



# Computational Spectroscopy

## II. *ab initio* Methods

---

from part (e) NMR Spectra  
Chemistry 713

Updated: February 21, 2008

# (e) Computation of NMR Spectra

- Optimize geometry at Hartree-Fock level and check "NMR"

with  
SPARTAN

Calculations

Calculate: Equilibrium Geometry at Ground state  
with Hartree-Fock 6-31G\*  Pseudopotential

Start From: Initial geometry

Subject To:  Constraints  Frozen Atoms  Symmetry  
Total Charge: Neutral

Compute:  UV/vis  IR  NMR  
Multiplicity: Singlet

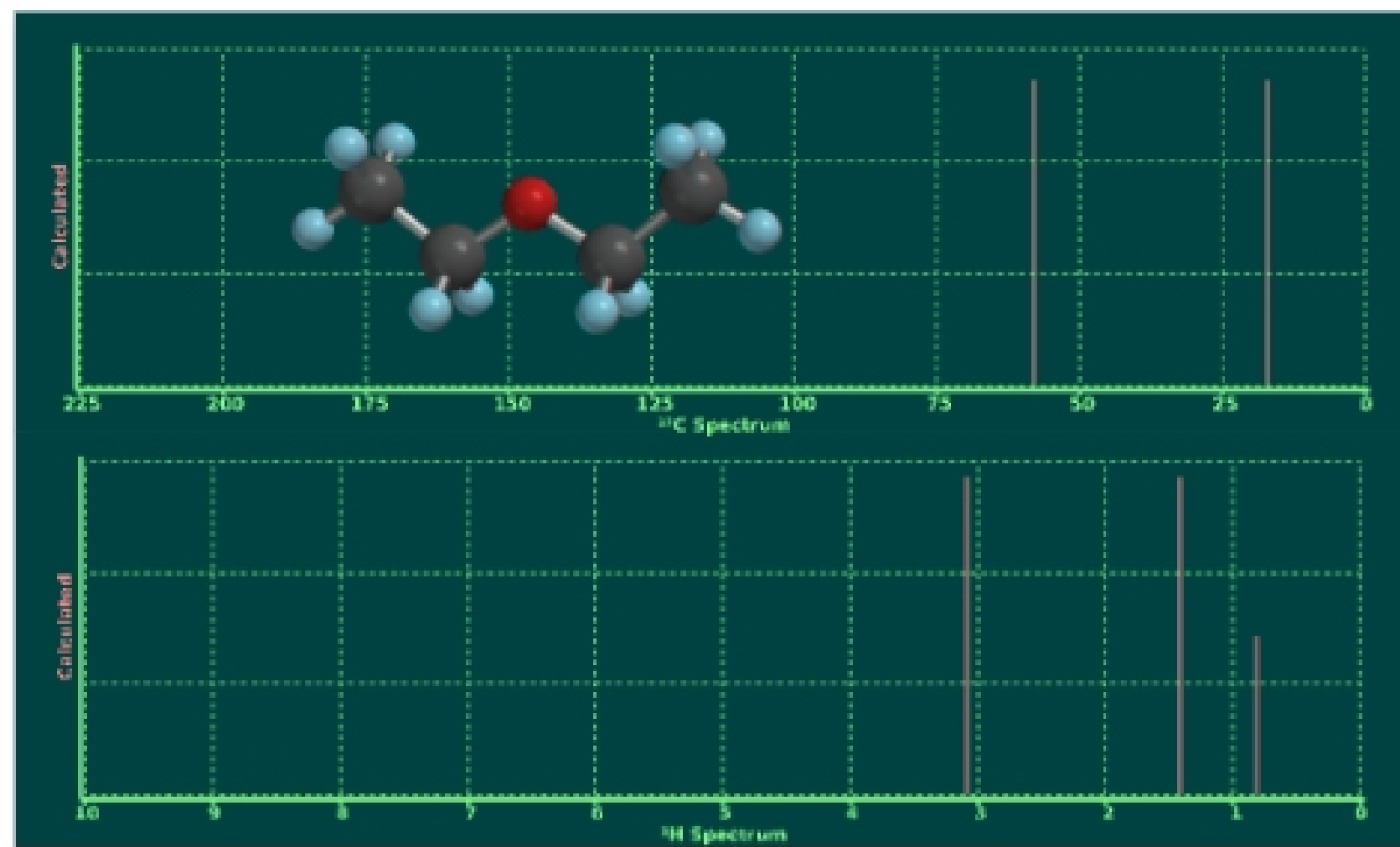
Print:  Orbitals & Energies  Thermodynamics  Vibrational Modes  Atomic Charges

Options:  Converge

Global Calculations

# Computed NMR for Diethylether

$^{13}\text{C}$



$^1\text{H}$