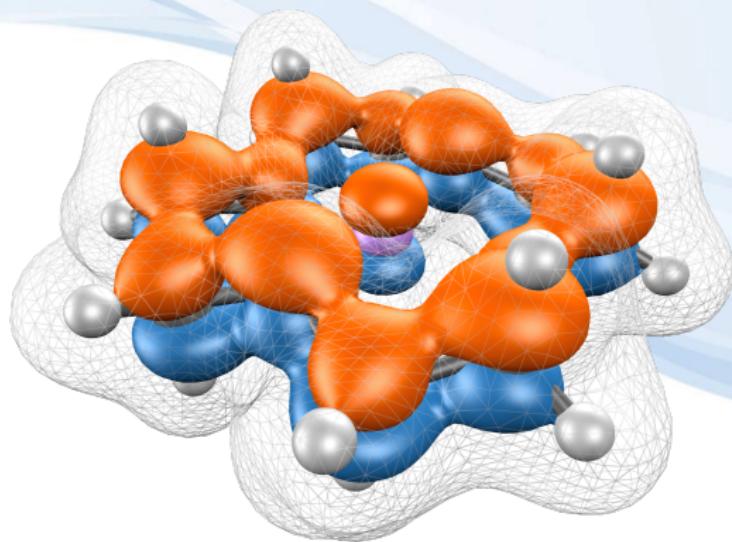


Introduction to Q-CHEM and IQMOL



9:30 - 10:00 Basic QM calculations using IQMOL

10:00 - 10:45 Freezing String Method



IQMOL is an open-source molecular editor and visualization package which runs under Windows, Mac OS X and Linux.

- ▶ Supported file formats include: xyz, cml, pdb, mol, fchk, cube data and Q-CHEM input/output
- ▶ Free-form molecular builder:
 - ▶ Structure optimization using MM
 - ▶ Symmetrization of structures
 - ▶ Built-in library of molecules
- ▶ Analysis features:
 - ▶ Animations: reaction pathways and vibrational frequencies
 - ▶ Surface plots: MOs and (spin) densities
 - ▶ Surface properties: ESP and cube data



IQMOL is a standalone program, but has been optimized to work best in a Q-CHEM work flow:

- ▶ Building structures
- ▶ Generating Q-CHEM input
- ▶ Submitting Q-CHEM calculations
- ▶ Visualizing results

This is due to several Q-CHEM specific features:

- ▶ Comprehensive Q-CHEM input file generator
- ▶ Embedded Q-CHEM keyword documentation
- ▶ Submission of Q-CHEM jobs to local and cloud servers including PBS, SGE and Web



- ▶ Binary packages can be downloaded from:
www.iqmol.org/downloads.html
- ▶ **Windows** double-click the installer in your downloads folder and follow the prompts.
- ▶ **OS X** double-click the dmg file in your downloads folder. The application bundle should be copied to the /Applications directory, or any other location.
- ▶ **Linux** RPM and Deb packages are available:

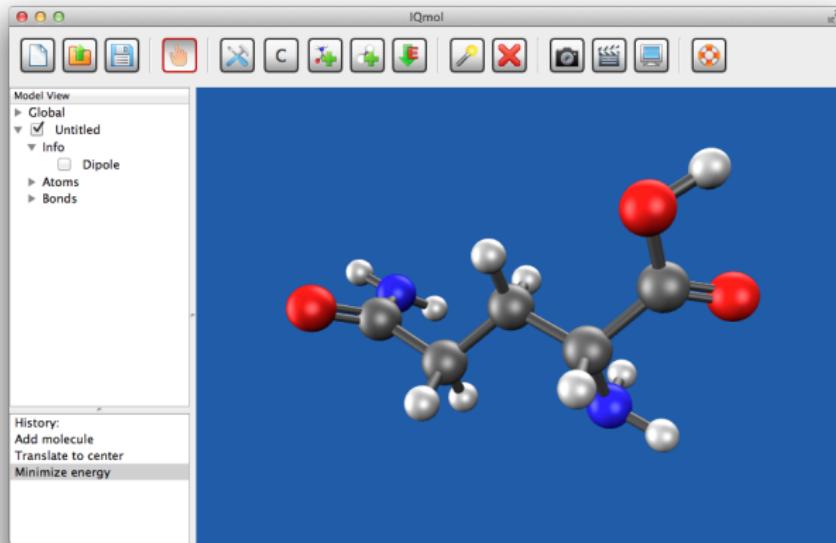
```
sudo dpkg -i iqmol_2.9.2.deb
```

```
sudo apt-get install -f
```

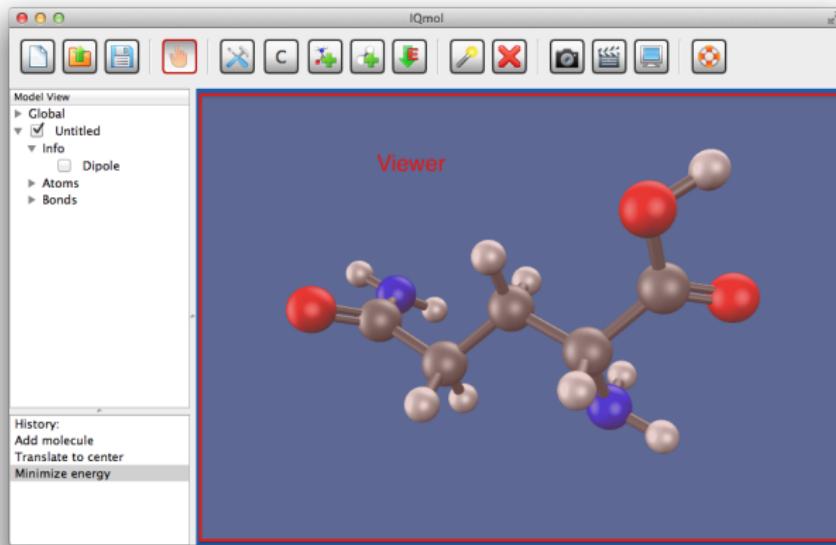
The second command resolves dependencies.



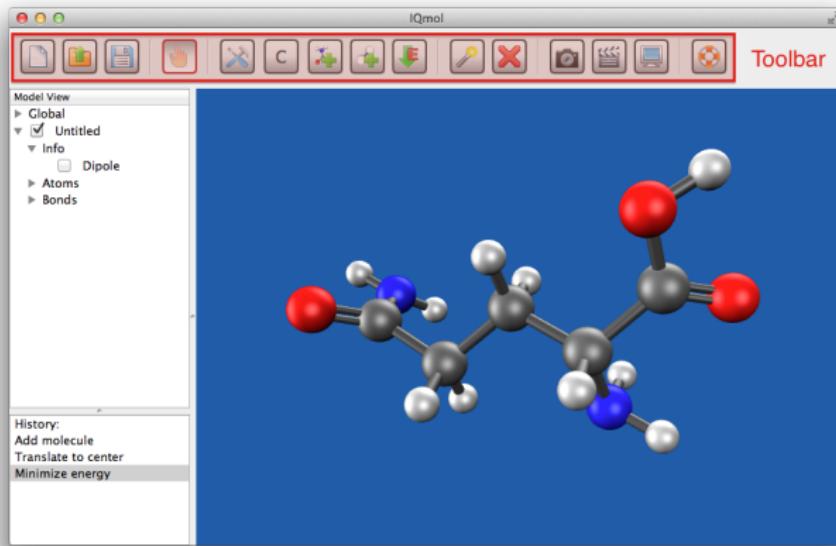
The main IQMOL window looks like this:



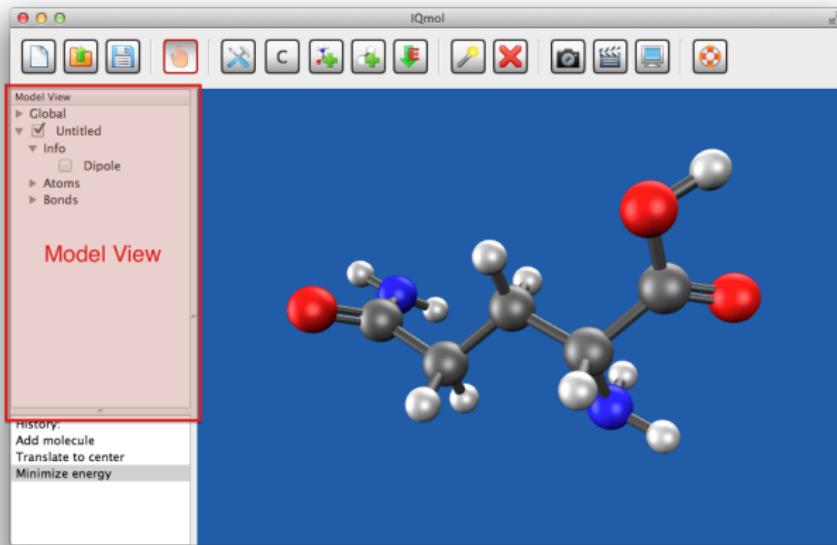
The Viewer is where the molecule is built and manipulated

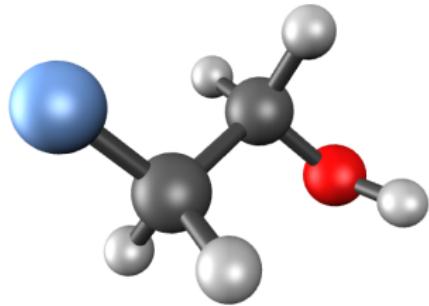


The Toolbar includes common commands operations



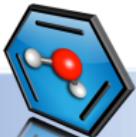
The Model View shows you what data is available





2-Fluoroethanol

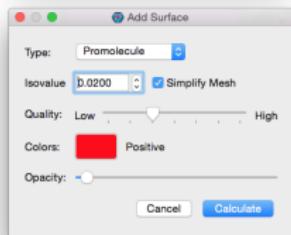
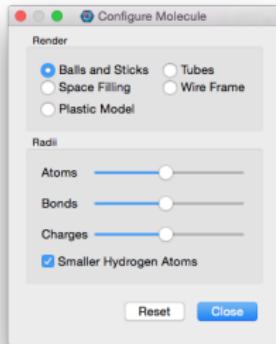
1. Ensure build mode then click and drag in the Viewer to form C-C
2. Change the build element
3. Click on one of the C atoms and drag to form a C-F bond
4. Click Add Fragment and select the alcohol group
5. Click on the other C atom and drag to form the C-OH bond
6. Finish by adding hydrogens



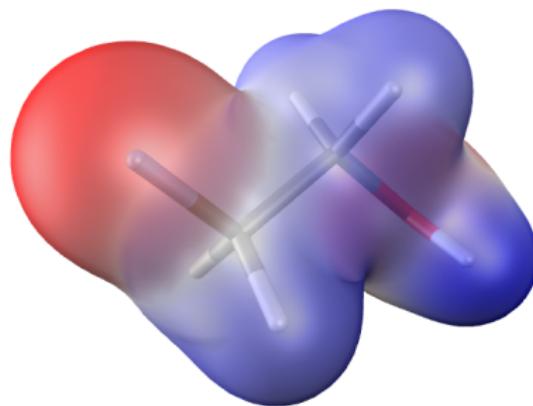
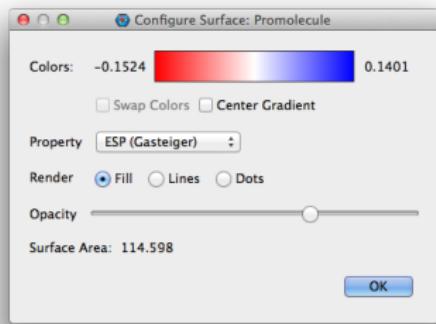
- ▶ IQMOL has a free-form builder, so your initial structure may not be very good. Click the minimize button  to optimize the structure using molecular mechanics.
- ▶ Bond lengths, angles and dihedrals can be measured by selecting 2, 3 or 4 atoms using select mode 
- ▶ Select the atoms C-C-O-H and set the torsion angle to 180° via Build→Set Geometric Constraint
- ▶ Symmetrize the structure using Build→Symmetrize Molecule, you should obtain a C_s structure.



- ▶ Double-clicking a Model View item brings up a Configurator.
- ▶ The Molecule Configurator allows you to change the appearance of the molecule (double-click the molecule name, Untitled)
- ▶ The Surfaces configurator allows you to add various surface types. Create a promolecule density for your molecule.



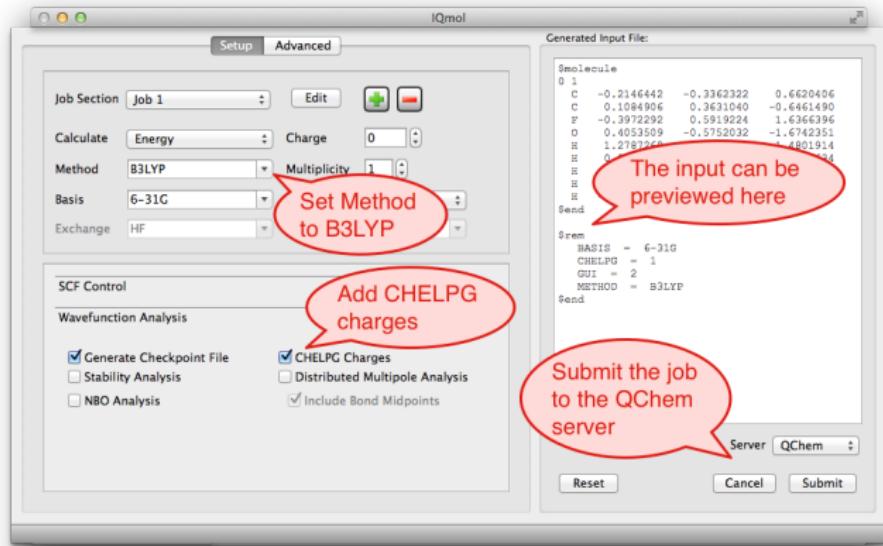
The Promolecule surface will appear in the Model View under Surfaces, double-click it to bring up the Surface Configurator.



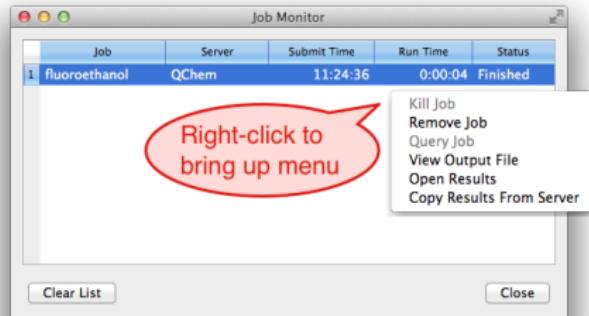
Change the property to ESP and adjust the opacity so you can still see the molecule. Click the checkbox to hide it.



Open the Q-CHEM User Interface (QUI) via the menu
Calculation→Q-Chem Setup

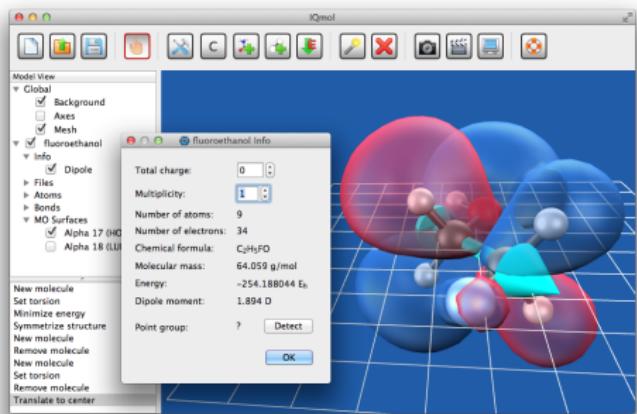


After submitting the calculation, its progress can be seen on the Job Monitor, which can be opened via the Calculation→Job Monitor menu option

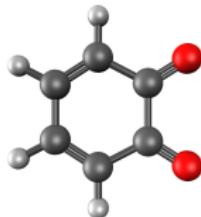


Once the job has finished, save the results into a folder, the output will be automatically opened.

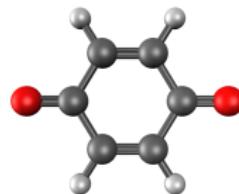
- ▶ Open the Info Configurator to get the energy
- ▶ Visualize the dipole
- ▶ Open the Canonical Orbitals item under Surfaces and plot the HOMO & LUMO.
- ▶ Use the File Configurator to view the Q-CHEM output



Benzoquinone exists in two isomeric forms:



o-Benzoquinone



p-Benzoquinone

1. Compute the HF/6-31G frequencies for both isomers.
2. Which vibrational band most easily differentiates between the two spectra?

Remember to optimize the structures first!

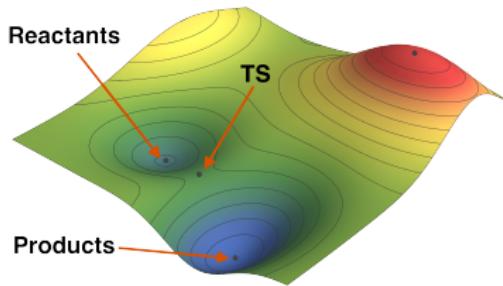


9:30 - 10:00 Basic QM calculations using IQMOL

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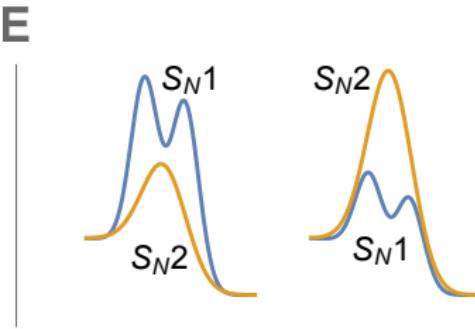
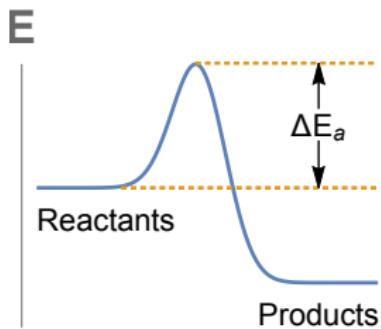
Transition states correspond to **first-order saddle points** on the molecular potential energy surface (PES):



They correspond to the highest point on the lowest-energy pathway connecting two minima (reactants and products).



Finding transition states is crucial for accurately predicting kinetic constants and reaction mechanisms.



$$k = Ae^{E_a/k_b T}$$



However, transition states are intrinsically more difficult to find than optimized structures:

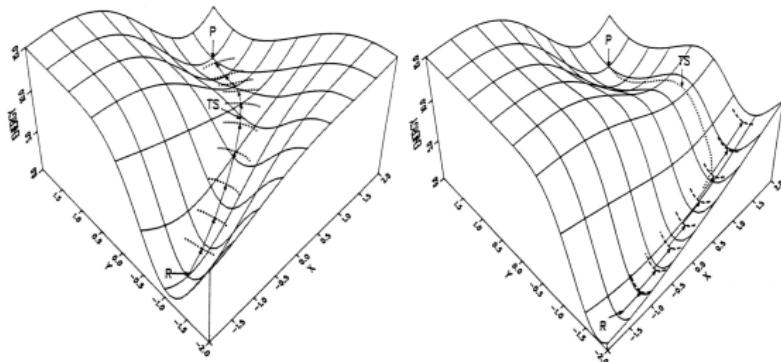
- ▶ Structures corresponding to transition states are **less predictable** via chemical intuition.
- ▶ Saddle points are more difficult to locate on a surface - **Hessian signature** needs to be correct.

The success of a TS algorithm depends critically on the initial guess structure.



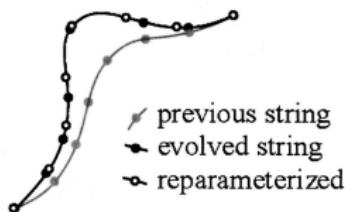
Eigenvector following methods attempt to maximise the energy in the direction of the eigenvector corresponding to the reaction coordinate, whilst minimizing the energy in the other directions.

This may or may not work:



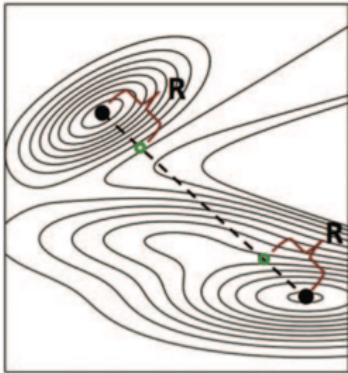
String methods provide a systematic way to obtain a **guess** structure for the transition state. They interpolate a chain of states between the reactants and products.

- ▶ String Method
- ▶ Nudged Elastic Band
- ▶ Growing String Method

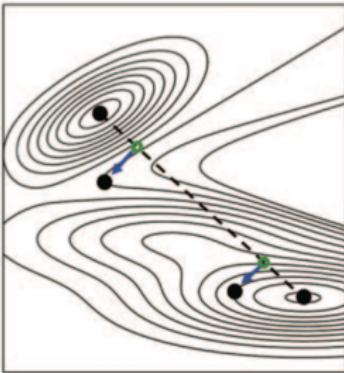


The Freezing String Method (FSM) attempts to minimize redundant QM calculations, thus making it more efficient.

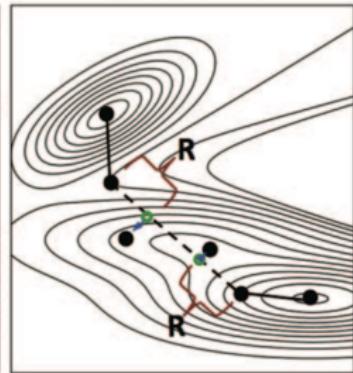
Inward growth along tangent



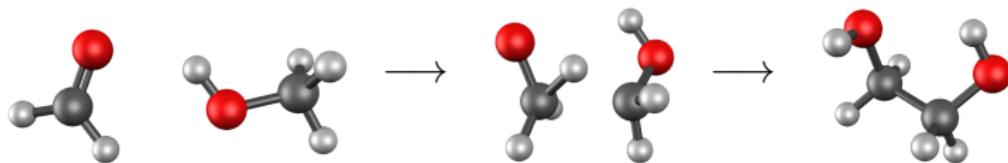
Perpendicular optimization



Repeat growth and optimization



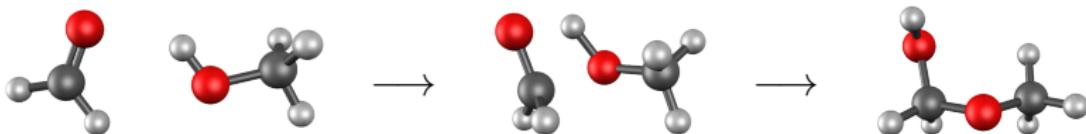
Formation of ethylene glycol from formaldehyde and methanol.



Turn off Generate Checkpoint file option!



Formation of methoxy-methanol from CH₂O and CH₃OH:

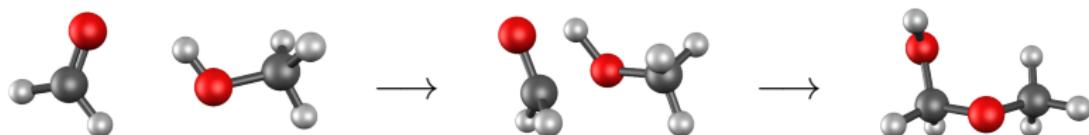


1. Download the dimer geometry from iqmol.org/geom1.xyz
2. Compute the HF/6-31G geometry for methoxy-methanol.
3. Use your geometries for a HF/6-31G FSM calculation.

Use 21 Nodes and 6 gradient steps
Turn off Generate Checkpoint file option!

4. Compute the frequencies for your selected geometry.
5. Perform a TS search following the appropriate mode.





If you have time:

1. Perform any additional calculations required to compute the HF/6-31G barrier for the methoxy-methanol reaction.
2. Try finding the TS for the ethylene glycol reaction (this is a little trickier).

