MOPAC

Molecular Orbital PACkage

MOPAC is the most popular software for semiempirical thermochemistry. It has been at the forefront of semiempirical model development for over 40 years, with many features and robust, efficient solvers. It is also integrated with many popular graphical user interfaces (GUIs) for molecular modeling.

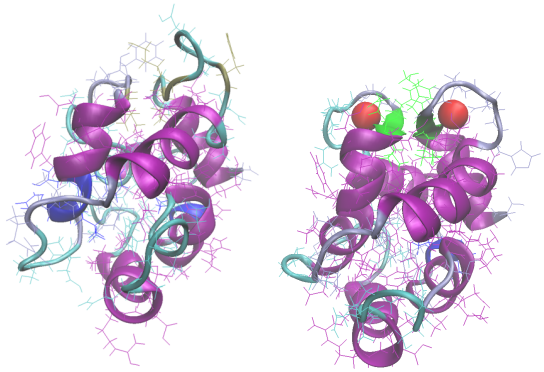
Features

MOPAC calculates quantum mechanical properties of molecules in a fraction of a second to meet the demands of modern high-throughput computational chemistry. MOPAC's features include:

- Parameterized models for all main group elements and transition metals
- Energy corrections for hydrogen bonds and van der Waals interactions
- Robust geometry optimization
- COSMO implicit solvent model
- Vibrational frequency calculations
- Periodic boundary conditions for polymers, surfaces, and crystals
- Transition state optimization
- INDO spectroscopy model

MOZYME & Protein Modeling

MOPAC's unique MOZYME solver can perform rapid calculations of covalent and ionic systems with thousands of atoms. Originally designed for protein modeling, this feature also works for a wide variety of systems such as metal-organic frameworks (MOFs), zeolites, and organic liquids. MOPAC also has specialized features for processing PDB files and protein structures, to insert missing hydrogen atoms and assign charges to side chains of amino acids.



Availability & Integration

MOPAC is available for Windows, Mac, and Linux. It is available as a standalone package or on the Conda package manager. MOPAC is integrated with many other popular software packages including:

- WebMO
- Molecular Operating Environment (MOE)
- Amsterdam Modeling Suite (AMS)
- Maestro
- Chem3D
- MedeA
- Mercury
- Phenix
- Avogadro
- Jmol
- Atomic Simulation Environment (ASE)
- SEAMM
- QCEngine

For more information about MOPAC, visit its legacy website at http://openmopac.net or its new website in development at https://openmopac.github.io.