HyperChem® 8

F E A T U R E S U M M A R Y

The First Choice for PC-Based Molecular Modeling

What is HyperChem?

HyperChem is a sophisticated molecular modeling environment that is known for its quality, flexibility, and ease of use. Uniting 3D visualization and animation with quantum chemical calculations, molecular mechanics and dynamics, HyperChem puts more molecular modeling tools at your fingertips than any other Windows program. It includes all the components of structure, thermodynamics, spectra, and kinetics.

What is New in HyperChem 8?

HyperChem 8.0 is the latest release of HyperChem. It introduces extensive new features that add to its industry-leading position. This is particularly true with regard to its "open architecture" and HyperChem's ability to interact with other programs such as Excel and Word or third-party packages in computational chemistry.

Third-Party Interfaces

In spite of the fact that HyperChem has extensive and elegant number crunching capabilities, it can't be all things to all computational chemists. With Release 8, an effort to enable HyperChem as a universal component in computational chemistry begins. Release 8 includes an interface to six third-party packages that are in common use in computational chemistry. None of these packages includes a native graphical user interface. Each benefits from the capabilities of HyperChem and each set of users now has capabilities never imagined before. Now PC Gamess, WinGamess, PQS, Q-Chem, Gaussian, and Mopac2007 can all be transparently executed by HyperChem. Now each of these can act as a computational engine for HyperChem. They add to the large number of native computational engines already in HyperChem, such as HyperGauss, HyperDFT, etc. The world just got easier.

Other Additions

- Double precision everywhere
- Additions to model builder (substituents)
- Render POINT, LINE, and PLANE
- Calculation of zero-point energies
- Undo and Redo of Model Builder
- CI separated from SCF dialog box
- Vista compatibility
- Vibrations for molecular mechanics
- Expanded use of MP2
- Electric fields for molecular mechanics
- Options for units (kCal, kJ, or a.u.)
- New Geometry measurements (POINT to PLANE, etc)
- New semi-empirical RM1 method
- Calculation of Entropies, Heat Capacities, FreeEnergies
- Additions to toolbar (C, N, O, etc), and Model Builder
- A recent file list has been added for ease of use
- Batch calculations which spawn back ends and return
- Line width envelopes for IR and UV spectra
- Named FIXEDATOMS and MECHANICALATOMS
- Calculation of Equilibrium Constants w/ Temperature
- Calculation of Kinetic Rate Constants w/ Temperature
- Calc. of particle-in-box energy and wave function

Windows and More

Hypercube, Inc.'s principal product is HyperChem Professional for Windows, the world's first chemistry software product on Windows. Other products and other platforms are also available. HyperChem Student, HyperChem Lite, Pocket HyperChem, and Personal HyperChem all satisfy specific markets. HyperChem for Mac is also now available. Look for others as well.