

\* Wyckoff site: 6a, site symmetry: 4. .

Table 1: Wyckoff bond: 6a@6a

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

Table 2: Wyckoff bond: 12b@6a

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

Table 3: Wyckoff bond: 24c@6a

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

continued ...

Table 3

No.	vector	center	mapping
13	$[Y, X, -Z]$	$[0, x, 0]$	[13]
14	$[-Y, -X, -Z]$	$[0, -x, 0]$	[14]
15	$[Y, -X, Z]$	$[0, -x, 0]$	[15]
16	$[-Y, X, Z]$	$[0, x, 0]$	[16]
17	$[X, Z, -Y]$	$[x, 0, 0]$	[17]
18	$[-X, Z, Y]$	$[-x, 0, 0]$	[18]
19	$[-X, -Z, -Y]$	$[-x, 0, 0]$	[19]
20	$[X, -Z, Y]$	$[x, 0, 0]$	[20]
21	$[Z, Y, -X]$	$[0, 0, -x]$	[21]
22	$[Z, -Y, X]$	$[0, 0, x]$	[22]
23	$[-Z, Y, X]$	$[0, 0, x]$	[23]
24	$[-Z, -Y, -X]$	$[0, 0, -x]$	[24]

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

Table 4: Wyckoff bond: 8a@8b

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

Table 5: Wyckoff bond: 24b@8b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, x]$	[1]
2	$[-X, -Y, Z]$	$[-x, -x, x]$	[2]
3	$[-X, Y, -Z]$	$[-x, x, -x]$	[3]
4	$[X, -Y, -Z]$	$[x, -x, -x]$	[4]
5	$[Z, X, Y]$	$[x, x, x]$	[5]
6	$[Z, -X, -Y]$	$[x, -x, -x]$	[6]
7	$[-Z, -X, Y]$	$[-x, -x, x]$	[7]
8	$[-Z, X, -Y]$	$[-x, x, -x]$	[8]
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]

*continued ...*

Table 5

No.	vector	center	mapping
13	$[Y, X, -Z]$	$[x, x, -x]$	[13]
14	$[-Y, -X, -Z]$	$[-x, -x, -x]$	[14]
15	$[Y, -X, Z]$	$[x, -x, x]$	[15]
16	$[-Y, X, Z]$	$[-x, x, x]$	[16]
17	$[X, Z, -Y]$	$[x, x, -x]$	[17]
18	$[-X, Z, Y]$	$[-x, x, x]$	[18]
19	$[-X, -Z, -Y]$	$[-x, -x, -x]$	[19]
20	$[X, -Z, Y]$	$[x, -x, x]$	[20]
21	$[Z, Y, -X]$	$[x, x, -x]$	[21]
22	$[Z, -Y, X]$	$[x, -x, x]$	[22]
23	$[-Z, Y, X]$	$[-x, x, x]$	[23]
24	$[-Z, -Y, -X]$	$[-x, -x, -x]$	[24]

\* Wyckoff site: 12c, site symmetry:  $\dots 2$

Table 6: Wyckoff bond: 12a@12c

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

Table 7: Wyckoff bond: 12b@12c

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

*continued ...*

Table 7

No.	vector	center	mapping
9	$[X, X, 0]$	$[y, y, 0]$	[9,21]
10	$[-X, X, 0]$	$[-y, y, 0]$	[10,23]
11	$[X, -X, 0]$	$[y, -y, 0]$	[11,22]
12	$[-X, -X, 0]$	$[-y, -y, 0]$	[12,24]

Table 8: Wyckoff bond: 24c@12c

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

\* Wyckoff site: 24d, site symmetry: 1

Table 9: Wyckoff bond: 24a@24d

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]

*continued ...*

Table 9

No.	vector	center	mapping
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]