

A Practical Introduction to Molecular Modeling

Eight hours of lectures and eight hours of “hands-on” exercises over two days cover a number of important aspects of molecular modeling and provide practical experience in the use of models to address a variety of chemical problems.

First Day:

Lecture Topics:

1. **Getting Started. Potential Energy Surfaces**
2. **Schrödinger Equation to Molecular Orbital Theory**
3. **Finding Geometries and Calculating Infrared Spectra**
4. **Calculating Reaction Energies**
5. **Finding Transition States and Calculating Activation Energies**
6. **Calculating Molecular Properties, Charges and Spectra**
7. **Molecular Modeling with Pictures**

Hands-on activities include:

1. Spartan basics
2. Using Hartree-Fock models to obtain equilibrium geometries and reaction energies, transition-state geometries and activation energies and properties and spectra.
3. Using graphical models to describe molecular properties and chemical reactivity/selectivity.
4. Use of molecular databases (Spartan Molecular Database, Cambridge Structural Database).
5. Access to web-based chemical data (retrieval of IR & UV/vis spectral data from NIST; retrieval of NMR Spectral Data from the University of Cologne NMR database; retrieval of protein / nucleotide structures from Protein Data Bank).

Second Day

Lecture Topics:

8. **Beyond Molecular Orbital Theory. MP2 Models**
9. **A Practical Alternative to MP2. Density Functional Models**
10. **Molecular Orbital Theory on Diet. Semi-Empirical Models**
11. **Conformational Preferences in Organic Molecules**
12. **Molecular Mechanics Models and Conformations of Molecules**
13. **Practical Aspects of Molecular Modeling**
14. **Finding "Similar" Molecules**

Hands-on activities include:

1. Applications for which Hartree-Fock models are not satisfactory.
2. Accurate thermochemical predictions.
3. Applications to systems that are too large for Hartree-Fock Models.
4. Applications to organometallic chemistry.
5. Conformational analysis.
6. Similarity analysis.

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