{2}, -z, -y]$	[19,-42]
20	$[X, 0, 0]$	$[\frac{1}{2}, -z, y]$	[20,-41]
21	$[0, 0, -X]$	$[z, y, \frac{1}{2}]$	[21,-48]
22	$[0, 0, X]$	$[z, -y, \frac{1}{2}]$	[22,-47]
23	$[0, 0, X]$	$[-z, y, \frac{1}{2}]$	[23,-46]
24	$[0, 0, -X]$	$[-z, -y, \frac{1}{2}]$	[24,-45]

Table 71: Wyckoff bond: 48c@241

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, y, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2}, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[\frac{1}{2}, y, -z]$	[3]
4	$[X, -Y, -Z]$	$[\frac{1}{2}, -y, -z]$	[4]
5	$[Z, X, Y]$	$[z, \frac{1}{2}, y]$	[5]
6	$[Z, -X, -Y]$	$[z, \frac{1}{2}, -y]$	[6]
7	$[-Z, -X, Y]$	$[-z, \frac{1}{2}, y]$	[7]
8	$[-Z, X, -Y]$	$[-z, \frac{1}{2}, -y]$	[8]
9	$[Y, Z, X]$	$[y, z, \frac{1}{2}]$	[9]
10	$[-Y, Z, -X]$	$[-y, z, \frac{1}{2}]$	[10]
11	$[Y, -Z, -X]$	$[y, -z, \frac{1}{2}]$	[11]
12	$[-Y, -Z, X]$	$[-y, -z, \frac{1}{2}]$	[12]
13	$[Y, X, -Z]$	$[y, \frac{1}{2}, -z]$	[13]
14	$[-Y, -X, -Z]$	$[-y, \frac{1}{2}, -z]$	[14]
15	$[Y, -X, Z]$	$[y, \frac{1}{2}, z]$	[15]
16	$[-Y, X, Z]$	$[-y, \frac{1}{2}, z]$	[16]
17	$[X, Z, -Y]$	$[\frac{1}{2}, z, -y]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{2}, z, y]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{2}, -z, -y]$	[19]
20	$[X, -Z, Y]$	$[\frac{1}{2}, -z, y]$	[20]
21	$[Z, Y, -X]$	$[z, y, \frac{1}{2}]$	[21]
22	$[Z, -Y, X]$	$[z, -y, \frac{1}{2}]$	[22]
23	$[-Z, Y, X]$	$[-z, y, \frac{1}{2}]$	[23]
24	$[-Z, -Y, -X]$	$[-z, -y, \frac{1}{2}]$	[24]
25	$[-X, -Y, -Z]$	$[\frac{1}{2}, -y, -z]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{2}, y, -z]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{2}, -y, z]$	[27]
28	$[-X, Y, Z]$	$[\frac{1}{2}, y, z]$	[28]
29	$[-Z, -X, -Y]$	$[-z, \frac{1}{2}, -y]$	[29]
30	$[-Z, X, Y]$	$[-z, \frac{1}{2}, y]$	[30]
31	$[Z, X, -Y]$	$[z, \frac{1}{2}, -y]$	[31]

continued ...

Table 71

No.	vector	center	mapping
32	$[Z, -X, Y]$	$[z, \frac{1}{2}, y]$	[32]
33	$[-Y, -Z, -X]$	$[-y, -z, \frac{1}{2}]$	[33]
34	$[Y, -Z, X]$	$[y, -z, \frac{1}{2}]$	[34]
35	$[-Y, Z, X]$	$[-y, z, \frac{1}{2}]$	[35]
36	$[Y, Z, -X]$	$[y, z, \frac{1}{2}]$	[36]
37	$[-Y, -X, Z]$	$[-y, \frac{1}{2}, z]$	[37]
38	$[Y, X, Z]$	$[y, \frac{1}{2}, z]$	[38]
39	$[-Y, X, -Z]$	$[-y, \frac{1}{2}, -z]$	[39]
40	$[Y, -X, -Z]$	$[y, \frac{1}{2}, -z]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2}, -z, y]$	[41]
42	$[X, -Z, -Y]$	$[\frac{1}{2}, -z, -y]$	[42]
43	$[X, Z, Y]$	$[\frac{1}{2}, z, y]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2}, z, -y]$	[44]
45	$[-Z, -Y, X]$	$[-z, -y, \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[-z, y, \frac{1}{2}]$	[46]
47	$[Z, -Y, -X]$	$[z, -y, \frac{1}{2}]$	[47]
48	$[Z, Y, X]$	$[z, y, \frac{1}{2}]$	[48]

* Wyckoff site: $24m$, site symmetry: $\dots m$

Table 72: Wyckoff bond: $24a@24m$

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]

continued ...

Table 72

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

Table 73: Wyckoff bond: 24b@24m

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]
23	$[0, -X, X]$	$[-z, x, x]$	[23,-30]
24	$[0, X, -X]$	$[-z, -x, -x]$	[24,-29]

Table 74: Wyckoff bond: 48c@24m

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]

continued ...

Table 74

No.	vector	center	mapping
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]
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: 48n, site symmetry: 1

Table 75: Wyckoff bond: 48a@48n

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]
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]

continued ...

Table 75

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