Howto: Generating your own linker files for AuToGraFS: Automatic Topological Generator for Framework Structures

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A Linker Specification

```
Data: SBUtype = linker
Data: shape = linear
Data: name = 15pyrene
GEOMETRY CARTESIAN
C       -5.36928632     -5.40538612      0.00597428     MMTYPE=C_R    QMMM=MM BOND=2/1.5:6/1.5:19/1.0
C       -3.97643832     -5.40538612      0.00597428     MMTYPE=C_R    QMMM=MM BOND=1/1.5:3/1.5:20/1.0
C       -3.26797532     -4.19690112      0.00597428     MMTYPE=C_R    QMMM=MM BOND=2/1.5:4/1.5:7/1.5
C       -3.98508832     -2.97229212      0.00601228     MMTYPE=C_R    QMMM=MM BOND=3/1.5:5/1.5:8/1.5
C       -5.40422232     -2.98162812      0.00604228     MMTYPE=C_R    QMMM=MM BOND=4/1.5:6/1.5:16/1.5
C       -6.08103232     -4.20804612      0.00593928     MMTYPE=C_R    QMMM=MM BOND=1/1.5:5/1.5:21/1.0
C       -1.82892032     -4.15481912      0.00603928     MMTYPE=C_R    QMMM=MM BOND=3/1.5:10/1.5:18/1.0
C       -3.27630232     -1.72648712      0.00623128     MMTYPE=C_R    QMMM=MM BOND=4/1.5:9/1.5:14/1.5
C       -1.85721432     -1.71716412      0.00626628     MMTYPE=C_R    QMMM=MM BOND=8/1.5:10/1.5:11/1.5
C       -1.15809632     -2.97568512      0.00612828     MMTYPE=C_R    QMMM=MM BOND=7/1.5:9/1.5:22/1.0
C       -1.18037132     -0.49067412      0.00642328     MMTYPE=C_R    QMMM=MM BOND=9/1.5:12/1.5:25/1.0
C       -1.89209432      0.70659688      0.00657428     MMTYPE=C_R    QMMM=MM BOND=11/1.5:13/1.5:23/1.0
C       -3.28500932      0.70659688      0.00660128     MMTYPE=C_R    QMMM=MM BOND=12/1.5:14/1.5:24/1.0
C       -3.99343532     -0.50183912      0.00639328     MMTYPE=C_R    QMMM=MM BOND=8/1.5:13/1.5:15/1.5
C       -5.43252232     -0.54396812      0.00618328     MMTYPE=C_R    QMMM=MM BOND=14/1.5:16/1.5:17/1.0
C       -6.10333832     -1.72308612      0.00602828     MMTYPE=C_R    QMMM=MM BOND=5/1.5:15/1.5:26/1.0
H       -5.97082932      0.41637988      0.00626528     MMTYPE=H_     QMMM=MM BOND=15/1.0
H       -1.29075732     -5.11521912      0.00574328     MMTYPE=H_     QMMM=MM BOND=7/1.0
H       -5.91350432     -6.36186912      0.00571128     MMTYPE=H_     QMMM=MM BOND=1/1.0
H       -3.42538532     -6.35767212      0.00588028     MMTYPE=H_     QMMM=MM BOND=2/1.0
H       -7.18118932     -4.22087812      0.00555928     MMTYPE=H_     QMMM=MM BOND=6/1.0
H       -0.05754732     -2.94774012      0.00584128     MMTYPE=H_     QMMM=MM BOND=10/1.0
H       -1.34796932      1.66316388      0.00654928     MMTYPE=H_     QMMM=MM BOND=12/1.0
H       -3.83598732      1.65895788      0.00661928     MMTYPE=H_     QMMM=MM BOND=13/1.0
X       -0.42042330     -0.48178557      0.00640117     MMTYPE=H_     QMMM=MM BOND=11/1.0
X       -6.86309145     -1.74245259      0.00566723     MMTYPE=H_     QMMM=MM BOND=16/1.0
END
```

Figure 1: A fragment (molecular) input file as required by AuToGraFS.

Explanation

1. Flags for AuToGraFS.

   This bit you'll have to add in on your own at the end.

   - Begins with `Data:` and contains a key/value pair separated by an equals sign
   - `SBUtype` is either **center** or **linker**
   - `shape` defines the shape of the fragment and determines how AuToGraFS will align it to the model. Currently understood shapes are:

     (a) blind (ZeroD) cap

     (b) point cap

(c) linear

(d) triangle

(e) tetrahedron, square, rectangle

(f) trigonal bipyramid, square pyramid

(g) octahedron, trigonal prism, hexagon

(h) cube

(i) icosahedron

(j) cuboctahedron

(k) elongated triangular orthobicupola

(l) rhombicuboctahedron

(m) MIL-53 (`mil53`), Kuratowski-type (`mfu4`)

...any spaces in shape names should be replaced with underscores e.g. (`point_cap`)

- `name` is solely for humans and so should be descriptive. It may be as long as you like so, "really fancy linker that took a long time to synthesize, notebook page 42" is perfectly appropriate. Likewise, "Linker from the excellent paper of S. McDuck *JACS* vol 314 p 2718 (2014)".

2. The actual molecule definition.

   (a) Atom symbols

   (b) Cartesian coordinates

   (c) UFF atom types.

   (d) Bond lists in the format *N/BO*, where N is the atom number in the list and BO is the bod order. e.g. Atom 1 is bonded to atoms 2 and 6 by aromatic (BO = 1.5)bonds and to atom 19 by a single bond.

3. Dummy atoms (symbol X) define the spatial extent of the fragment and are the points used to align the fragment with the model. The MMType is not important but should be left as "H_".

In future versions this may change to designate dummy atoms that must bond to Carbon or must bond to Nitrogen.

Using Avogadro

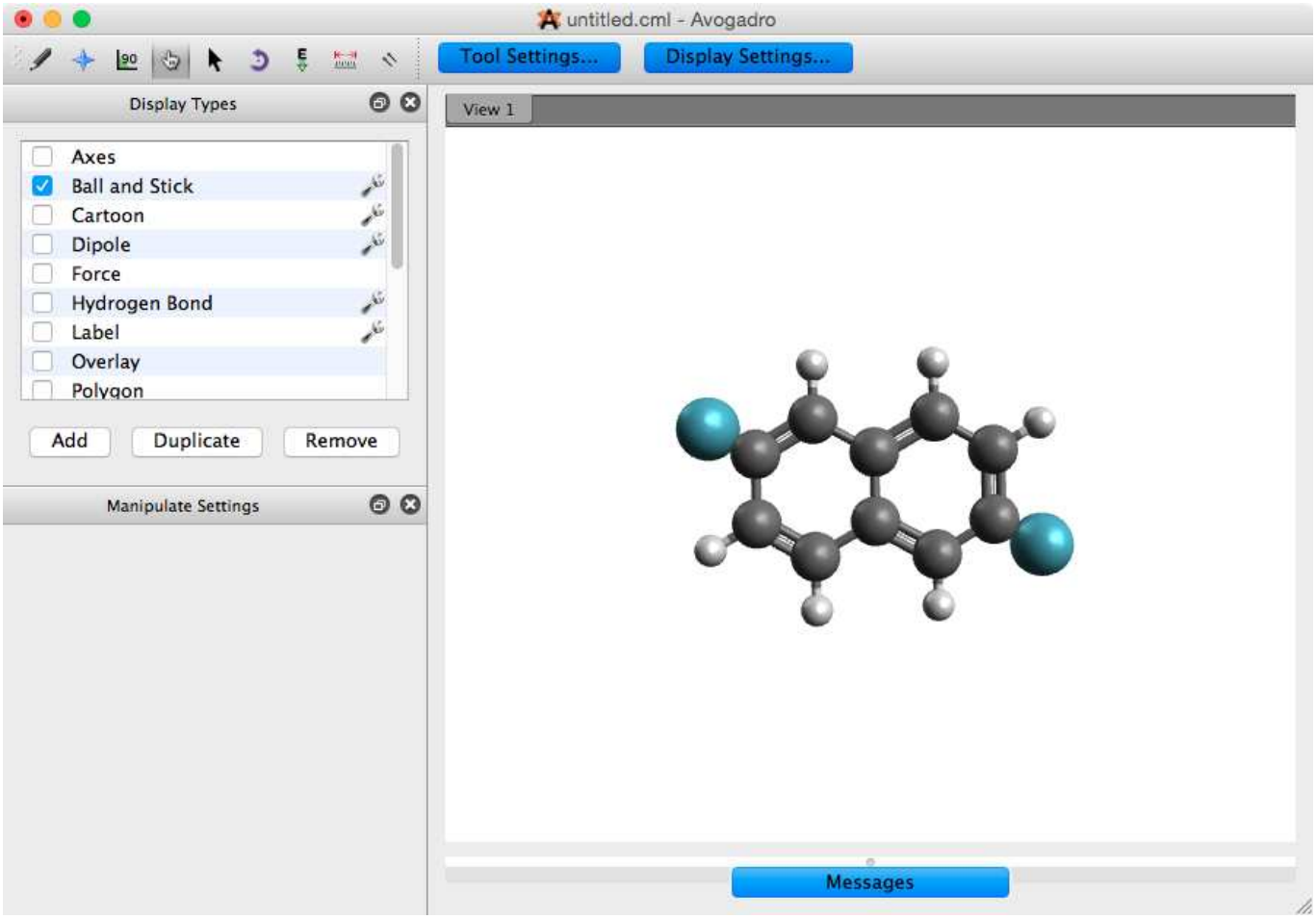

Figure 2: Building a molecule with Avogadro

1. Build the molecule. Here we've built naphthalene.

2. Change the desired connection points to Xe atoms. We'll change this later, so anything that doesn't appear in your actual molecule is OK. But Xe is easy to change to X. If you have optional connection points (i.e. where solvent may bind) make these atoms something else, Ba is rather uncommon and easy to change to Bq.

3. Change the Xe–Y bondlengths to half the desired bondlength in the finished framework. e.g. If you intend to form a carbon-carbon bond, make the bondlength 0.75Å.

4. Save your molecule using **Sybyl Mol2 (*.mol2)** format

5. From the command line, run `mol22inp YourMolecule` (without the extension!). This will yield a file, YourMolecule.inp. Open this file, change Xe atoms to X atoms, Ba to Bq (if any) and check the MMTypes are all there.

6. Add the three header (`Data:`) lines at the top and you're done!

Using GaussView

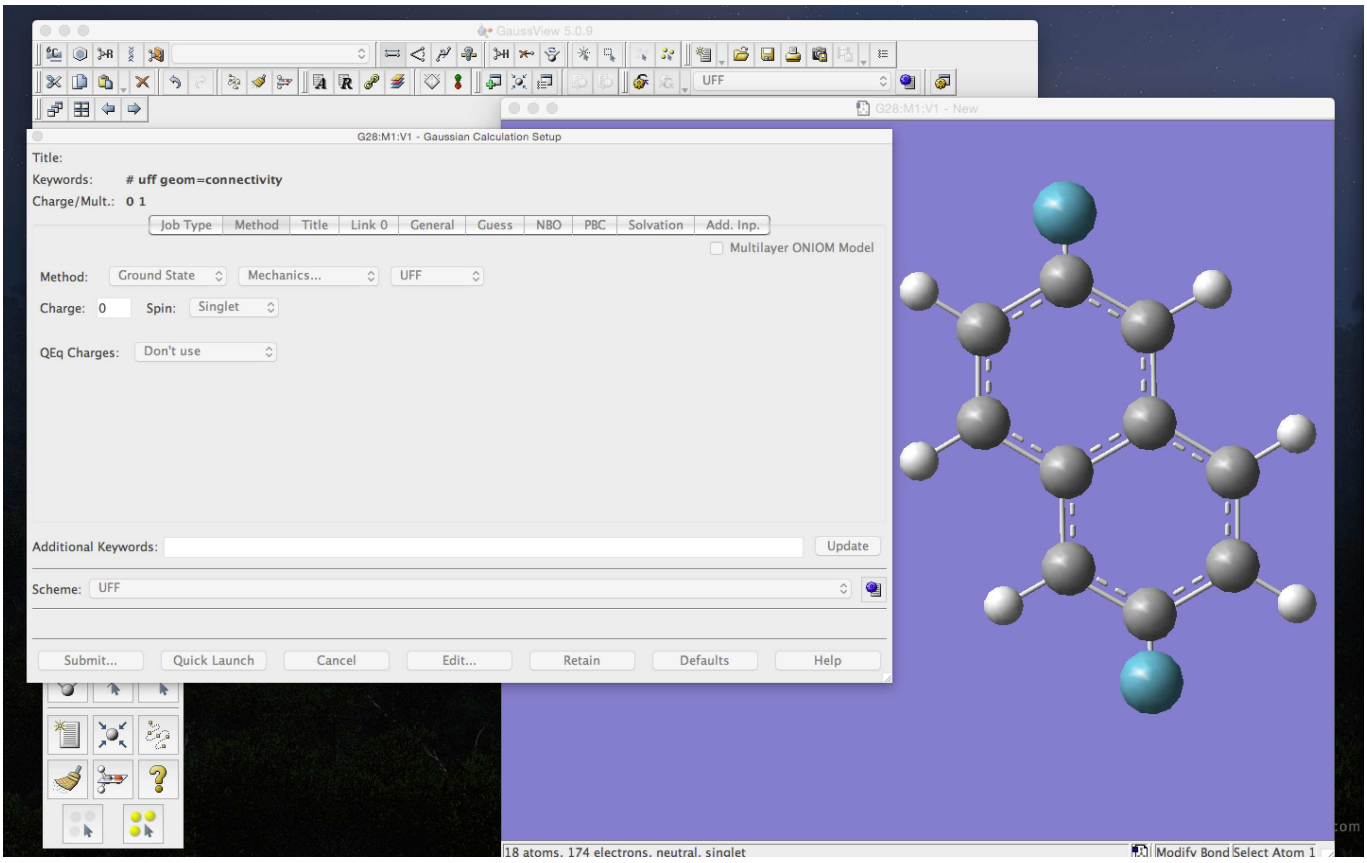

Figure 3: Building a molecule with Gaussview

1. Build the molecule. The bond orders you see are the bond orders you get.

2. IMPORTANT! Use Xe (or something else) for dummy atoms because Gaussview doesn't include dummy atoms in the connectivity list.

3. From the **Calculate** menu, select **Gaussian Calculation Setup**...

   - In **Method**, select **Mechanics**, then **UFF** or **Dreiding**
   - **geom=connectivity** should automatically appear
   - To save the file, click on **Edit...**
   - Save the file using the extension **.gjf** .com is also a legal gaussian file extension, but AuToGraFS won't read the atoms types or bonding information from a .com file.

4. From the command line, run `g0x2inp YourMolecule` (without the extension!). This will yield a file, YourMolecule.inp. Open this file, change Xe atoms to X atoms, Ba to Bq (if any) and check the MMTypes are all there.

5. Add the three header (`Data:`) lines at the top and you're done!