

WebMO: A User Friendly Computational Platform for Chemical Educators

Jun (Eva) Yi

Department of Chemistry and Biochemistry

University of Oklahoma

WebMO

WebMO is a WWW-based interface for computational chemistry software

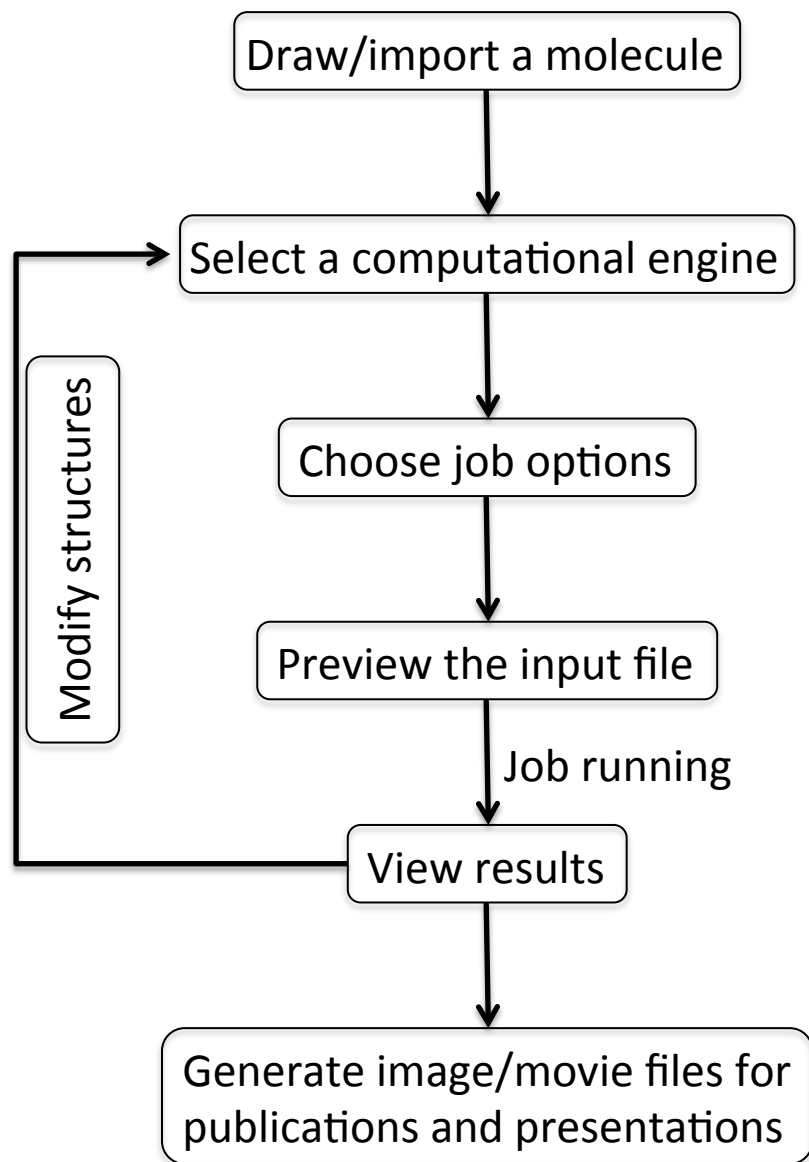
Key features

- Supports Gaussian 09 and many other computational engines
- Allows for drawing of molecules, submitting calculations, running jobs and viewing results using a web browser
- Simple enough for undergraduate computational chemistry educational/research projects
- Flexible enough for advanced computational chemistry research projects

Useful Links

- WebMO official website:
<http://www.webmo.net/index.html>
- Computational Chemistry for Chemistry Educators:
<http://www.computationalscience.org/ccce/about/sessions/sessions.php>
- WebMO login window on OSCER:
<http://webmo.oscer.ou.edu>

Flowchart for running a computational job using WebMO



Application for undergraduate research

- Case study using nitric oxide (NO): comparison of physical/chemical properties of nitroxyl anion (NO^-), NO and nitrosonium (NO^+)
 - geometry optimizations
 - calculation of vibrational frequencies
 - calculation of molecular orbitals
- OBJECTIVE: subtracting/adding an electron into an ANTIBONDING ORBITAL (using NO as an example), predict effects on
 - bond length,
 - IR stretching freq,
 - nature of the HOMO/LUMO

Choose job options

WebMO Job Manager

Configure Gaussian Job Opti

https://webmo.oscer.ou.edu/~webmo/cgi-bin/webmo/build_molecule.cgi

OU EMAIL CHEM_OU libraries_OU Google Maps Wikipedia WebMO Research Grants PX google voice Other Bookmarks

Configure Gaussian Job Options

Status

- evayi263
- webmo
- unlimited
- unlimited
- 0 jobs

Progress

- Job manager
- Build molecule
- Job options

Configure options for the selected job and computational engine.

- Submit job
- Help

Job Options | Advanced | Custom | Preview | Notes

Job Name: NO_GO_Freq

Calculation: Optimize + Vib Freq

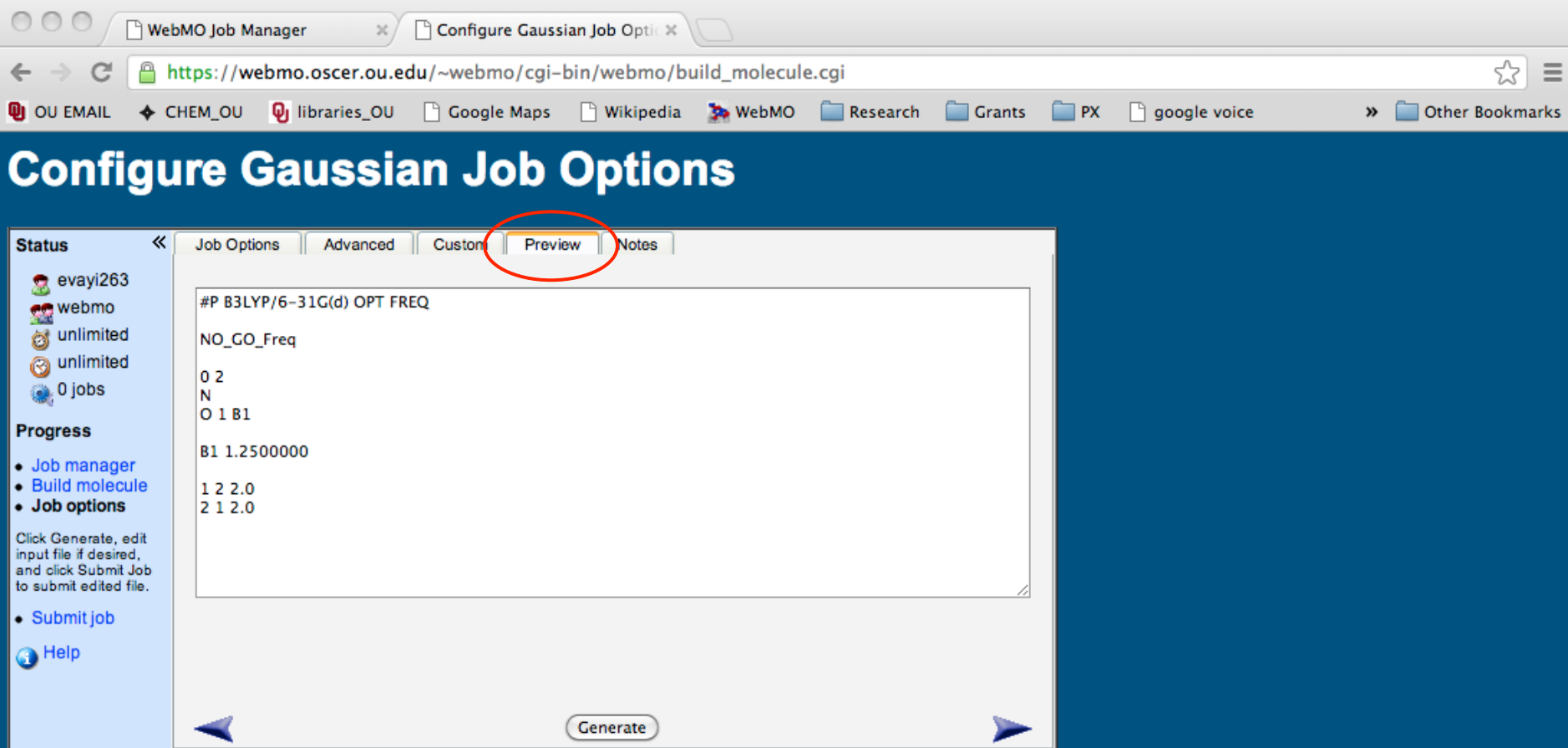
Theory: B3LYP

Basis Set: Routine: 6-31G(d)

Charge: 0

Multiplicity: Doublet

Preview the input file



The screenshot shows a web browser window with the URL https://webmo.oscer.ou.edu/~webmo/cgi-bin/webmo/build_molecule.cgi. The page title is "Configure Gaussian Job Options". The interface has a blue header and a white content area. On the left, there is a sidebar with user information (evayi263, webmo, unlimited, 0 jobs) and progress links (Job manager, Build molecule, Job options, Submit job, Help). The main content area has a tabbed interface with "Job Options", "Advanced", "Custom", "Preview", and "Notes". The "Preview" tab is selected and circled in red. The preview window displays the following Gaussian input file content:

```
#P B3LYP/6-31G(d) OPT FREQ
NO_GO_Freq
0 2
N
O 1 B1
B1 1.2500000
1 2 2.0
2 1 2.0
```

At the bottom of the main content area, there is a "Generate" button.

View the Job Manager

WebMO Job Manager | WebMO Job Manager | WebMO Job Manager | 1261 - View Job

https://webmo.oscer.ou.edu/~webmo/cgi-bin/webmo/jobmgr.cgi?t=1349143808284?t=1349145159378

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WebMO Job Manager

Status << New Job Refresh Download Move To Delete Utilities Logout

Show all Show all Show all Show all

Number	Name	Description	Date	Status	Time	Actions
1261	NO_GO2_Freq	Optimize + Vib Freq - Gaussian	10/1/2012 21:00	Complete	11.5 sec	
1257	NO_GO_Freq	Optimize + Vib Freq - Gaussian	10/1/2012 20:54	Complete	6.9 sec	
1244	PF3ImONO_GO13	Geometry Optimization - Gaussian	10/1/2012 14:36	Running	0.0 sec	
1105	2HNO_2H2O_GO5_scan	Coordinate Scan - Gaussian	9/28/2012 12:58	Failed	39:01:25	

Folders

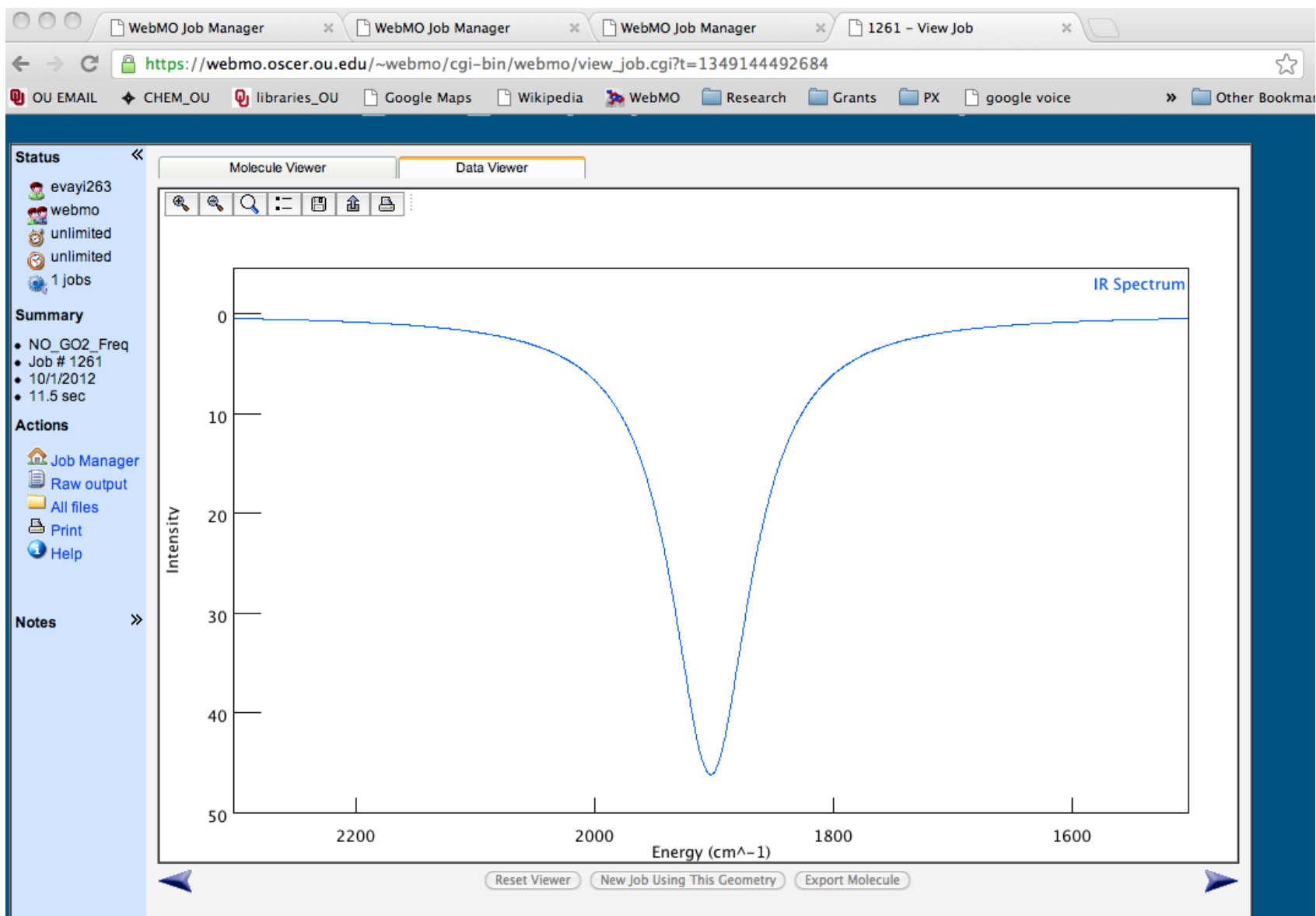
- Inbox
- Failed_Cal
- Fe_Chlorin_N...
- Fe_nitrite
- Fe_Porphine_...
- HNO_cal
- SO_Cal
- Trash

Manage folders
Empty trash

Search

Displayed jobs

Visualize the results (e.g., spectrum)



Visualize the results (e.g., HOMO)

WebMO Job Manager x WebMO Job Manager x WebMO Job Manager x WebMO Job Manager x 1270 - View Job x 1261 - View Job

https://webmo.oscer.ou.edu/~webmo/cgi-bin/webmo/jobmgr.cgi?t=1349146075339

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View Job 1270: NO_MO, Molecular Orbitals - Gaussian

Status

evayi263
webmo
unlimited
unlimited
0 Jobs

Summary

- NO_MO
- Job # 1270
- 10/1/2012
- 2.0 sec

Actions

- Job Manager
- Raw output
- All files
- Print
- Help

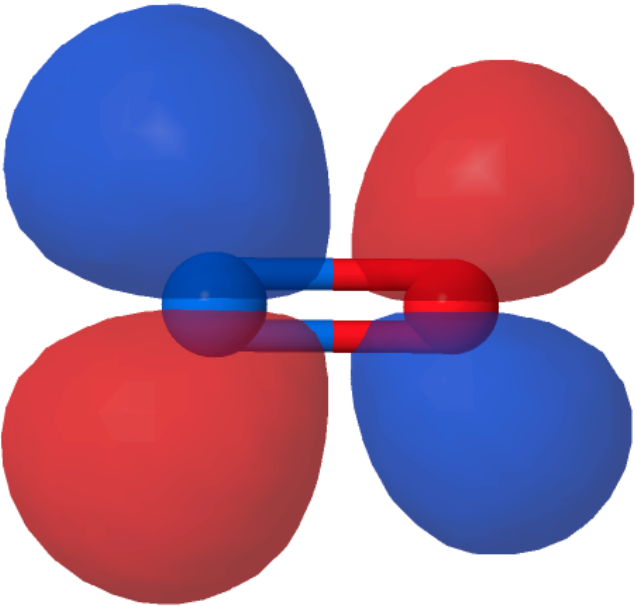
Notes

Molecule Viewer Data Viewer MO Viewer

File Edit View Help

job1270_mo8

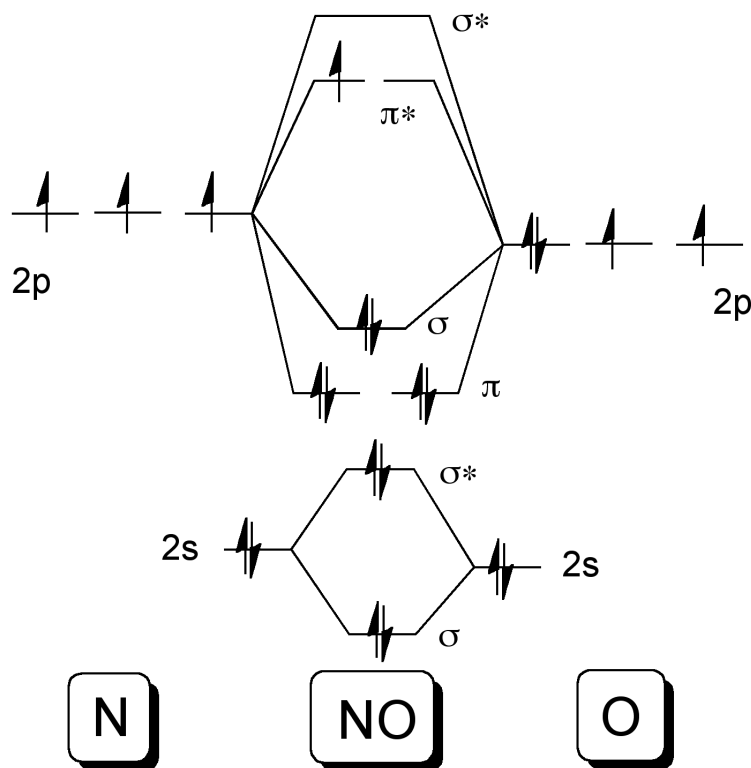
MO	Occ.	Energy
9	0	-0.11886
10	0	0.0422
11	0	0.0874
12	0	0.09544
13	0	0.09713
14	0	0.17173
15	0	0.19858
16	0	0.2021
17	0	0.3186
18	0	0.39684
19	0	0.71414
20	0	0.72368
21	0	0.74152
22	0	0.96516
23	0	0.99563
24	0	0.99992
25	0	1.01179
26	0	1.46376
27	0	1.80647
28	0	1.80909
29	0	1.8171
30	0	1.8206
31	0	2.57116



Electron density
Electrostatic pot
Elec (HOMO) density
Nuc (LUMO) density
Radical density

Reset Viewer New Job Using This Geometry Export Molecule

M.O. Diagrams and occupied/unoccupied antibonding orbitals (the case of NO)

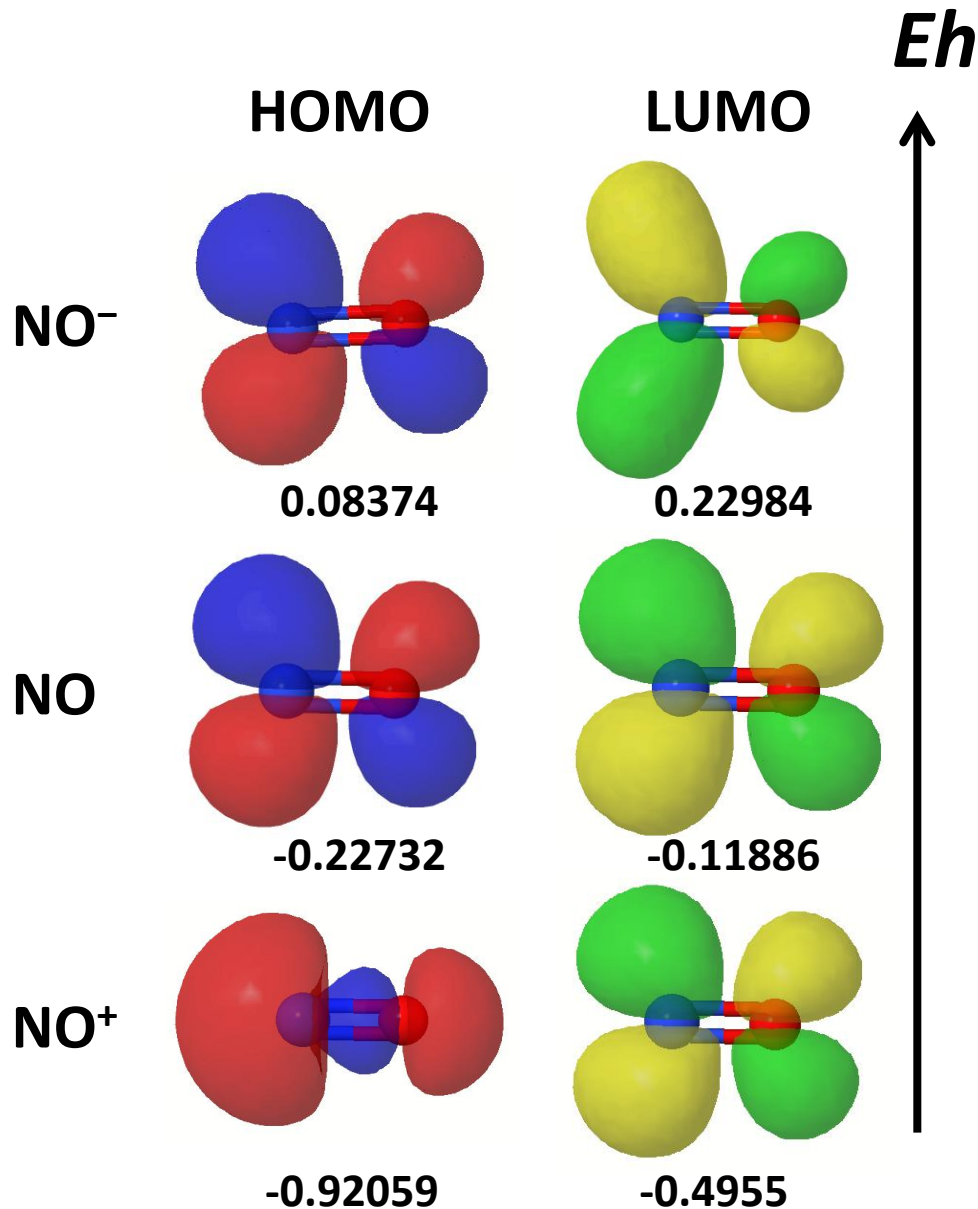
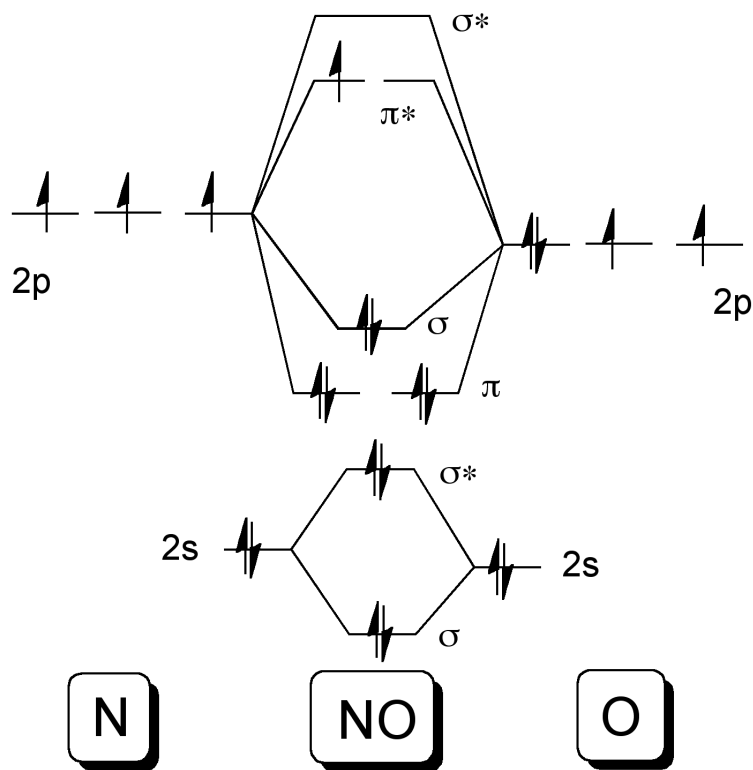


	N-O (Å)	IR (cm ⁻¹)
NO⁻(t)	1.264 (1.200)	1415 (2591) [1450]
NO (d)	1.148 (1.127)	1980 (2340) [1880]
NO⁺(s)	1.060 (1.074)	2491 (2591) [2300]

basis set: B3LYP/6-311+G(d), (PM3)

Experimental data in (***bold/italics***)

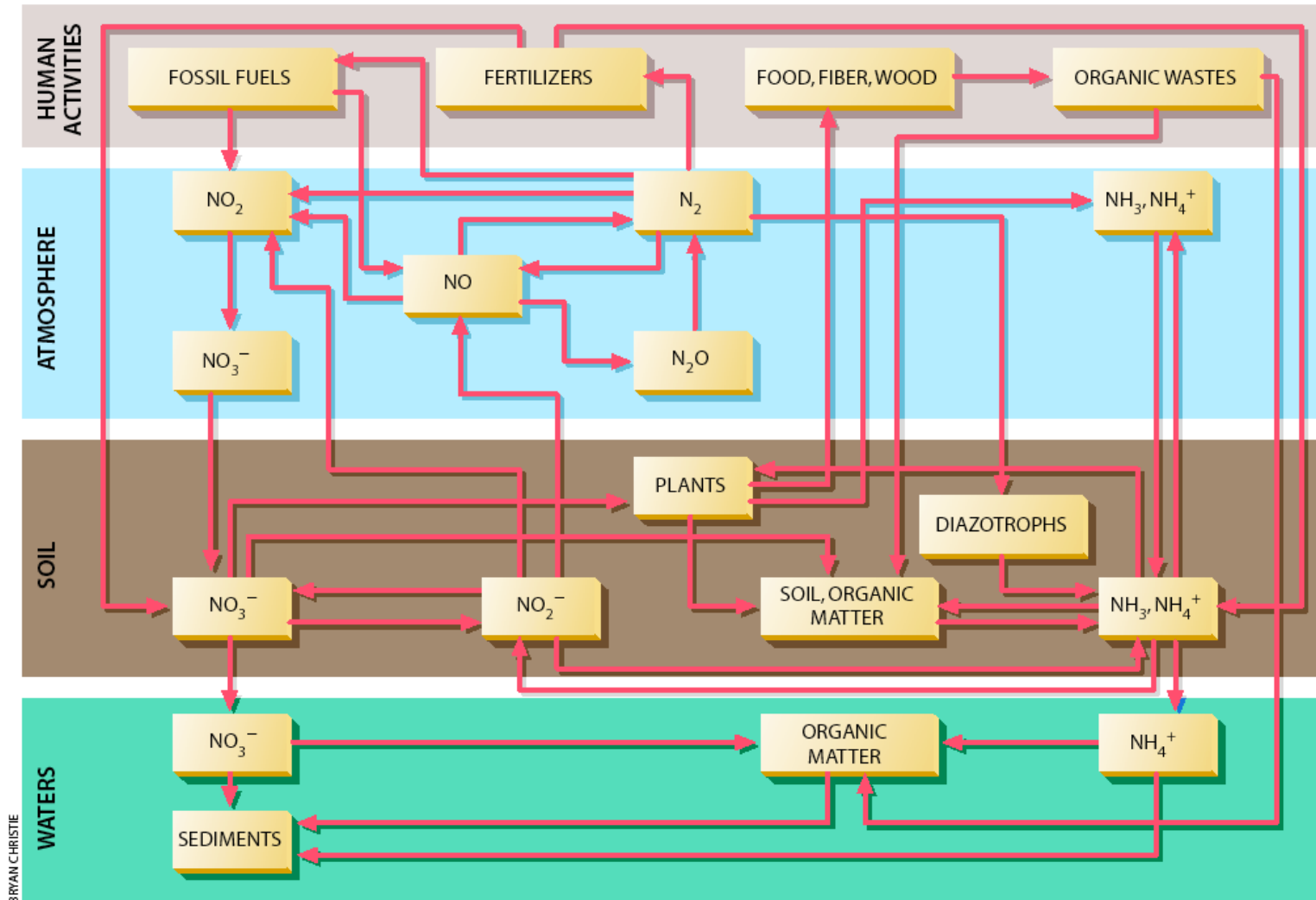
M.O. Diagrams and occupied/unoccupied antibonding orbitals



Presented at CCCE 2011
(JY, GBRA, PS)

basis set: B3LYP/6-311+G(d)

Nitrogen reservoirs in the environment



BRYAN CHRISTIE

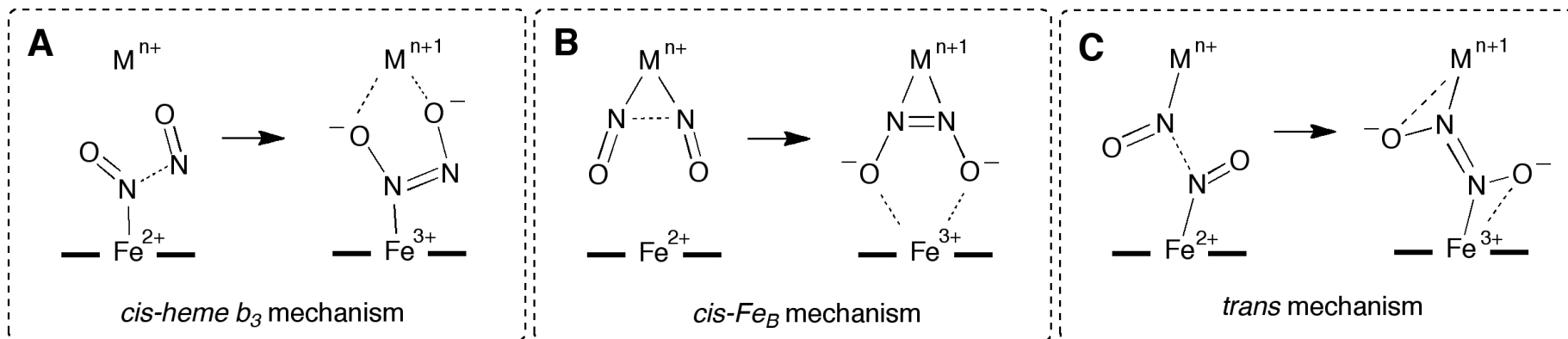
“Global Population and the Nitrogen Cycle” by Vaclav Smil in *Scientific American* July 1997, pp 76-81.

Heme-assisted reductions of NOx

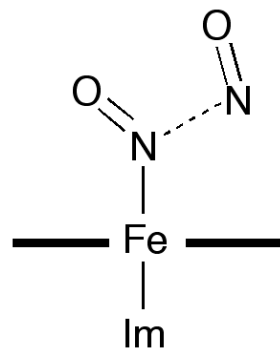


via
heme-(NO₂)

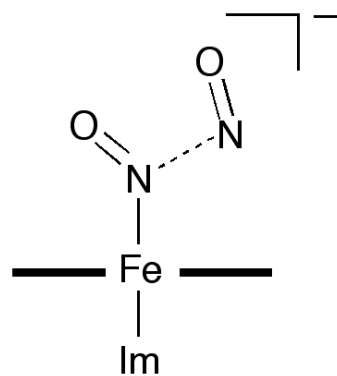
via
heme-(N₂O₂)



The “(P)Fe(NO)(Im) + NO” question



N-N = 1.957 Å
(5C = 1.974 Å)

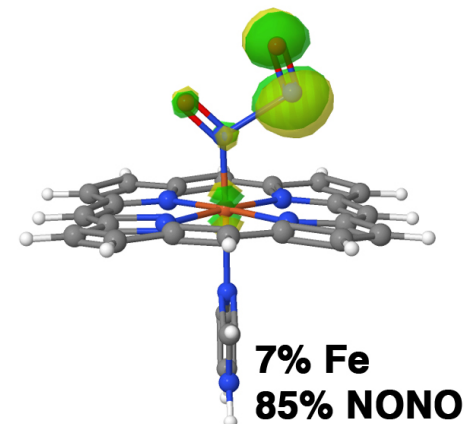
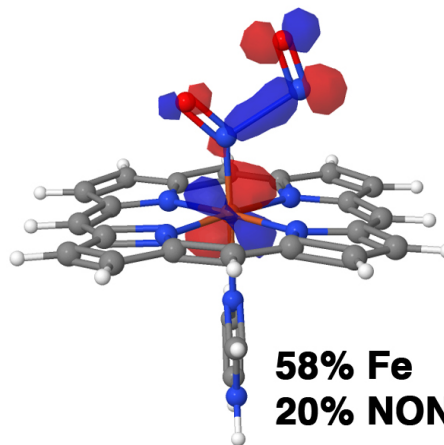


N-N = 1.708 Å
(5C = 1.898 Å)

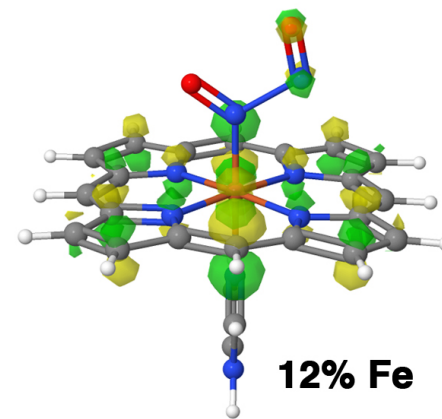
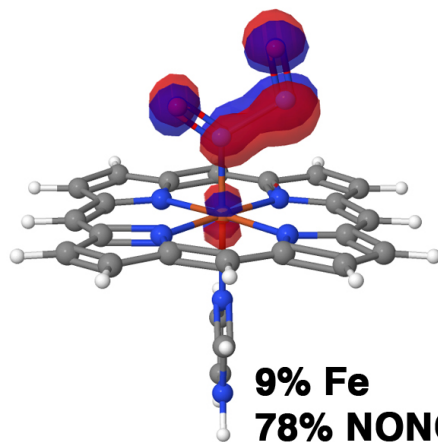
α -HOSO

α -LUSO

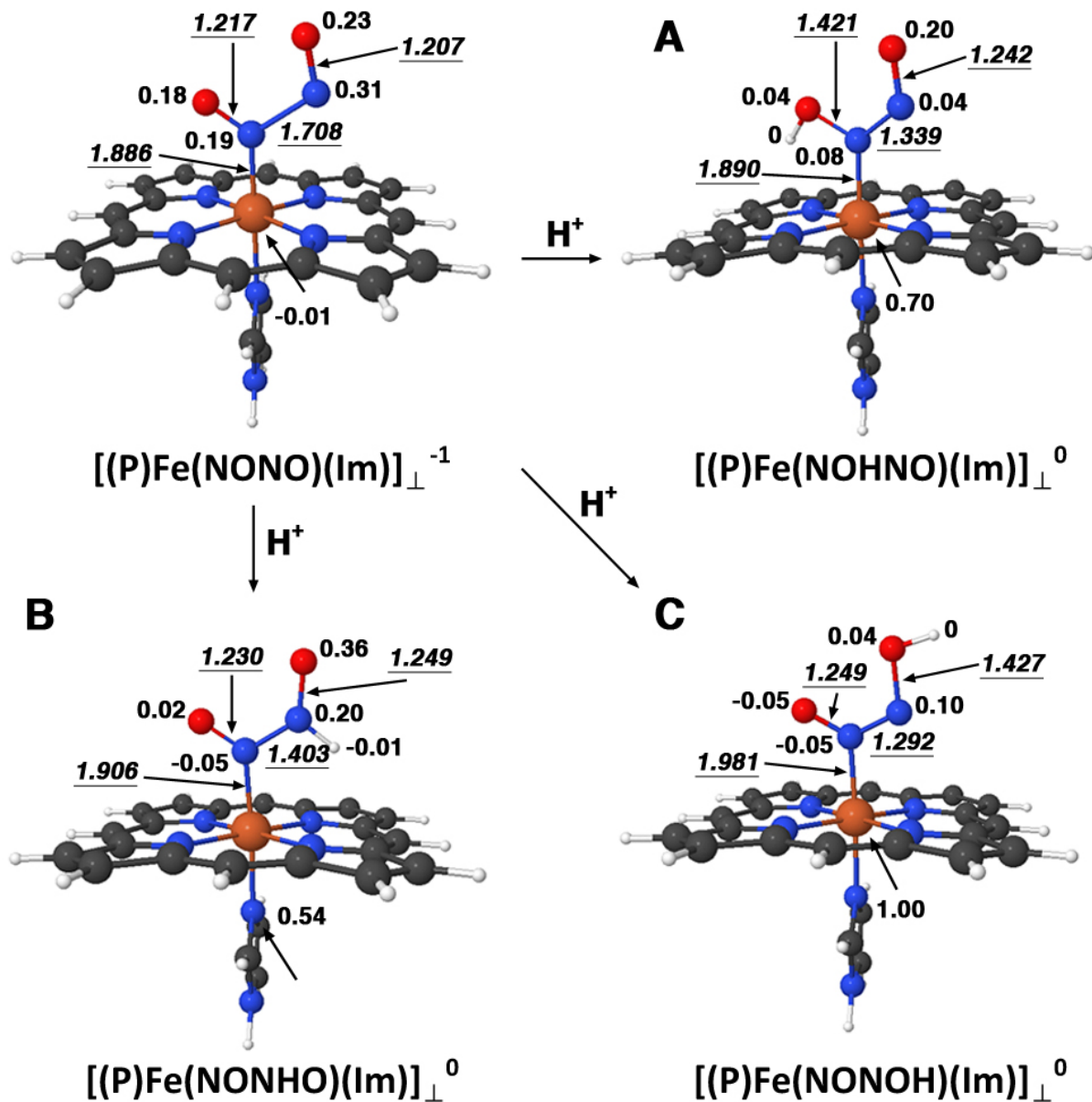
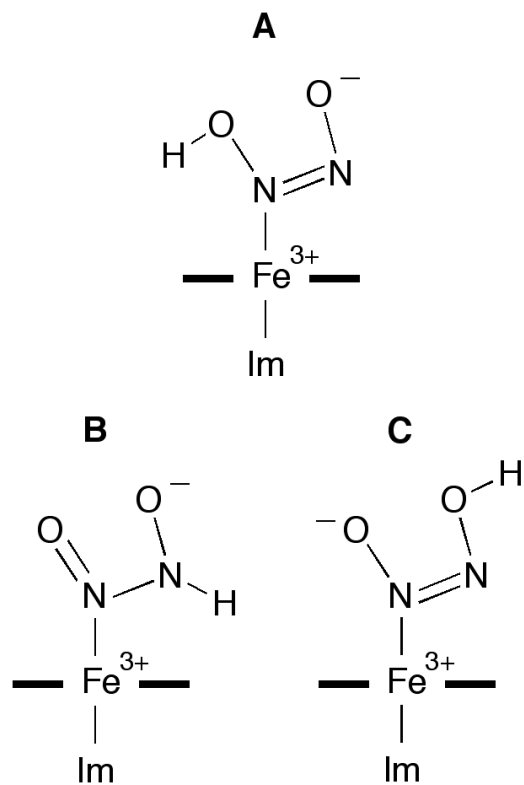
$[(P)Fe(NONO)(Im)]_{\perp}^0$



$[(P)Fe(NONO)(Im)]_{\perp}^{-1}$



**Protonation shortens
the N–N bond length**



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