

# PG No. 28 $T$ 23 [ cubic ]

\* Wyckoff site: 4a, site symmetry: .3.

Table 1: Wyckoff bond: 4a@4a

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]

Table 2: Wyckoff bond: 12b@4a

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]

\* Wyckoff site: 6b, site symmetry: 2..

Table 3: Wyckoff bond: 6a@6b

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]

Table 4: Wyckoff bond: 6b@6b

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

Table 5: Wyckoff bond: 12c@6b

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]

\* Wyckoff site: 12c, site symmetry: 1

Table 6: Wyckoff bond: 12a@12c

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]