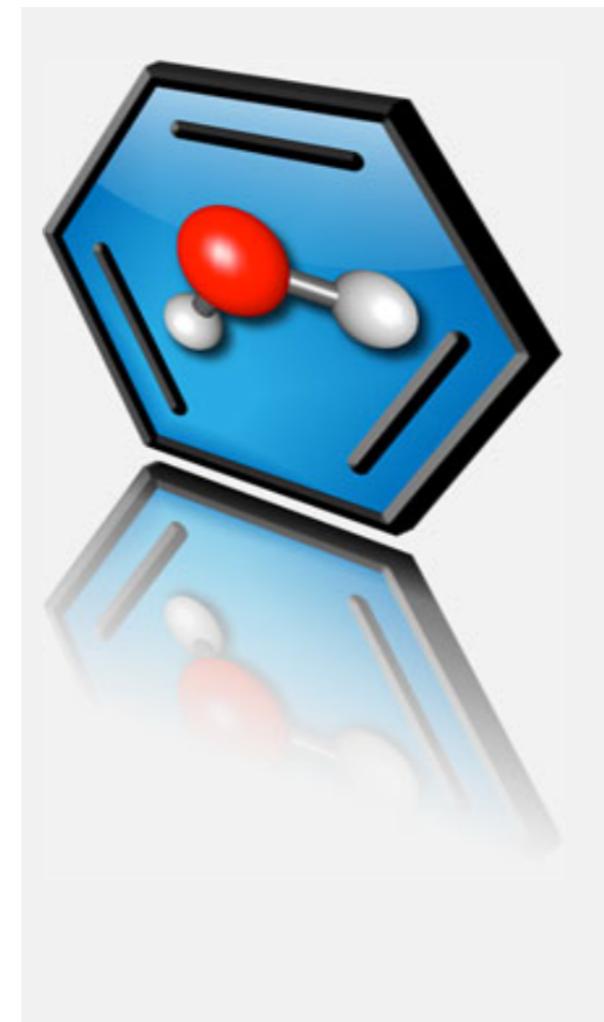


# Introduction to IQmol: Part II

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- 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

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

The screenshot shows the IQmol software interface with the 'Advanced' setup for a CH2O molecule. The 'Wavefunction Analysis' section has 'NBO Analysis' checked. The 'Generated Input File' preview shows the resulting input file with 'NBO = 1' and the optimized coordinates for the CH2O molecule.

**Job Section:** CH2O

**Calculate:** Energy

**Method:** Omega-B97X-D

**Basis:** 6-31G\*

**Exchange:** HF

**Charge:** 0

**Multiplicity:** 1

**ECP:** None

**Correlation:** None

**Wavefunction Analysis:**

- Generate Checkpoint File
- Stability Analysis
- NBO Analysis
- CHELPG Charges
- Distributed Multipole Analysis
- Include Bond Midpoints

**Generated Input File:**

```

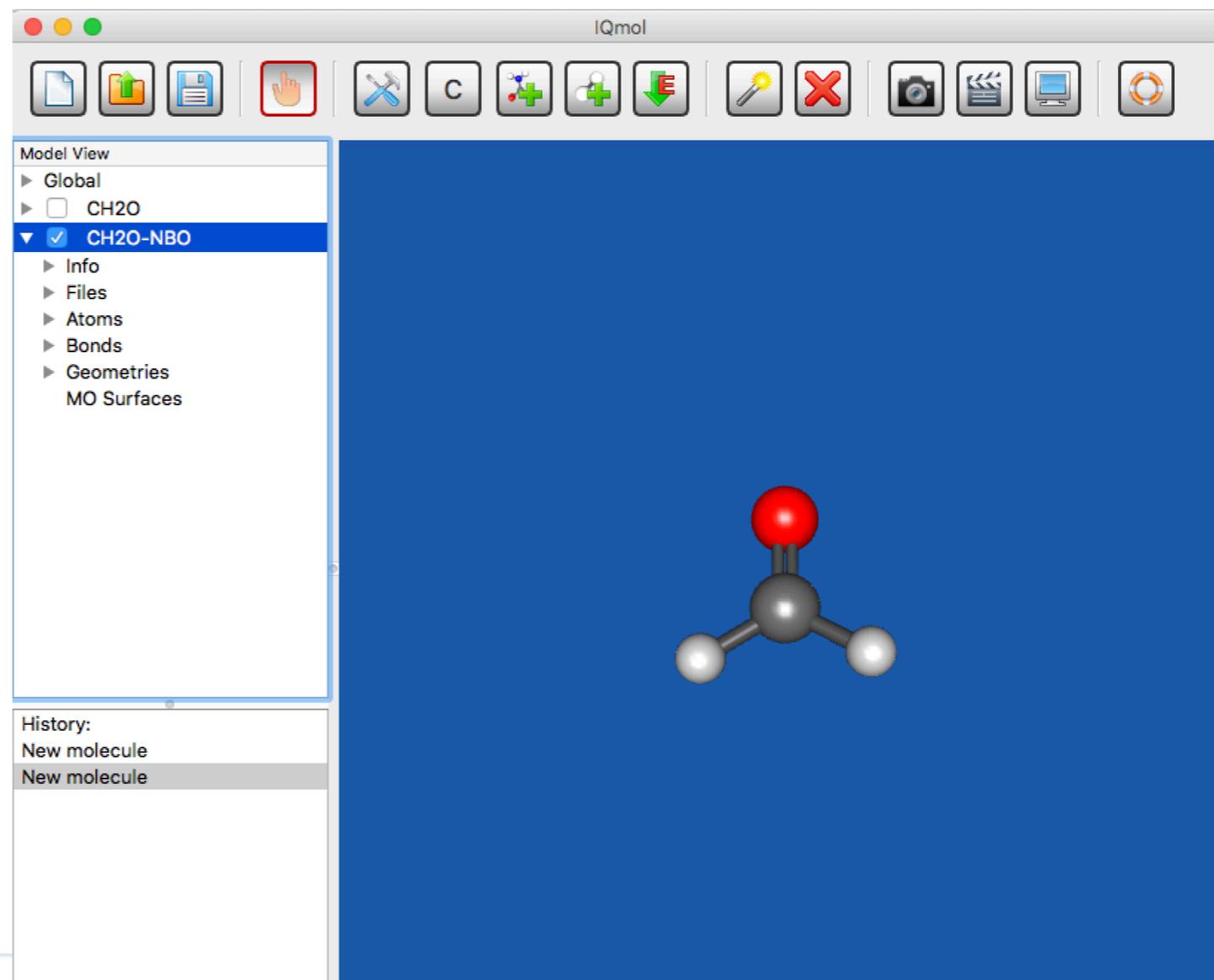
$comment
CH2O
$end

$molecule
0 1
C 0.0000000 0.0000000 0.5278061
O 0.0000000 0.0000000 -0.6751563
H 0.9389194 0.0000000 1.1172067
H -0.9389194 0.0000000 1.1172067
$end

$rem
BASIS = 6-31G*
GUI = 2
METHOD = wB97XD
NBO = 1
$end
  
```

**NBO = 1**

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



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

Output from NBO calculations

The screenshot shows the IQmol software interface. On the left, the 'Model View' panel is expanded to 'Files', where 'CH2O-NBO.out' is selected. An arrow points from the text 'Output from NBO calculations' to this file. The main window, titled 'CH2O-NBO.out', displays the following text:

```

XXXX  -17.3373  XXX1   0.0000  XX11  -4.8884
YYYY   0.0000  YYYY  -9.1548  XXXZ   0.0000
XXYZ   0.0000  XYYZ   0.0000  YYYZ   0.0000
XZZZ  -9.8281  XYZZ   0.0000  YZZZ  -8.8044
ZZZZ   0.0000  YZZZ   0.0000  ZZZZ  -43.6770
-----
Begin NBO analysis for the ground state

***** NBO 5.0 *****
  NATURAL ATOMIC ORBITAL AND
  NATURAL BOND ORBITAL ANALYSIS
*****
(c) Copyright 1996-2002 Board of Regents of the University of Wisconsin System
on behalf of the Theoretical Chemistry Institute. All Rights Reserved.

Cite this program as:

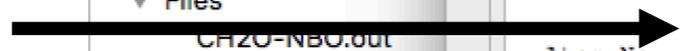
NBO 5.0. E. D. Glendening, J. K. Badenhoop, A. E. Reed,
J. E. Carpenter, J. A. Bohmann, C. M. Morales, and F. Weinhold
(Theoretical Chemistry Institute, University of Wisconsin,
Madison, WI, 2001); http://www.chem.wisc.edu/~nbo5

/PRINT / : Print level set to 1
This is a closed-shell NBO calculation

Job title: Starting NBO analysis.

Storage needed:      6000 in NPA,      4757 in NBO ( 7748700 available)
  
```

Atomic charges



Model View

- Global
- CH2O
- CH2O-NBO
  - Info
  - Files
    - CH2O-NBO.out
    - CH2O-NBO.inp
    - CH2O-NBO.FChk
  - Atoms
  - Bonds
  - Geometries
  - MO Surfaces

History:

- New molecule
- New molecule

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
C 1	0.22414	1.99972	3.74732	0.02883	5.77586
O 2	-0.50430	1.99983	6.48283	0.02164	8.50430
H 3	0.14008	0.00000	0.85714	0.00278	0.85992
H 4	0.14008	0.00000	0.85714	0.00278	0.85992
* Total *	0.00000	3.99955	11.94443	0.05603	16.00000

Natural Population	
Core	3.99955 ( 99.9887% of 4)
Valence	11.94443 ( 99.5369% of 12)
Natural Minimal Basis	15.94397 ( 99.6498% of 16)
Natural Rydberg Basis	0.05603 ( 0.3502% of 16)

Atom No	Natural Electron Configuration
C 1	[core]2s( 1.05)2p( 2.70)3s( 0.01)3p( 0.01)3d( 0.01)
O 2	[core]2s( 1.71)2p( 4.77)3d( 0.01)
H 3	1s( 0.86)
H 4	1s( 0.86)

Close

Atomic orbital populations

