

PG No. 30  $O$  432 [ cubic ]

\* 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: .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: . . 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]