- Display atom labels such as symbol, name, number, type, charge, spin, mass, basis set, chirality, and gradient.
- Display bond labels such as length and bond order or residue labels such as type and number.
- Display custom user-defined atom labels as annotations to a structure.
- Display inertial axes and moments of inertia for any selected portion of a molecular system.
- Display POINT, LINE, and PLANE in a graphical way as structural features of any molecule or selection.
- Display periodic boundary conditions
- Hide any selected portion of system.
- Display overlap of two molecular systems as per their RMS fit.
- Use a variety of user selected colors for window backdrops, atoms, selections, orbitals, and isosurfaces; color portions of a system according to your own needs and tastes.
- Display/Edit molecular mechanics or semi-empirical parameters for selected atoms, bonds, and angles.
- Copy displayed images to file or clipboard for incorporation into another program such as Microsoft PowerPoint or for display on a web page.
- Capture structure, orbitals, or spectra and immediately create an active web page allowing rotation of molecule, inspection of orbitals, or animation of normal mode; freely distribute web control to allow others to view your active content.
- Apply and display names for individual molecules of a system.
- Immediately display potential energy surfaces for one or two independent structural variables; save as potential energy plot for presentations.
- Display spectra including frequency, intensity and line-width envelopes. Click on any line for further information.
- Display vectors attached to atoms indicating the relative force on the atom or its direction of motion in a normal mode.
- Display animations of normal modes from vibrational analysis (IR Spectra).

Selections

- Apply most operations either to the current selection or alternatively to the whole system.
- Select and name sets of atoms for custom display or monitoring of properties.
- Select a set of atoms and apply pre-defined properties POINT, LINE, PLANE, REACTANT, PRODUCT, PLOT1, PLOT2, GHOST ATOMS, NMR ATOMS, FIXED ATOMS, MECHANICAL ATOMS, and QUANTUM ATOMS to the atoms.
- Select with unit of selection being atoms, residues, or whole molecules.
- Select atoms based on their individual properties - such as all atoms within a specified range of energy gradient.
- Select atoms associated with a secondary structure such as beta-turn atoms, helix atoms, etc.
- Logically complement a selection.

Annotations

- Draw text, lines, ellipses and rectangles (filled or unfilled) on annotation layer to document your modeling results; apply z-ordering to your annotations for proper visual effect. In essence, a small general drawing program is include in HyperChem.
- Create symbol annotations as text in a particular font and size.
- Hide annotation layer or place it in front of or behind modeling layer.
- Save annotations in same file as molecular system to save/restore a general-purpose drawing or a specific set of annotations.
- Select and zoom/translate annotations as you would atoms of a molecule.
- Draw the bottom of a one-dimensional box and see the “particle-in-a-box” energies and wave functions.

Database

HyperChem 8.0 includes a separate database package that interacts intimately with HyperChem to provide molecules for input to modeling calculations and to store results of those calculations.

- Create a new database of 2D molecular drawings with associated 3D structures and molecular data.
- Open a default existing database of over 10,000 common molecules.
- Create a new database record from HyperChem with the push of a button.
- Create 2D drawings for publication and presentation purposes.
- Query a database for 2D structure and values of the database fields.
- Run a script over a database of molecules to automate HyperChem calculations.
- Create a general-purpose 3D query but associating query with (true, false) result of any HyperChem script.
- Create a database of molecules to carry around on your phone or Pocket PC.