**Manual for ToBaCCo**

ToBaCCo (*To*pologically *B*ased *C*rystal *Co*nstructor) is a code to make crystalline structures based on a given topology, nodes, and edges. This current version of the code only deals with edge-transitive nets, which were obtained from RCSR. Briefly, the code reads a net, chooses appropriate nodes and edges, scales the unit cell to fit the building blocks and subsequently, places and connects them, generating a crystal in .cif format. It uses python 2.7.

**Topology**

A topology, or net, template file contains the name of the topology, the unit cell vectors, the number of types of vertices, or nodes, as well as the number of types of edges. It also contains the coordination and symmetry key information of each type of node as well as the total number and the fractional coordinates of each building block. Below is an example of a net template:

topology SHE

unit\_cell\_vectors

28.284 0.0000 0.0000

0.0000 28.284 0.0000

0.00000 0.0000 28.284

2 types\_of\_vertices

type number coordination symmetry\_key

1 12 4 5

2 8 6 0

1 types\_of\_edges

type number half\_length

12 48 5.00

fract\_coordinates\_vertices

first type

0.2500 0.0000 0.5000

0.7500 0.0000 0.5000

0.2500 0.5000 0.0000

0.5000 0.2500 0.0000

0.5000 0.7500 0.0000

0.0000 0.5000 0.2500

0.0000 0.5000 0.7500

0.5000 0.0000 0.2500

0.0000 0.2500 0.5000

0.0000 0.7500 0.5000

0.7500 0.5000 0.0000

0.5000 0.0000 0.7500

second type

0.2500 0.2500 0.2500

0.7500 0.7500 0.2500

0.7500 0.2500 0.7500

0.2500 0.7500 0.7500

0.2500 0.2500 0.7500

0.7500 0.7500 0.7500

0.2500 0.7500 0.2500

0.7500 0.2500 0.2500

fract\_coordinates\_edges

first type

0.2500 0.1250 0.3750

0.7500 0.8750 0.3750

0.7500 0.1250 0.6250

0.2500 0.8750 0.6250

0.3750 0.2500 0.1250

0.3750 0.7500 0.8750

0.6250 0.7500 0.1250

0.6250 0.2500 0.8750

0.1250 0.3750 0.2500

0.8750 0.3750 0.7500

0.1250 0.6250 0.7500

0.8750 0.6250 0.2500

0.1250 0.2500 0.6250

0.8750 0.7500 0.6250

0.1250 0.7500 0.3750

0.8750 0.2500 0.3750

0.2500 0.3750 0.8750

0.7500 0.3750 0.1250

0.7500 0.6250 0.8750

0.2500 0.6250 0.1250

0.3750 0.1250 0.7500

0.3750 0.8750 0.2500

0.6250 0.1250 0.2500

0.6250 0.8750 0.7500

0.7500 0.8750 0.6250

0.2500 0.3750 0.1250

0.2500 0.1250 0.6250

0.2500 0.8750 0.3750

0.7500 0.1250 0.3750

0.6250 0.7500 0.8750

0.1250 0.2500 0.3750

0.6250 0.2500 0.1250

0.3750 0.2500 0.8750

0.3750 0.7500 0.1250

0.8750 0.6250 0.7500

0.3750 0.1250 0.2500

0.1250 0.6250 0.2500

0.8750 0.3750 0.2500

0.1250 0.3750 0.7500

0.8750 0.7500 0.3750

0.8750 0.2500 0.6250

0.1250 0.7500 0.6250

0.7500 0.6250 0.1250

0.2500 0.6250 0.8750

0.7500 0.3750 0.8750

0.6250 0.8750 0.2500

0.6250 0.1250 0.7500

0.3750 0.8750 0.7500

**Building Blocks**

A building block can be an edge or a node. They should be in a .cif file and the connection points should be marked with X’s in the first column. It is important to note that *these files cannot have an empty line at the end of the file*. Below is an example of a .cif file for a node.

data\_sym\_4\_mc\_1

\_audit\_creation\_date 2014-09-12

\_audit\_creation\_method 'Materials Studio'

\_symmetry\_space\_group\_name\_H-M 'P1'

\_symmetry\_Int\_Tables\_number 1

\_symmetry\_cell\_setting triclinic

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

x,y,z

\_cell\_length\_a 20.0000

\_cell\_length\_b 20.0000

\_cell\_length\_c 20.0000

\_cell\_angle\_alpha 90.0000

\_cell\_angle\_beta 90.0000

\_cell\_angle\_gamma 90.0000

loop\_

\_atom\_site\_label

\_atom\_site\_type\_symbol

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

\_atom\_site\_U\_iso\_or\_equiv

\_atom\_site\_adp\_type

\_atom\_site\_occupancy

C1 C -0.10182 0.05995 -0.07511 0.00000 Uani 1.00

H2 H -0.09897 0.09775 -0.03653 0.16000 Uiso 1.00

C3 C -0.14698 0.06723 -0.12789 0.00000 Uani 1.00

H4 H -0.17950 0.11037 -0.13046 0.17800 Uiso 1.00

C5 C -0.06270 -0.04251 -0.12036 0.00000 Uani 1.00

H6 H -0.02914 -0.08471 -0.11793 0.16000 Uiso 1.00

C7 C -0.10721 -0.03695 -0.17393 0.00000 Uani 1.00

H8 H -0.10868 -0.07489 -0.21245 0.17800 Uiso 1.00

N9 N -0.06133 0.00531 -0.07188 0.00000 Uani 1.00

C10 C -0.00999 -0.01534 0.13924 0.00000 Uani 1.00

H11 H 0.04400 -0.01632 0.13603 0.16000 Uiso 1.00

C12 C -0.04143 -0.02215 0.20123 0.00000 Uani 1.00

H13 H -0.01220 -0.02817 0.24634 0.17800 Uiso 1.00

C14 C -0.11509 -0.00723 0.08480 0.00000 Uani 1.00

H15 H -0.14374 -0.00246 0.03931 0.16000 Uiso 1.00

C16 C -0.14832 -0.01393 0.14589 0.00000 Uani 1.00

H17 H -0.20237 -0.01366 0.14792 0.17800 Uiso 1.00

Zn18 Zn -0.00049 0.00005 0.00051 0.00000 Uani 1.00

N19 N -0.04701 -0.00732 0.08267 0.00000 Uani 1.00

C20 C 0.05389 0.12110 0.05226 0.00000 Uiso 1.00

N21 N 0.05195 0.07889 -0.00115 0.00000 Uiso 1.00

C22 C 0.08556 0.09318 -0.05860 0.00000 Uiso 1.00

C23 C 0.12421 0.15116 -0.06329 0.00000 Uiso 1.00

C24 C 0.09200 0.17959 0.04944 0.00000 Uiso 1.00

C25 C 0.02427 -0.13758 -0.00349 0.00000 Uiso 1.00

C26 C 0.06223 -0.19604 -0.00802 0.00000 Uiso 1.00

C27 C 0.16156 -0.12851 -0.01938 0.00000 Uiso 1.00

C28 C 0.12193 -0.07116 -0.01468 0.00000 Uiso 1.00

N29 N 0.05442 -0.07668 -0.00761 0.00000 Uiso 1.00

H30 H 0.02565 0.10988 0.09688 0.00000 Uiso 1.00

H31 H 0.08232 0.05935 -0.10069 0.00000 Uiso 1.00

H32 H 0.15129 0.16253 -0.10871 0.00000 Uiso 1.00

H33 H 0.09390 0.21319 0.09178 0.00000 Uiso 1.00

H34 H -0.02932 -0.14058 0.00321 0.00000 Uiso 1.00

H35 H 0.03844 -0.24453 -0.00514 0.00000 Uiso 1.00

H36 H 0.21517 -0.12444 -0.02522 0.00000 Uiso 1.00

H37 H 0.14526 -0.02251 -0.01622 0.00000 Uiso 1.00

X38 C -0.11109 -0.02135 0.20440 0.00000 Uiso 1.00

X39 C -0.14961 0.01831 -0.17752 0.00000 Uiso 1.00

X40 C 0.13133 -0.19129 -0.01608 0.00000 Uiso 1.00

X41 C 0.12740 0.19453 -0.00877 0.00000 Uiso 1.00

loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_ccdc\_geom\_bond\_type

C1 N9 1.362 . S

C1 C3 1.397 . D

C1 H2 1.082 . S

C3 H4 1.082 . S

C3 X39 1.395 . S

C5 N9 1.362 . D

C5 C7 1.397 . S

C5 H6 1.079 . S

C7 H8 1.082 . S

C7 X39 1.395 . D

N9 Zn18 1.894 . S

C10 N19 1.362 . S

C10 C12 1.397 . D

C10 H11 1.082 . S

C12 H13 1.082 . S

C12 X38 1.395 . S

C14 N19 1.362 . D

C14 C16 1.397 . S

C14 H15 1.079 . S

C16 H17 1.082 . S

C16 X38 1.395 . D

Zn18 N19 1.894 . S

Zn18 N21 1.894 . S

Zn18 N29 1.894 . S

C20 N21 1.362 . A

C20 C24 1.397 . A

C20 H30 1.080 . S

N21 C22 1.362 . A

C22 C23 1.397 . A

C22 H31 1.082 . S

C23 H32 1.082 . S

C23 X41 1.395 . D

C24 H33 1.082 . S

C24 X41 1.395 . S

C25 C26 1.397 . A

C25 N29 1.362 . A

C25 H34 1.082 . S

C26 H35 1.082 . S

C26 X40 1.395 . D

C27 C28 1.397 . A

C27 H36 1.082 . S

C27 X40 1.395 . S

C28 N29 1.362 . A

C28 H37 1.080 . S

**Running the code**

The code is written in python. In the directory of choice, simply run ‘main\_auto’. This will iterate through all the topologies found in the folder ‘templates’, fitting in appropriate nodes and edges found in the folders ‘nodes\_bb’ and ‘edges\_bb’, respectively. All these folders should be in the same directory as ‘main\_auto’ along with the modules: ‘connect\_edgeto2nodes’, ‘connect\_nodetonode’, ‘edges’, ‘neighbors’, ‘nodes’, ‘placing\_bb\_func’, ‘placing\_edge’, ‘placing\_edge\_1node’, ‘transformations’, and ‘write2cif’. If successful, the code will generate a folder called ‘output\_structures’ where the .cif files with the structures will be placed. The name of the structures will contain the topology as well as node, or nodes, and edge used.