Introduction to IQmol: Part II

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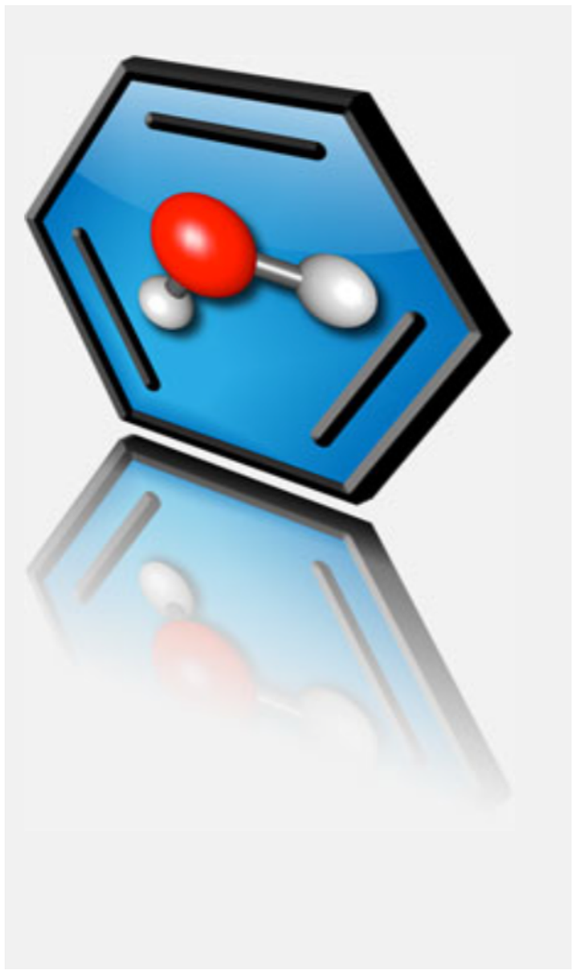
Resources

- Written by Dr. Andrew Gilbert

- Keep yourself up to date with IQmol website: http://iqmol.org

- **IQmol Youtube channel:** IQmol now has its own Youtube channel

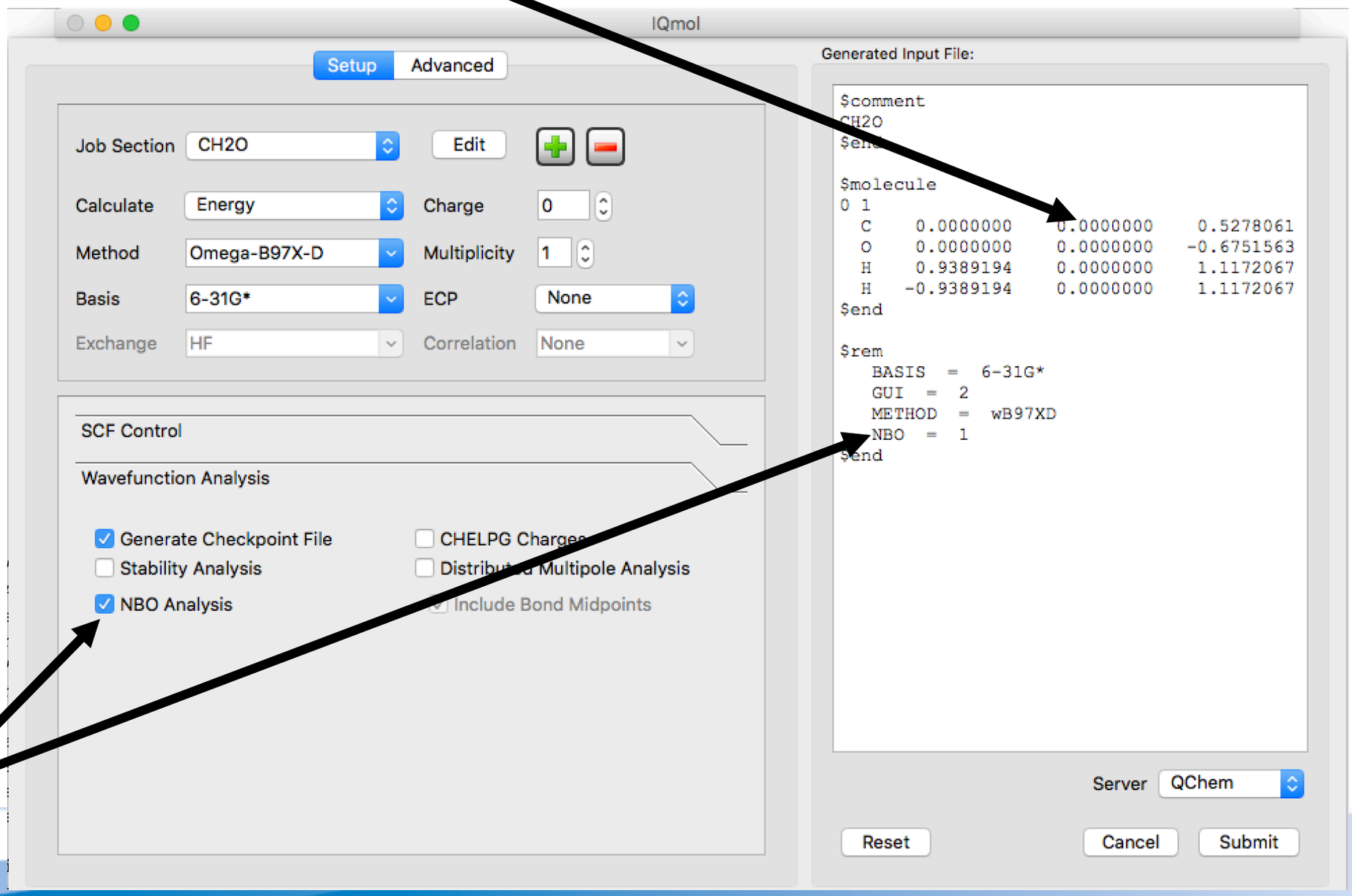


Performing Q-Chem calculations

Advanced examples

Advanced: NBO analysis

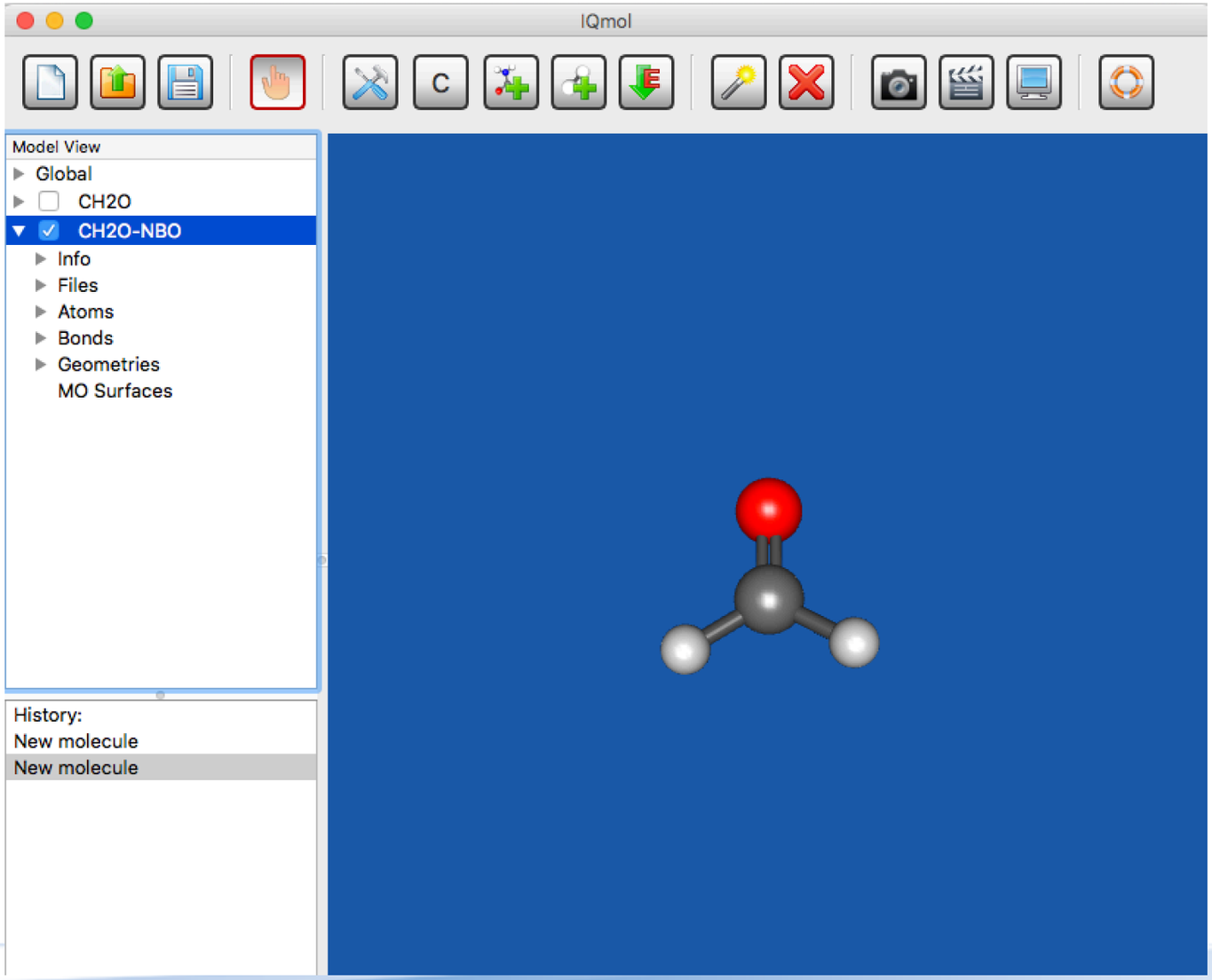
- Take the optimized geometry (final coordinate after geometry optimization) and copy in the preview of input file



NBO = 1

NBO analysis

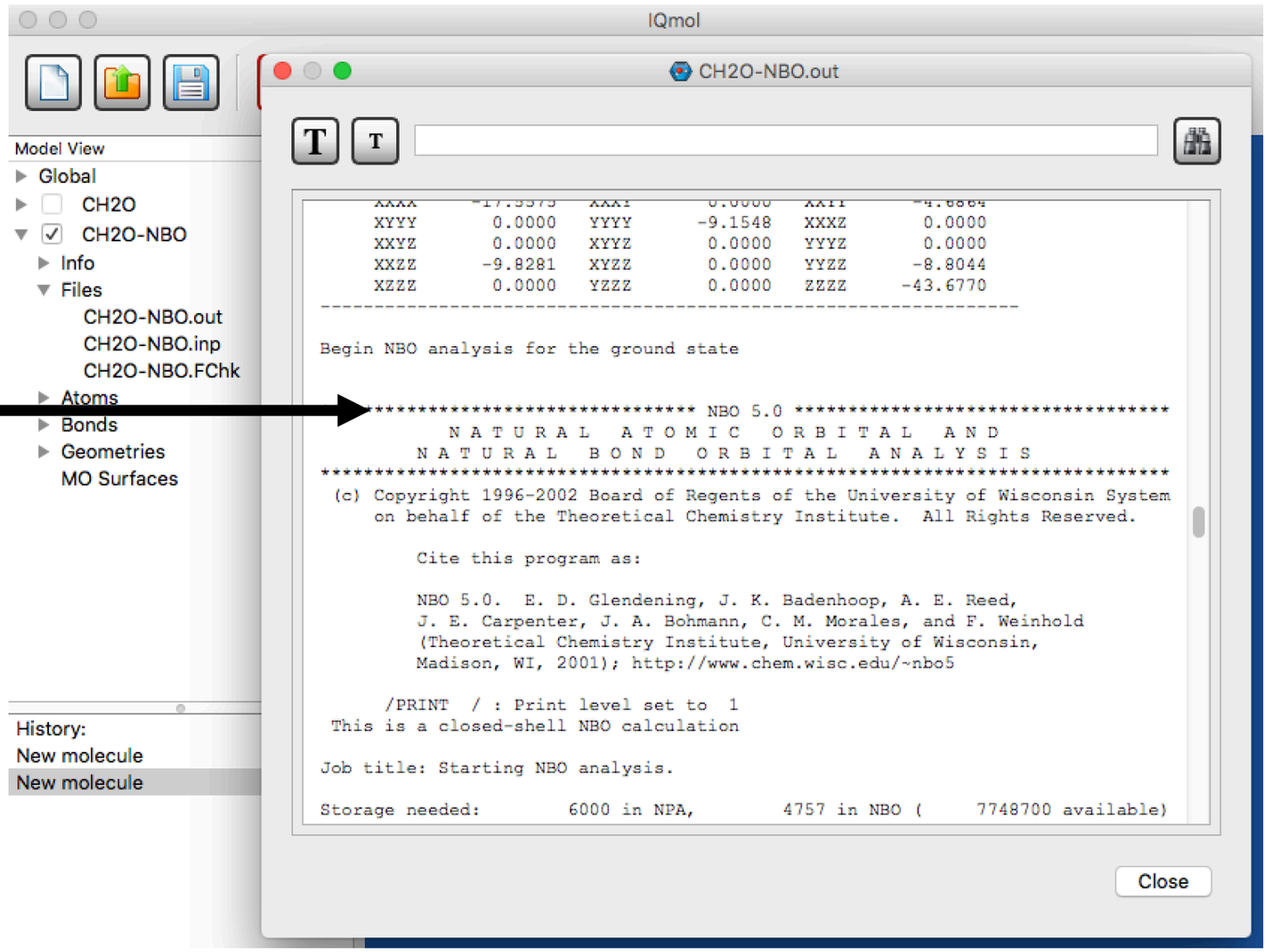
- Submit the job
- Copy back the output into your laptop
- Click the checkbox



NBO analysis

- Click on Files
- Open CH2O-NBO.out file

Output from NBO calculations



NBO analysis

Atomic charges

Atomic orbital populations