

Results with HyperChem

Display

- Rendering choices: Ball-and-stick, fused CPK spheres, ball and cylinders, or tubes with optional shading and highlighting. Also vdW dots added to any rendering.
- Ribbon rendering for protein backbones, with optional sidechain display.
- Cylinders, ribbon lines, thin solid ribbons, thick ribbons and coils for secondary structure rendering.
- 3D Isosurfaces or 2D contour plots of: Total charge density. Molecular orbitals, Spin density, Electrostatic potential (ESP).
- ESP mapped onto 3D charge density surface
- Isosurface rendering choices: wire mesh, Jorgensen-Salem, transparent and solid surfaces, Gouraud shaded surface. User-specified grid and isosurface value.
- Generate ray-traced graphical images.
- During simulations, display and average kinetic, potential, and total energy, as well as values of user-specified bond lengths, bond angles, or torsion angles.
- Spectra display of IR or UV-VIS.
- Animate vibrational modes.
- NMR spectra.
- Crystal structures.
- Slides (molecules plus annotations).

Customize and Automate

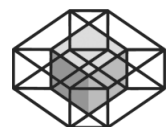
- Construct custom menus
- Automate routine operations with scripts
- Send selected data to files or workspace
- Add new features as menu items, or run from scripts

Interface and Extend

- Construct a custom interface to programs written in VB, C/ C++, or FORTRAN
- Send HyperChem results to MS Word or Excel.

HyperChem Release 8.0 is available for both standalone and networked installations. Site licensing is also available; ask us about it!

CONTACT YOUR HYPERCHEM RESELLER OR ASK US FOR FREE EVALUATION DISK



Hypercube

Good Chemistry

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Predict

- Relative stabilities of isomers
- Heats of formation
- Activation energies
- Atomic charges
- HOMO-LUMO energy gap
- Ionization potentials
- Electron affinities
- Dipole moments
- Electronic energy levels
- MP2 electron correlation energy
- CI excited state energy
- Transition state structures and properties
- Non-bonded interaction energy
- UV-VIS absorption spectra
- IR absorption spectra
- Rate constants - unimolecular or bimolecular reactions
- Equilibrium as a function of temperature
- Isotope effects on vibrations
- Collision effects on structural properties
- Stability of clusters
- Shielding and coupling constants
- Conformations of flexible systems
- Homologous proteins

Save Results

- Use Import/Export option to save results of quantum mechanics calculations or to view results generated by other programs.
- Use HyperChem Data to store structures and properties in a custom molecular database.
- Create Reaction Movies in AVI format

System Requirements

PC running Windows NT, 98, ME, 2000, XP, or Vista.

128 MB of RAM and 50-150 MB of hard disk space (the requirements for running Windows are generally more severe than for running HyperChem).

Raytracing and using the HTML controls requires a graphics card with more than 256 colors. Otherwise, any PC graphics card is acceptable as long as it supports OpenGL.