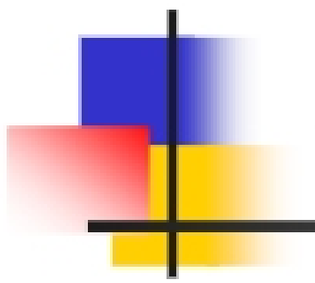


Computational Spectroscopy
II. *ab initio* Methods

from part (e) NMR Spectra

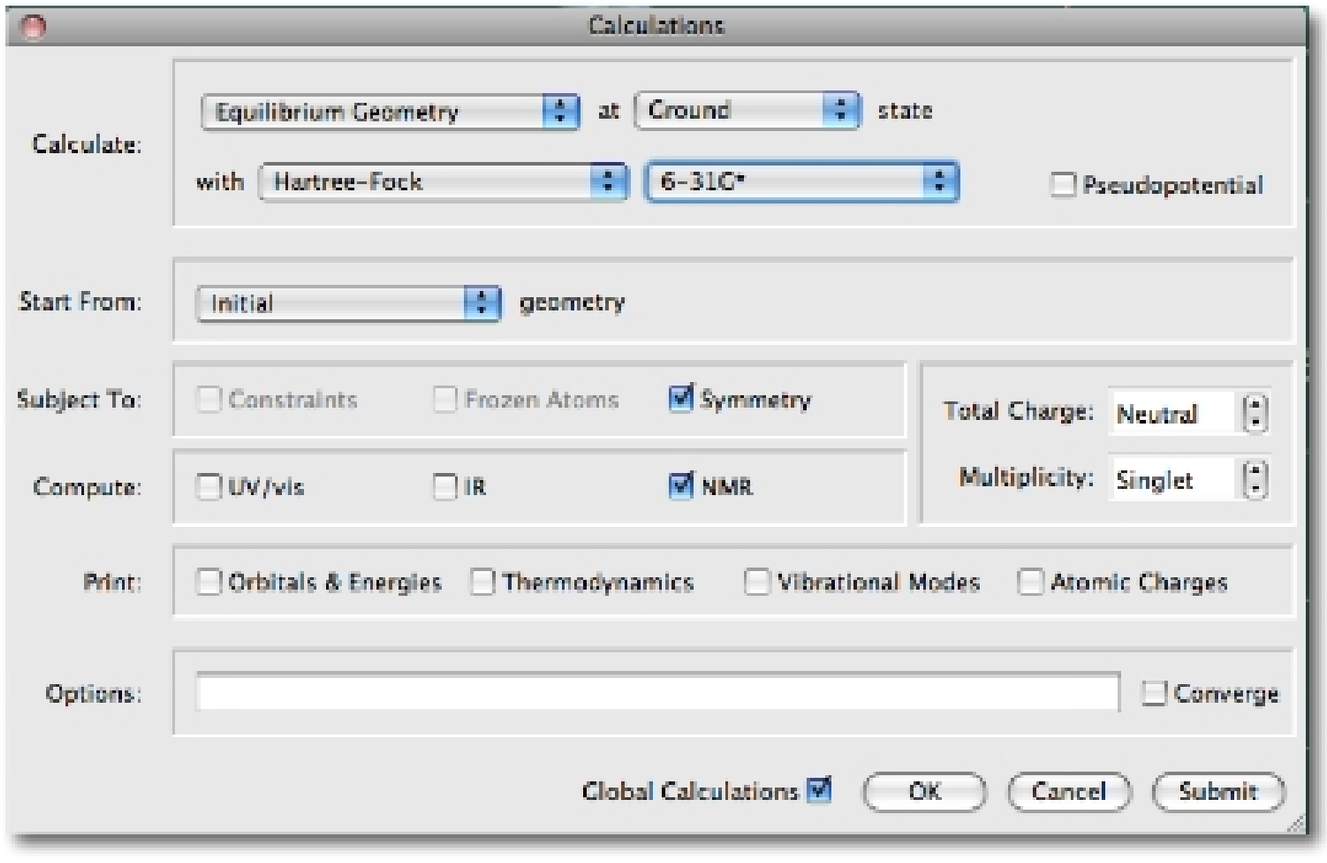
Chemistry 713

Updated: February 21, 2008

(e) Computation of NMR Spectra

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

with SPARTAN



Computed NMR for Diethylether

^{13}C

^{1}H