

# 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	$[-Y, -Z, X]$	$[-y, -z, x]$	$[12]$