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!

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 temperaure
- 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.

CONTACT YOUR HYPERCHEM RESELLER OR ASK US FOR FREE EVALUATION DISK

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