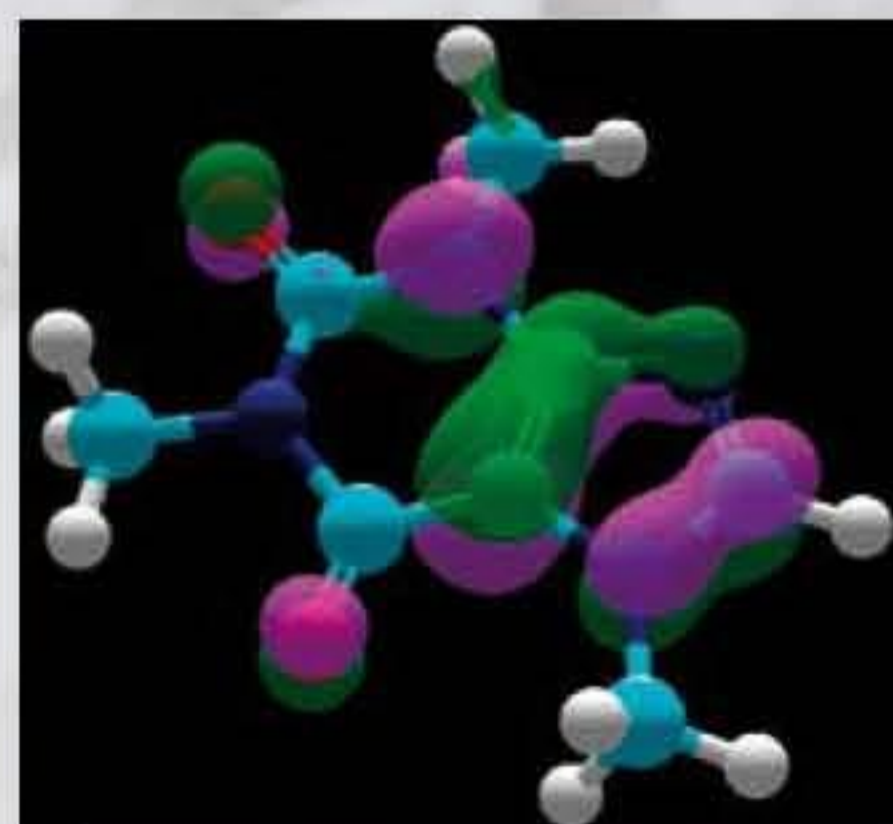




MOPAC is a general-purpose semi-empirical molecular orbital package for the study of solid state, solution and gas phase molecular structures and reactions. Quantum methods are used to compute structure and properties such as molecular orbitals, vibrational spectra, thermodynamic quantities, isotopic substitution effects, radicals, ions, peptides and polymers. MOPAC is also used to generate descriptors for quantitative structure-property (or activity) relationships and to predict a wide variety of biological and other properties including carcinogenicity, vapor pressure, water solubility, and reaction rates.

#### Use MOPAC to research

- Macromolecules: very fast, patented, linear-scaling MOZYME algorithm optimizes proteins and DNA.
- Materials: d-orbitals, crystals, geometry in electric fields, NLO, 2D/3D periodic boundaries.
- Polymers: band structures, phonon spectra, Young's modulus, tensile strength.
- Dyes: MOS-F for UV spectra prediction, intersystem crossing, excited states in solution.
- Synthesis: thermodynamics, kinetics, transition-states, reaction paths, solvation, catalysis.



#### Powerful Compute Engines

- Semi-empirical Hamiltonians: MNDO, MINDO/3, AM1, PM3, MNDO-d, and PM5.
- Transition metals: Sc, Ti, Zr, V, Cr, Mo, Fe, Co, Ni, Pd, Pt, Cu, Ag, Zn, Cd, and Hg.
- Optimization: MOPAC uses the very robust Baker's Eigenvector Following procedure as the default geometry optimizer. Other options include: Broyden-Fletcher-Goldfarb-Shanno

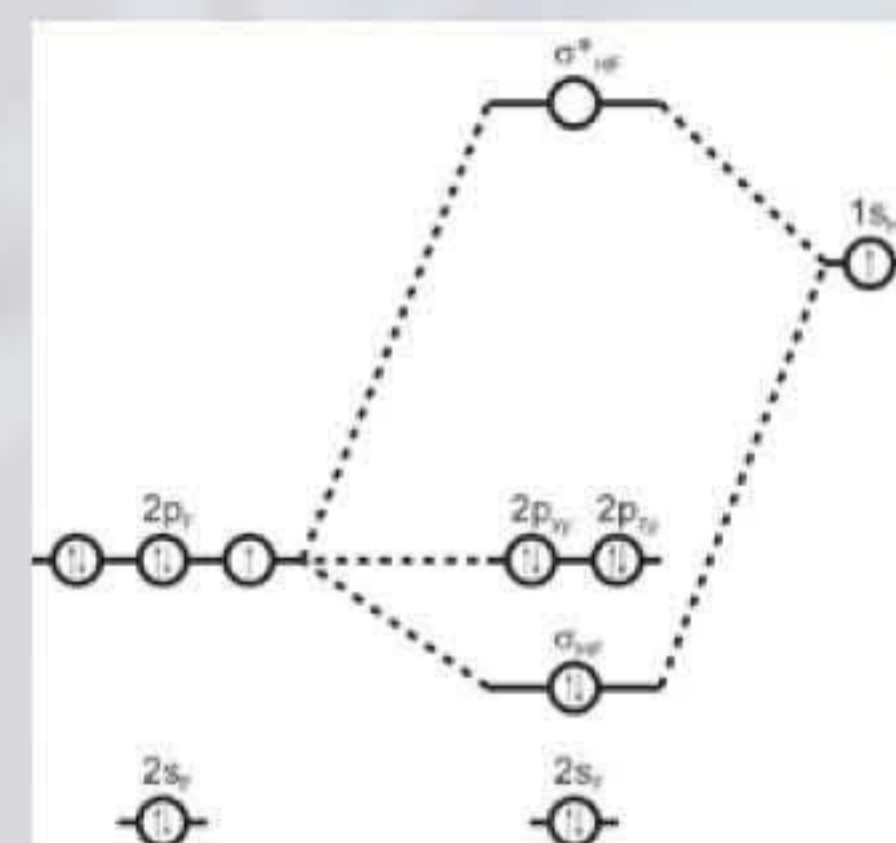
(BFGS), Davidon-Fletcher-Powell (DFP), Sigma, and McIver-Komornicki. Mixed internal and Cartesian coordinate input is allowed.



- SCF Procedures: Restricted Hartree-Fock, Unrestricted Hartree-Fock, SCF-CI.
- Giant Molecules: MOZYME method for solving the SCF equations is implemented that scales linearly in time and memory usage with the size of the system. The electronic properties of systems with more than 20,000 atoms, including proteins, polymers, semiconductors, and crystals can now be calculated in minutes.
- Solvent effects: the linear COSMO technique and the Tomasi method (MST).
- Electric Fields: the effect of applied external electric fields can be modeled.
- Electrostatic Potentials: MOPAC embodies two electrostatic potential methods, the Wang-Ford Parametric Electrostatic Potential (PMEP) and Merz-Besler ESP methods.
- Vibrations: the normal modes of vibration of ground state and transition state systems can be calculated, including the force constants and effective mass. Isotopic substitution effects can be modeled.

- Thermodynamic quantities: partition functions, enthalpies, heat capacities, and entropies can be calculated for any temperature, or range of temperatures.
- Quantum Molecular Dynamics: MOPAC can perform dynamics calculations as a function of time at constant total energy, controlled reduction of kinetic energy (cooling or simulated annealing) and controlled increasing kinetic energy (heating).

#### Hardware and software requirements



- Suggested hardware configuration for Windows version: Intel Pentium 4 2.0 GHz or higher, 512 MB RAM or more, 500MB HDD space or more.
- Operating systems: AIX (IBM), HP-UX, Fujitsu PrimePower, Windows 98/NT/2000/XP, and Linux.
- MOPAC has also been ported to various parallel computers.

