- Use standard Microsoft Access *.mdb database files.
- Convert 2D structures to 3D structures or vice versa.

Computational Chemistry

Use HyperChem to explore quantum or classical model potential energy surfaces with single point, geometry optimization, or transition state search calculations. Include the effects of thermal motion with molecular dynamics, Langevin dynamics or Metropolis Monte Carlo simulations. User-defined structural restraints may be added. Use translational, rotational, and vibrational partition functions to calculate entropies, heat capacities, and free energies.

Types of Calculations

- Single point calculations determine the molecular energy and properties for a given fixed geometry; SCF, configuration interaction, or MP2.
- Geometry optimization calculations employ energy minimization algorithms to locate stable structures. Six minimization algorithms are provided. Even calculate geometries with MP2 or for excited states.
- Vibrational frequency calculations find the normal vibrational modes of an optimized structure. The vibrational spectrum can be displayed (with IR intensities) and the vibrational motions associated with specific transitions can be animated.
- Electronic spectra with visual display of frequencies and intensities.
- Transition state searching locates the metastable structures corresponding to transition states using either Eigenvector Following or Synchronous Transit methods. Molecular properties are then calculated.
- Molecular dynamics (MD) simulations compute classical trajectories for molecular systems. Quantum forces can be used to model reactive collisions. Heating, equilibration, and cooling periods can be employed for simulated annealing and for studies of other temperature-dependent processes. Both constant energy and constant temperature simulations are available.
- Langevin dynamics simulations add frictional and stochastic forces to conventional molecular dynamics to model solvent collisional effects without inclusion of explicit solvent molecules.
- Metropolis Monte Carlo simulations sample configurations from a statistical ensemble at a given temperature and are useful for exploring the possible configurations of a system as well as for computing temperature-dependent equilibrium averages.
- Calculate the energy and entropy at a temperature T using an analysis of the translation, rotation, and vibration of a molecule. Subsequently obtain the free energy as A=E-TS.
- Calculate the equilibrium constant for any reaction and plot as a function of the temperature.
- Calculate the rate constant for unimolecular and bimolecular reactions from the HyperChem (or other) structures obtained for the transition state and the reactant species. Plot the rate constant as a function of temperature.
- Calculate heat capacities for molecules at temperature T from their translation, rotation, and vibration.
- Apply a superimposed electric field to any molecular system. See what changes this makes to any molecular modeling result such as structure, energetics, and reactivity.
- Apply a superimposed magnetic field to a molecular system for a subset of the semi-empirical methods.
- Specify that your results be described by any of the three system of units - kJ, kCal, or atomic units(Hartrees.).
- Calculations generally apply to any applicable method, e.g. *ab initio* MD or vibrational spectra with DFT, etc.
- QSAR properties (Gasteiger charges, surface area (2 methods), volume, hydration energy, log P, refractivity, sum of bond polarizabilities, mass).
- Conformational search (Monte Carlo generation of conformers, subsequent optimization, and simple collection of table of low energy conformers); easy inspection and manipulation of each conformer.
- NMR shielding and coupling constants with optional subsequent computation and display of 1-D spectra; special TNDO technology gives rapid computation of NMR parameters with improved accuracy over other semi-empirical methods.

***Ab Initio* Quantum Mechanics**

- Choose from many commonly-used basis sets (STO-1G to 6-311++g2d2p) including the standardized STO-3G, 3-21G, 6-31G*, and 6-31G** basis sets
- Extra basis functions (s, p, d, sp, spd) can be added to individual atoms or to groups of atoms.
- Users can define their own basis sets or modify existing basis sets easily using HyperChem's documented basis set file format.
- Different basis sets can be used on different atoms; use ghost orbitals to eliminate basis set extension.
- Use electric fields, configuration interaction, MP2, direct SCF and RHF or UHF.