WebMO: A User Friendly Computational Platform for Chemical Educators

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WebMO

WebMO is a WWW-based interface for computational chemistry software

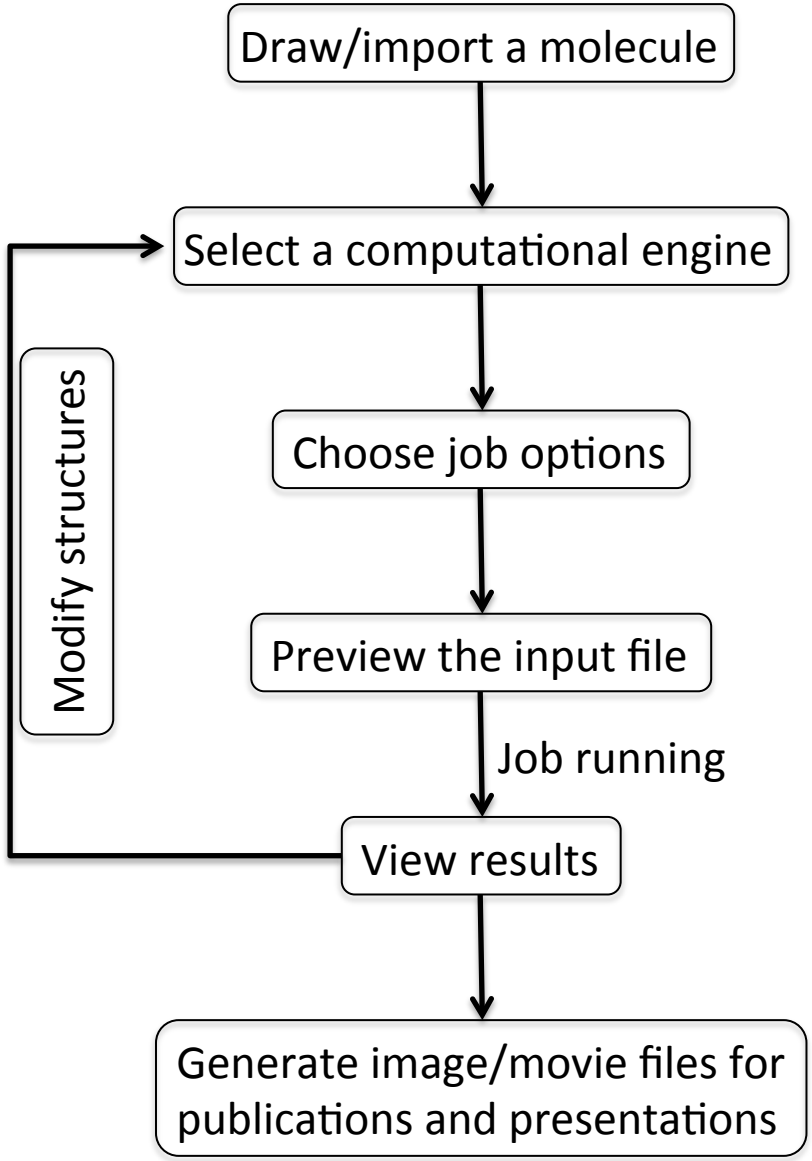
Key features

- 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

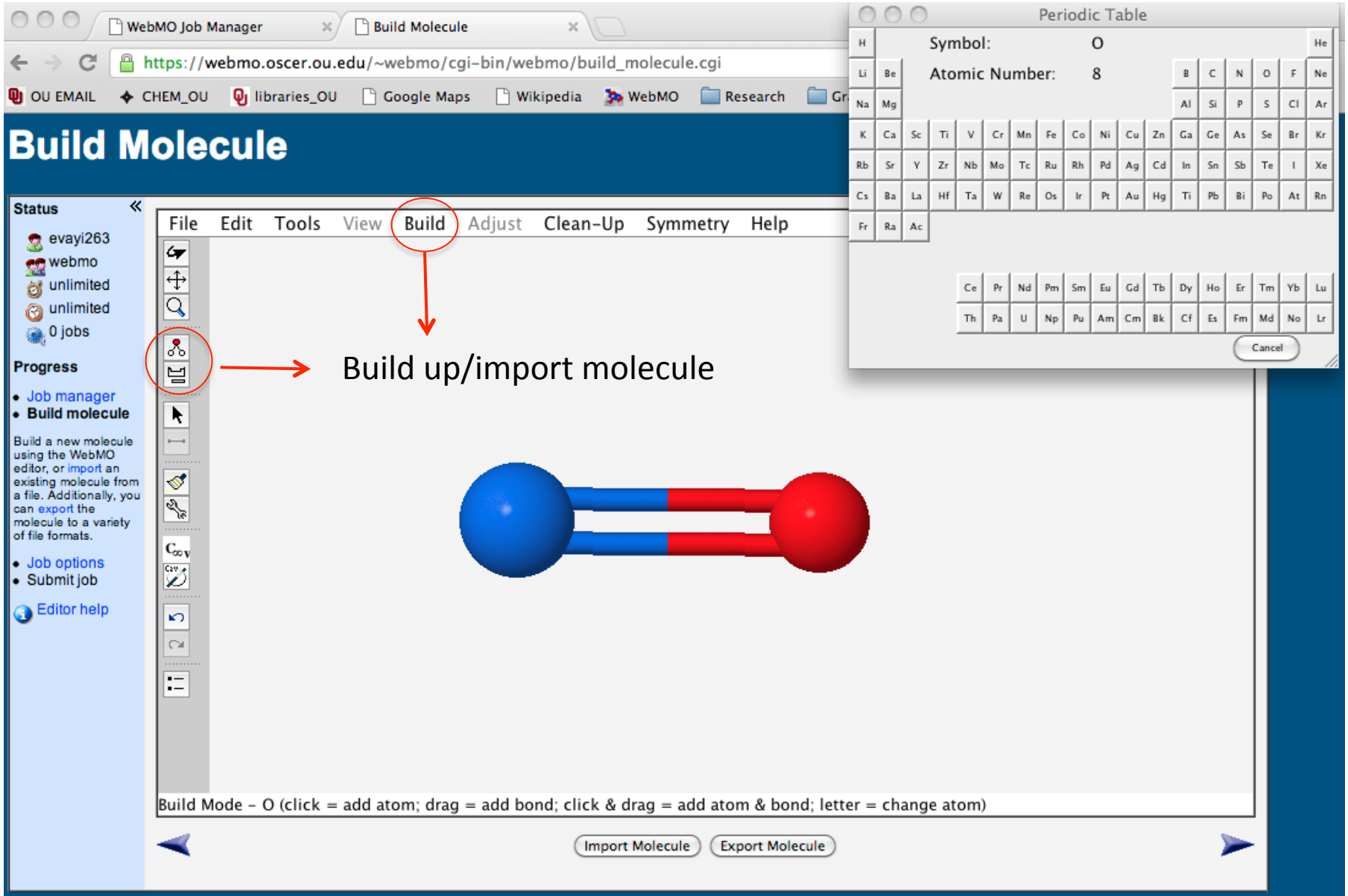


Application for undergraduate research

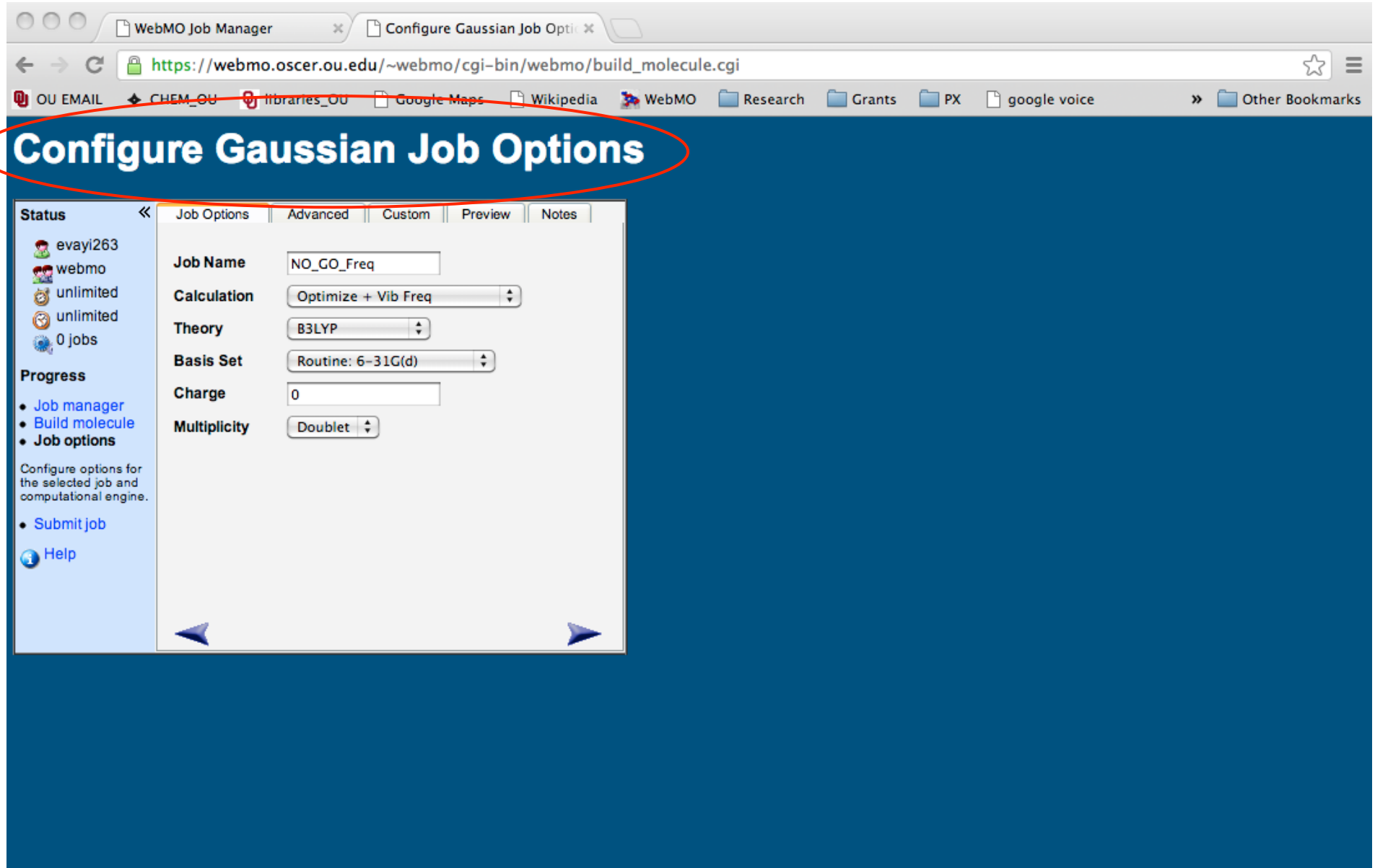
- Case study using nitric oxide (NO): comparison of physical/chemical properties of nitroxyl anion (NO^-), NO and nitrosonium (NO^+)
  - geometry optimizations
  - calculation of vibrational frequencies
  - calculation of molecular orbitals

- 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

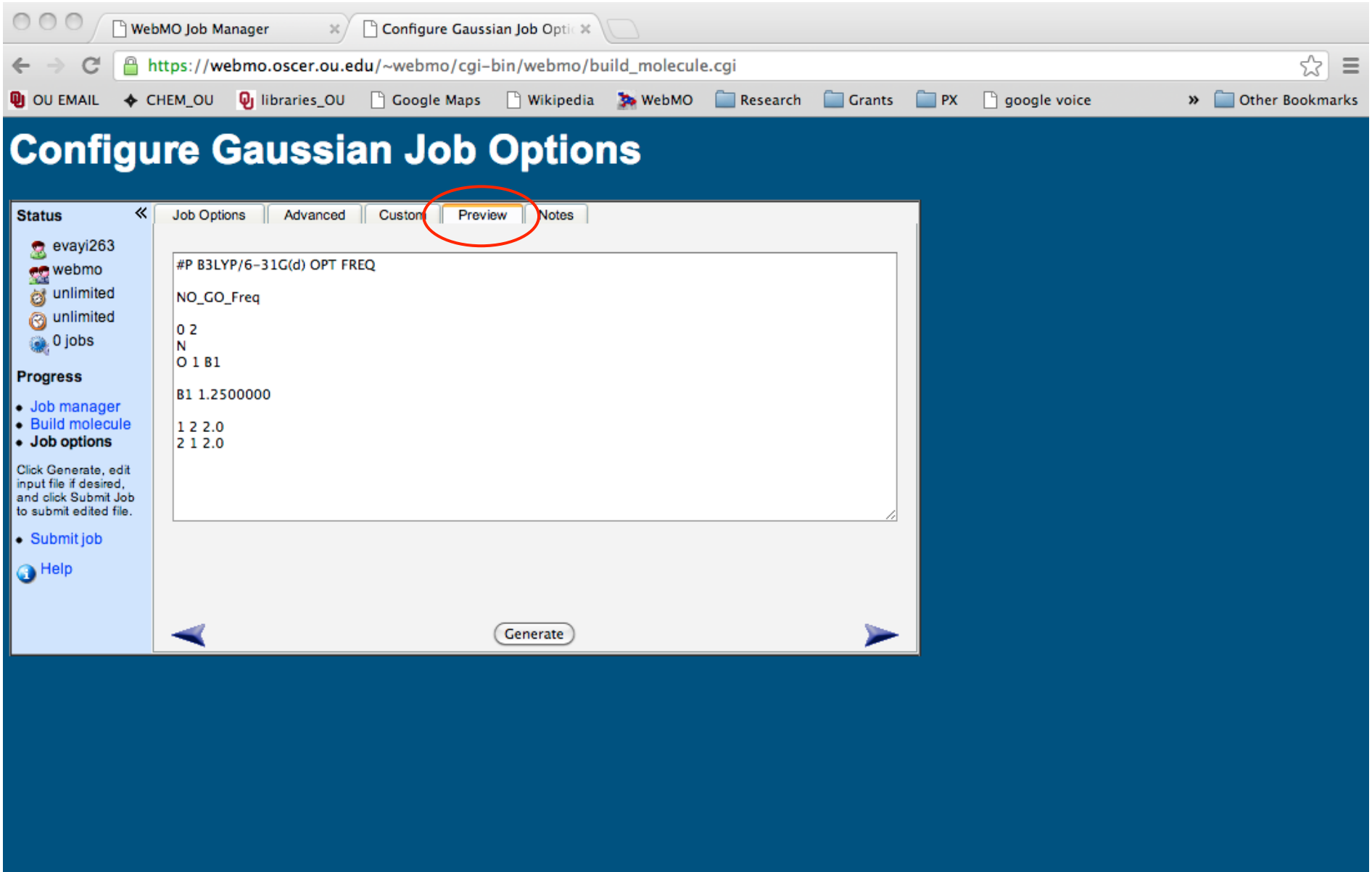
build the NO molecule



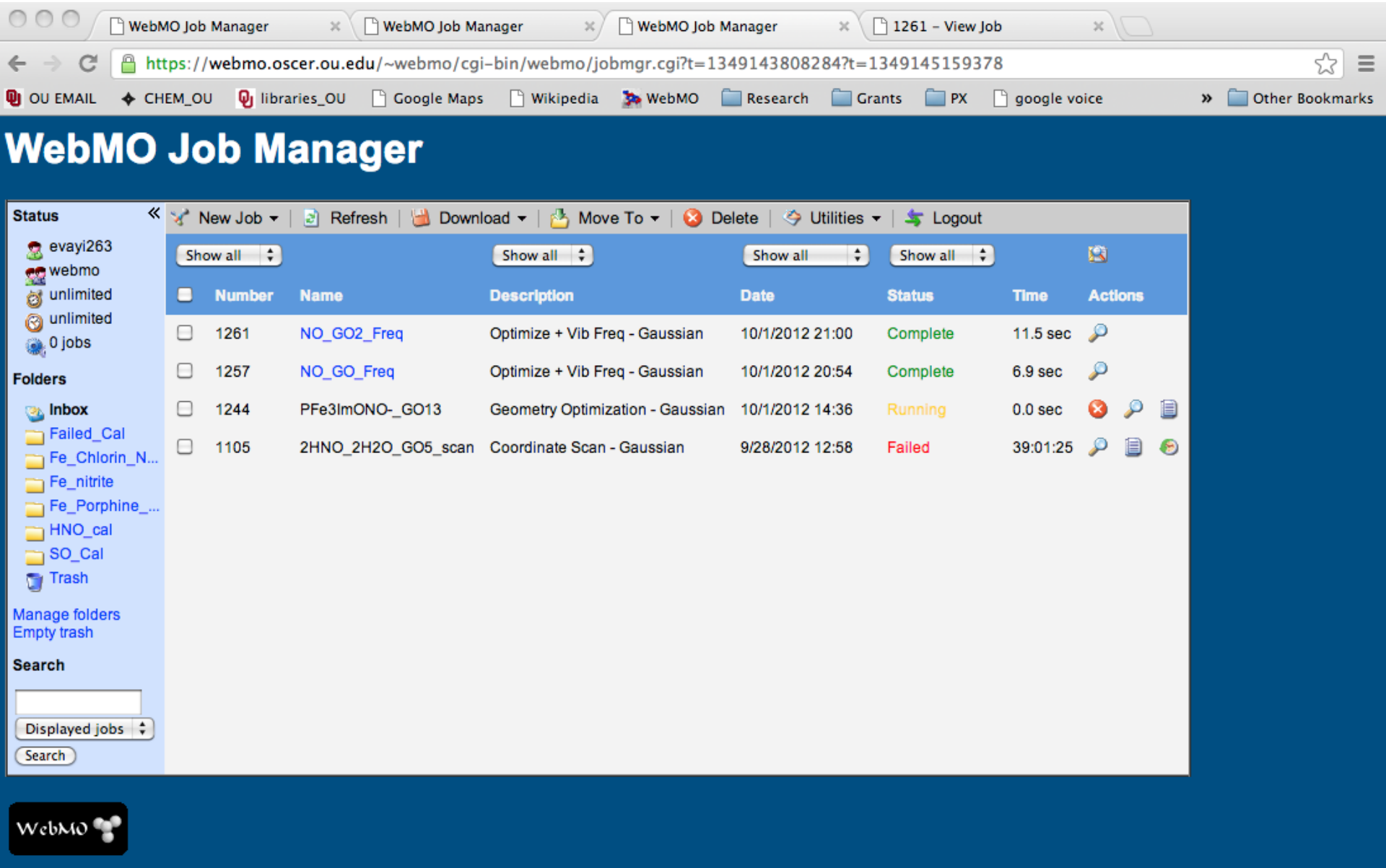
Choose job options



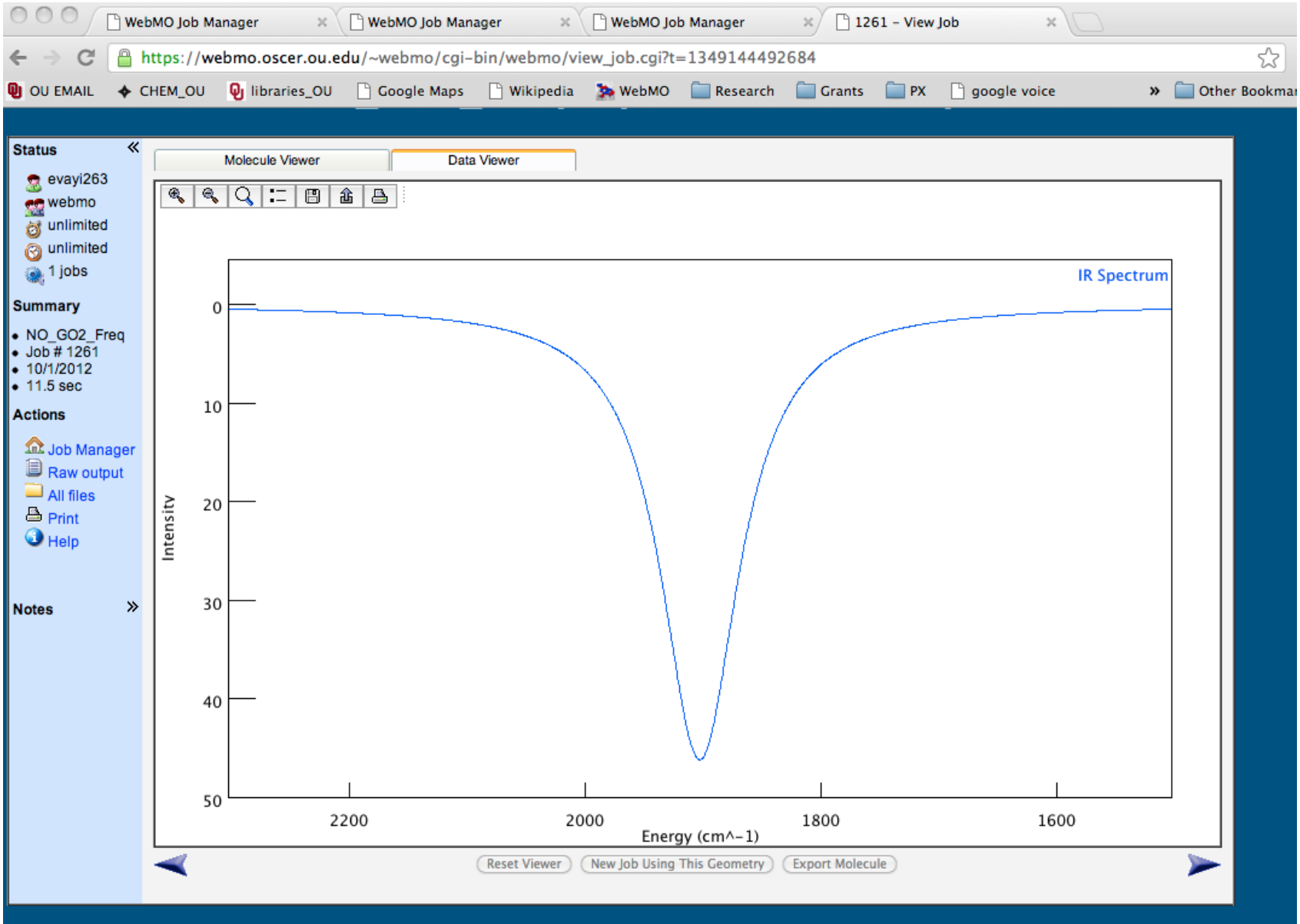
Preview the input file



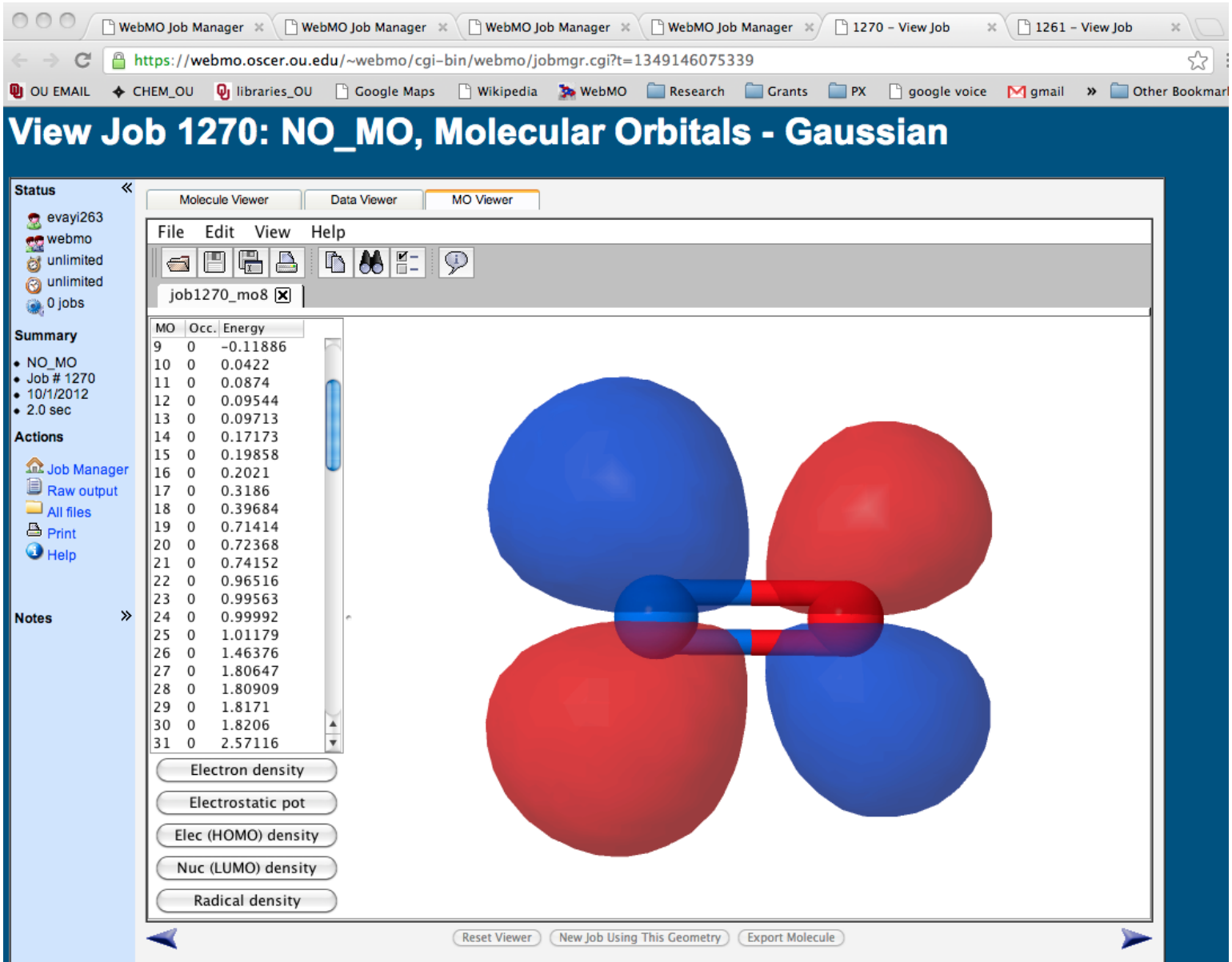
View the Job Manager



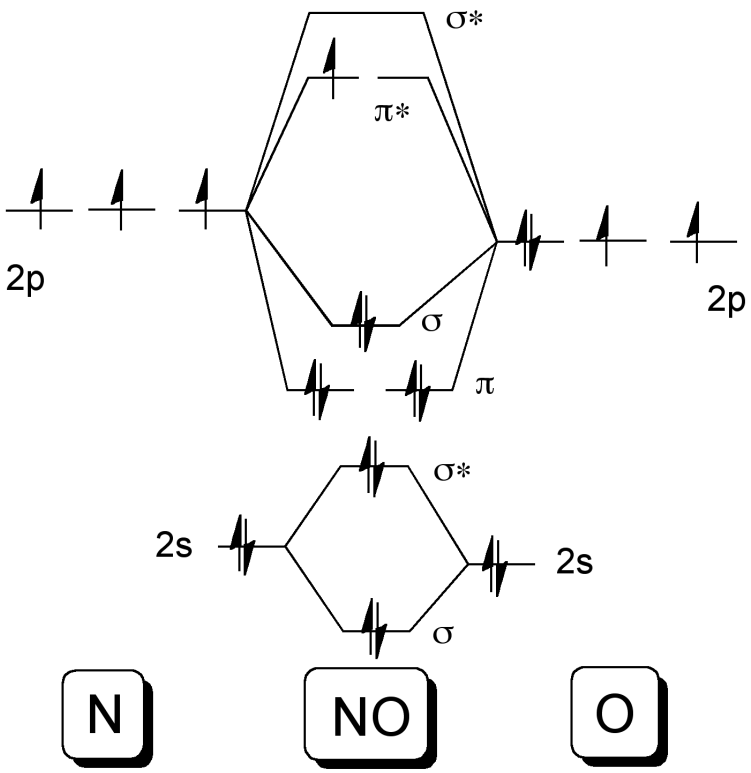
Visualize the results (e.g., spectrum)



Visualize the results (e.g., HOMO)



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

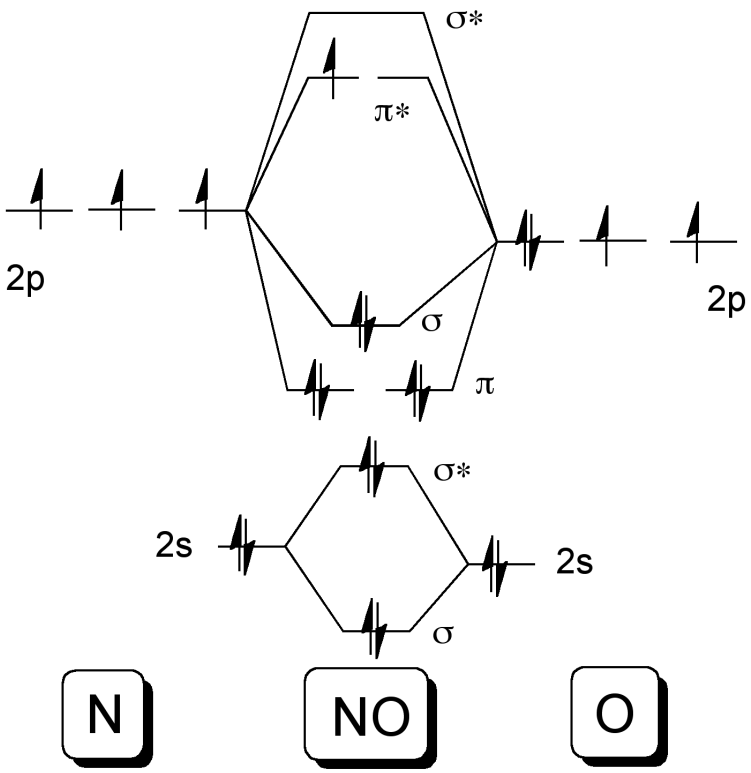


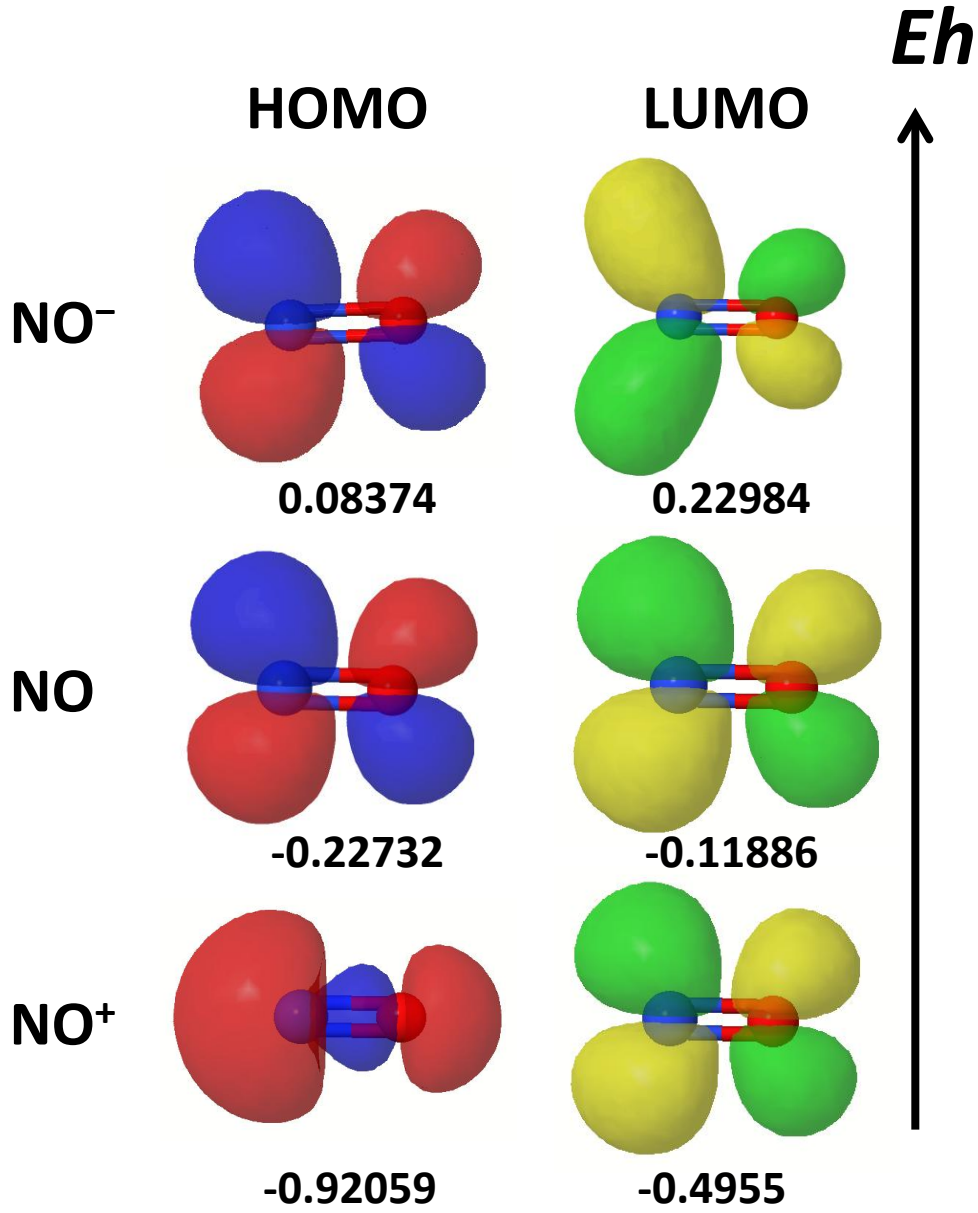
	N-O (Å)	IR (cm^{-1})
NO^-(t)	1.264 (1.200)	1415 (2591) [***1450***]
NO (d)	1.148 (1.127)	1980 (2340) [***1880***]
NO^+(s)	1.060 (1.074)	2491 (2591) [***2300***]

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

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

M.O. Diagrams and occupied/unoccupied antibonding orbitals

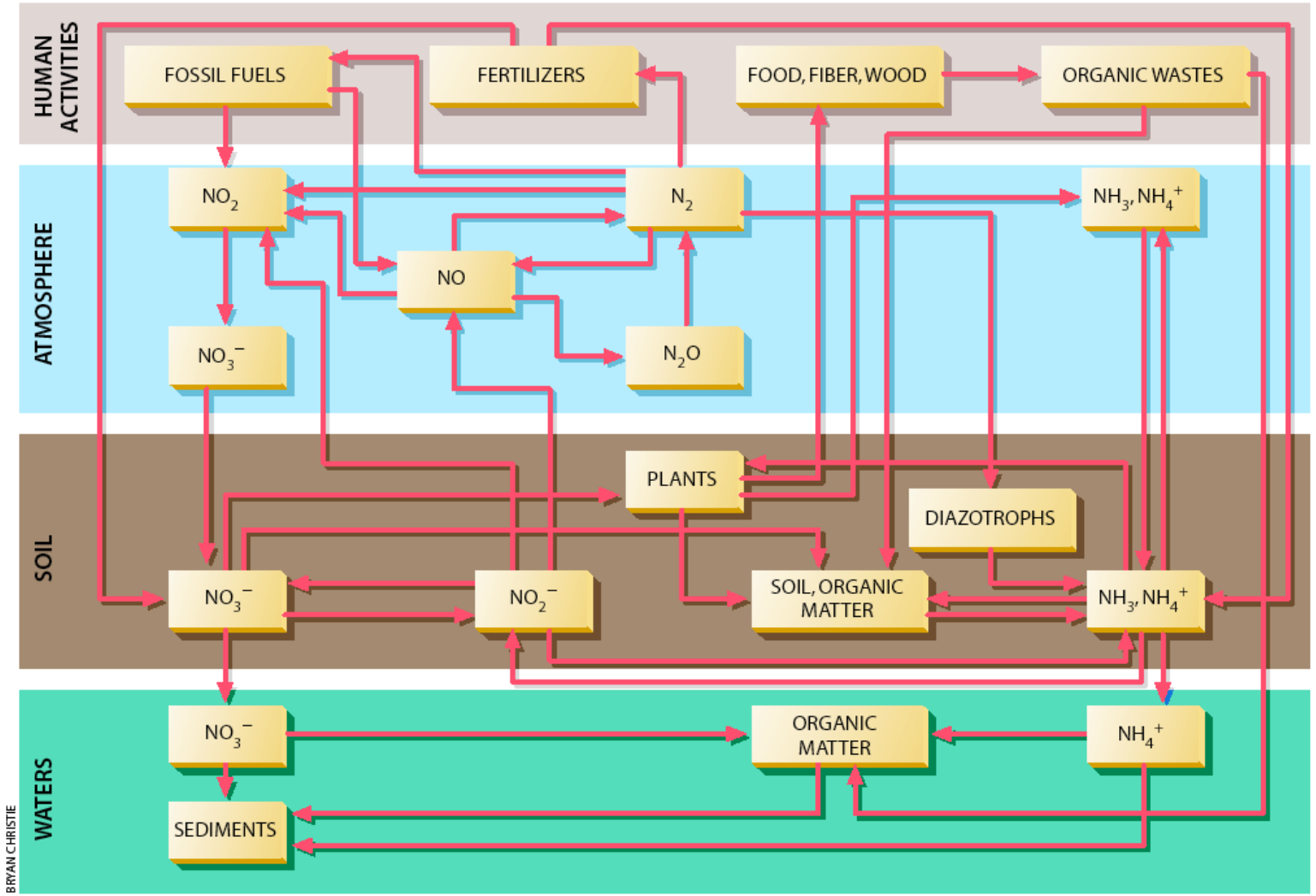




basis set: B3LYP/6-311+G(d)

Presented at CCCE 2011
(JY, GBRA, PS)

Nitrogen reservoirs in the environment

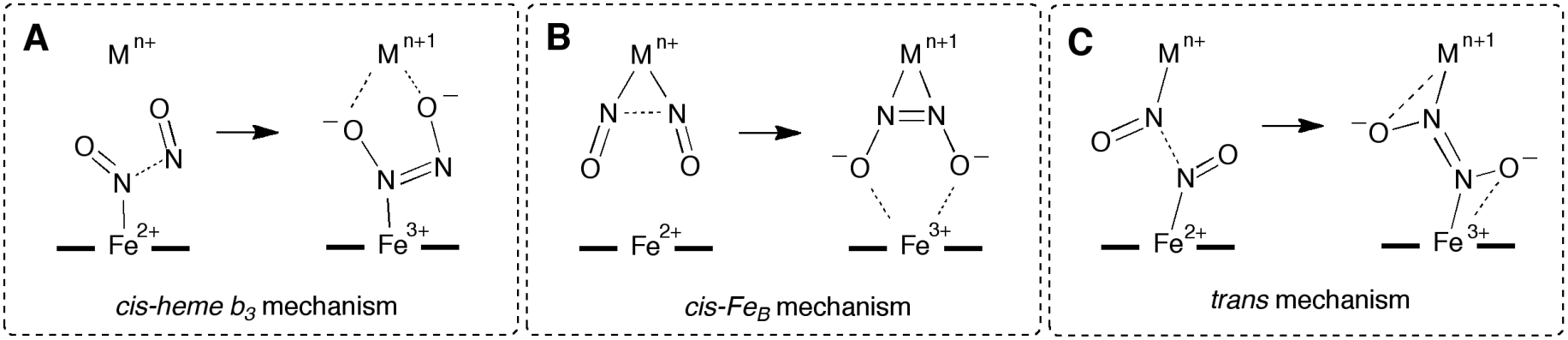


"Global Population and the Nitrogen Cycle" by Vaclav Smil in *Scientific American* July 1997, pp 76-81.

Heme-assisted reductions of NOx

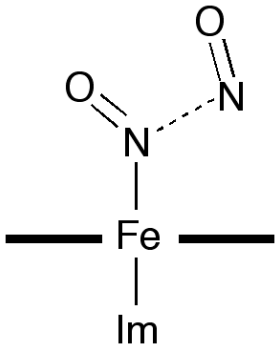
$$NO_2^- \xrightarrow{\text{NiR}} NO \xrightarrow{\text{NOR}} N_2O$$

via heme-(NO_2) via heme-(N_2O_2)



Moenne-Loccoz *Nat. Prod. Rep.* **2007**, *24*, 610-620 (bacNOR intermediates).

The "(P)Fe(NO)(Im) + NO" question

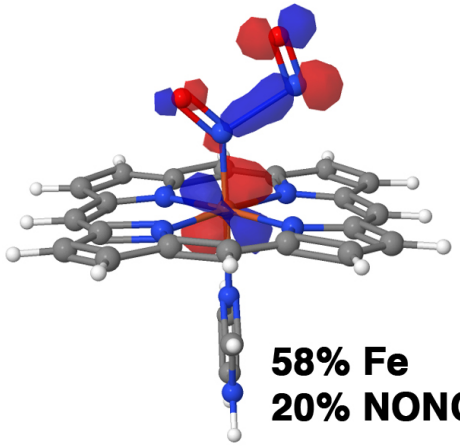


N–N = 1.957 Å
(5C = 1.974 Å)

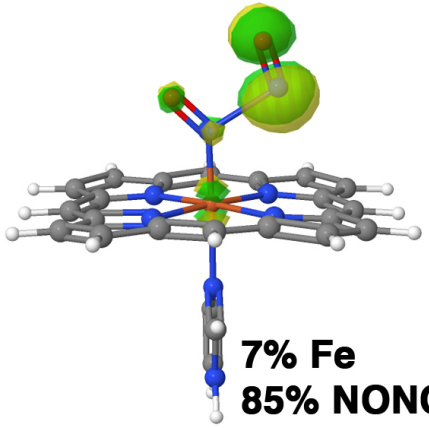
α-HOSO

α-LUSO

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

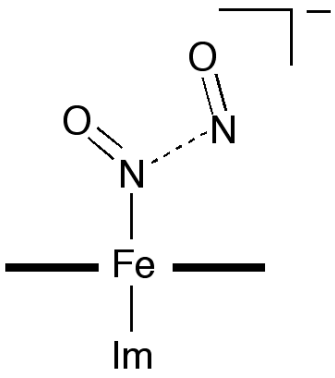


58% Fe
20% NONO

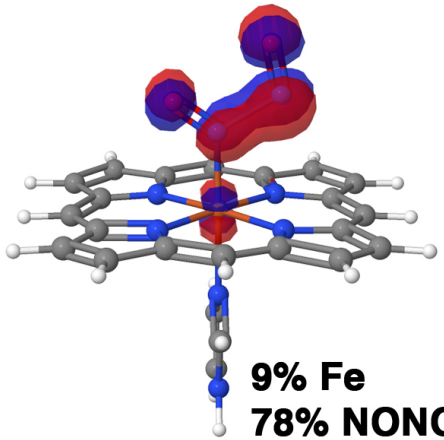


7% Fe
85% NONO

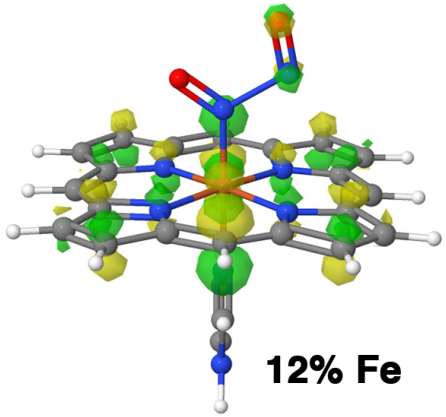
$[(P)Fe(NONO)(Im)]_{\perp}^{-1}$



N–N = 1.708 Å
(5C = 1.898 Å)



9% Fe
78% NONO

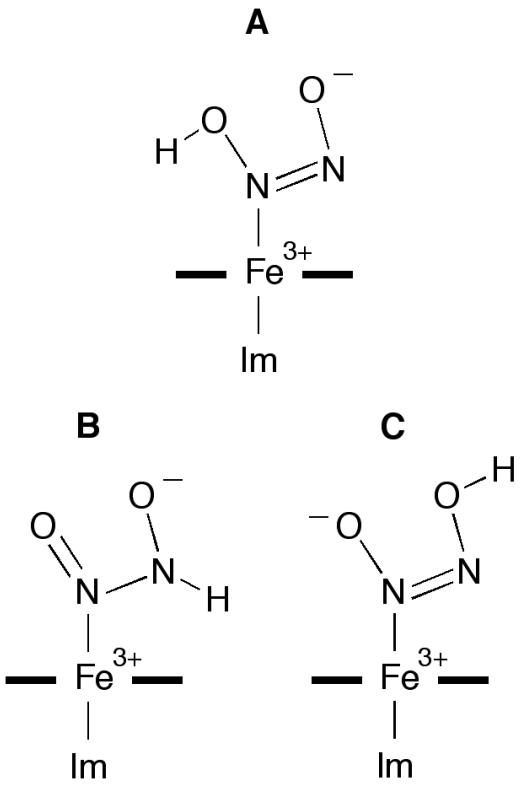


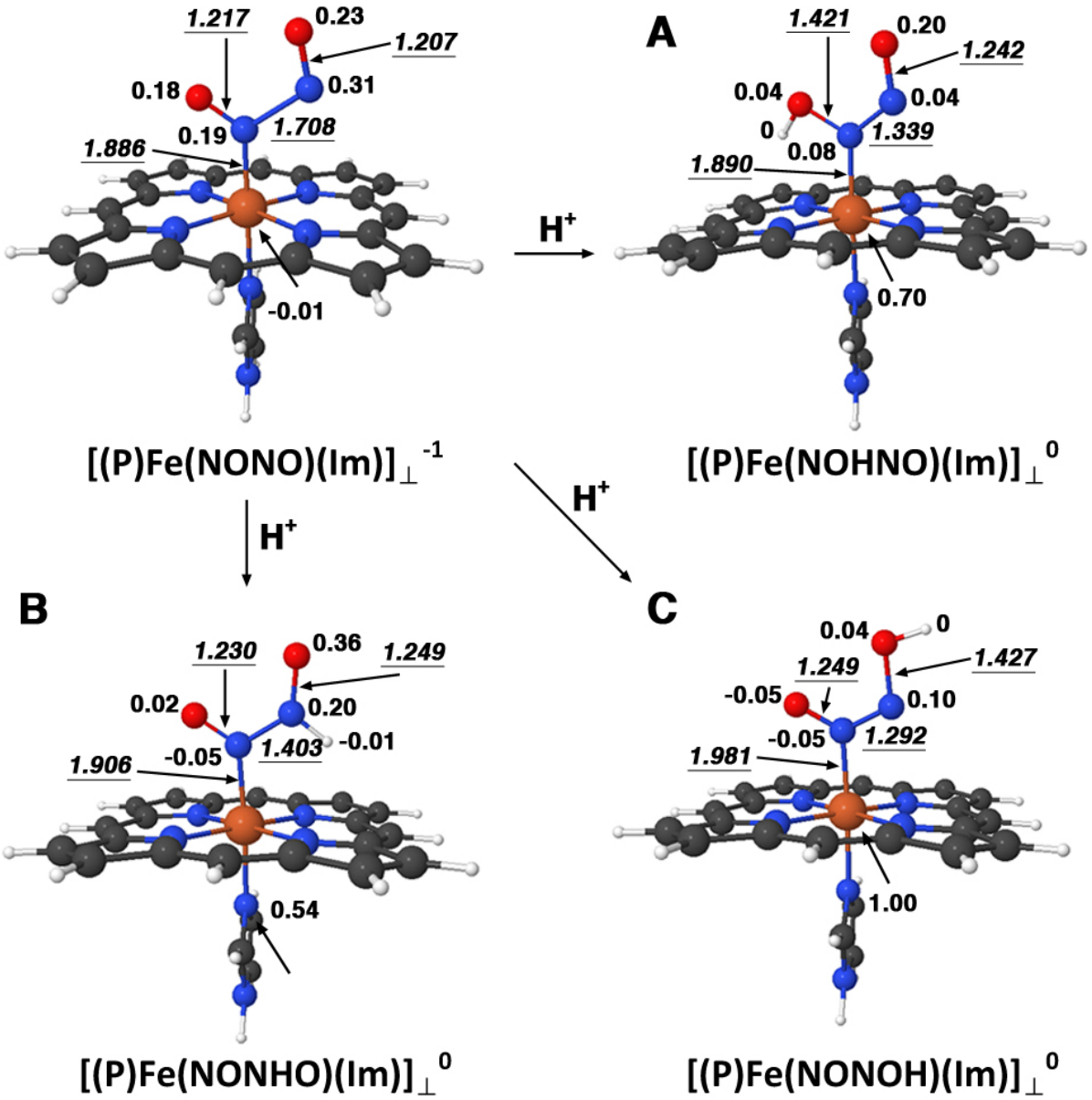
12% Fe

BP86/TZVP

J. Yi, G. B. Richter-Addo, *Chem. Commun.*, **2012**, *48*, 9041-9043

Protonation shortens the N–N bond length





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