Computational Chemistry

Computational Chemistry uses tools (software) to understand chemical reactions and processes (i.e., to enhance chemical knowledge).

Major Benefits

- Computational Chemistry tools can be used to investigate a much wider variety of chemical species than are normally accessible to the experimental chemist.

- Computational Chemistry tools allow chemists to think more clearly about issues that are really central to chemistry - structure, stability and reactivity - than would be possible without the use of a computer.

Applications

- molecular structures (both stable and unstable species)
- heats of formation and heats of reaction (ΔH_f^o and ΔH^o)
- dipole moments
- ionization potentials
- charge and spin densities
- reaction mechanisms
- activation energies
- vibrational modes

Considerations for Choosing a Computational Model

- Need to understand how the computational models are implemented and the nature of the databases used to parameterize the models.

- Use this knowledge to determine the most appropriate model for a specific investigation (i.e., the problem at hand) and to define the level of confidence required in the results.

- Evaluate available computational resources and relative computational cost.

The goals of Computational Chemistry can be to eliminate/reduce time-consuming experiments, provide insight into existing experimental data, or guide new experimental studies.