

## ChemSite Pro<sup>®</sup>

Computer-Aided Chemistry Modeling Set  
Build ANY Structure Quickly!

ChemSite Pro is an interactive 3D molecular graphics environment that empowers the chemist to build, study, and present molecules in an impressive visual environment. The intuitive Windows interface makes ChemSite Pro easy to learn and use. Interactive 3D modeling and real time animation lets you use molecular building blocks or atom by atom construction to visualize even the most complex structures. Easily build protein, DNA, organic, and inorganic molecules as fully realized, space-filling entities. Easily build molecules by sketching them as you would on paper and then automatically convert the sketch to an accurate 3D model. You can even create and playback molecular dynamics. Photo-realistic rendering tools such as Bezier curves, Ray tracing, Phong shading and texture-mapped atom symbols help create stunning presentations. ChemSite Pro images could then be exported to other Windows applications with a single mouse click-Works interactively with CISPro, MMP and NIST Mass Spec Search programs. Powerful analysis features include tools and techniques formerly found only on workstation level modeling programs. Full support for stereo chemistry, for example, with dashes and wedges around chiral centers and auto-determination of R and S stereo centers is included. Files can be freely imported and exported in all the most popular formats including Brookhaven, ChemDraw connectivity table, and Mopac Z-matrix. An extensive library of organic molecules suitable for college organic chemistry courses is included for use with lessons from organic chemistry textbooks such as McMurray. Can be used as a great teaching tool! The latest version displays molecular surfaces calculated with semi-empirical quantum mechanics and provides improved graphic performance. Easily draw any 2D structure for publication quality graphics and automatically convert to 3D modeling. Includes all of the features of ChemSite Std.

Lipid Builders

Lipid Bilayer Builder

Synthetic Polymer Builder

Build lipid bilayers and perform MD simulation in water under 2D periodic boundary conditions

Works interactively with CISPro, MMP+ and NIST Mass Spec Search programs

Perform semi-empirical extended huckel calculations

Performs Ab Initio Calculations: includes the STO-3G and 3-21G bases sets

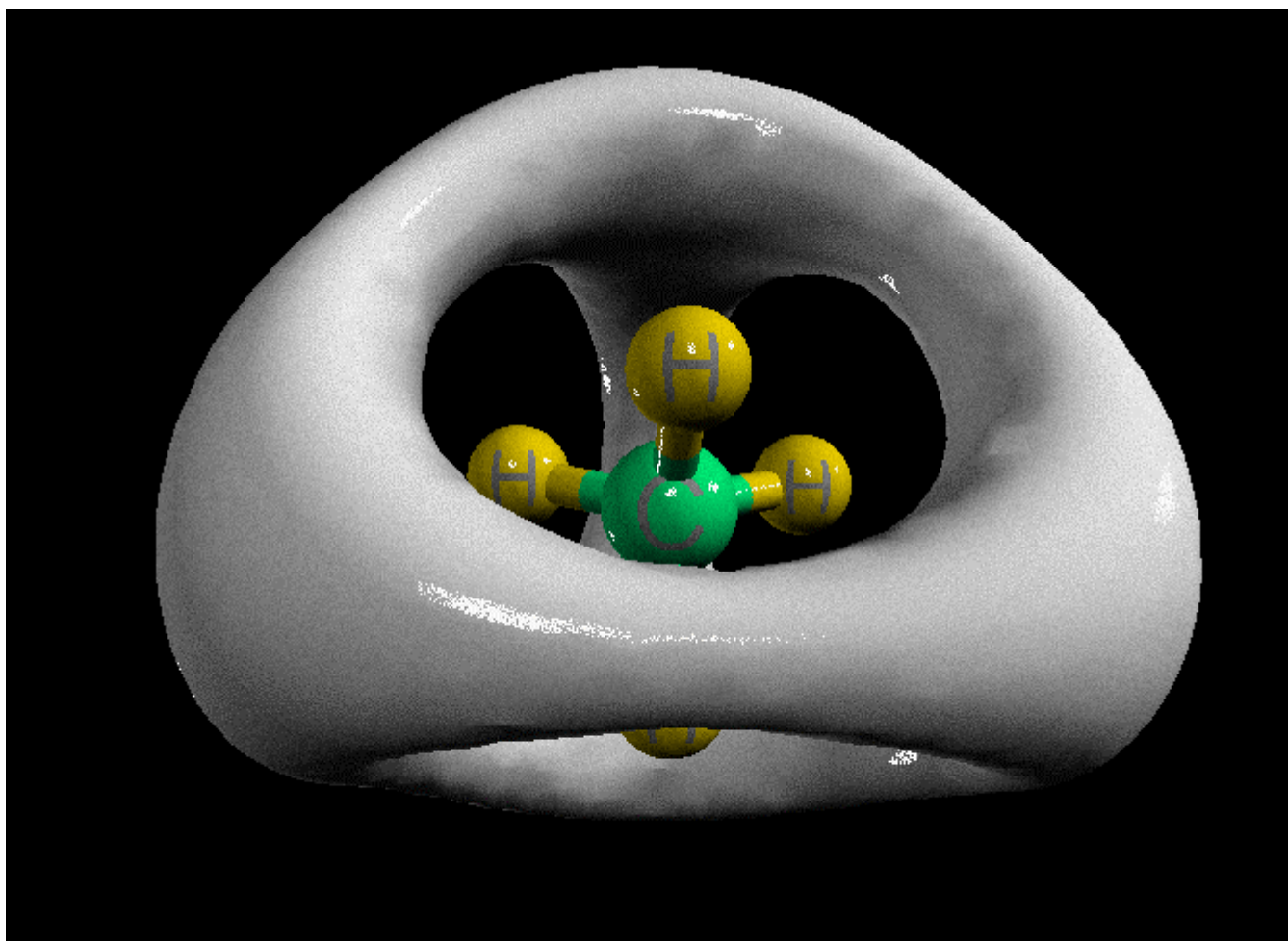
Build crystals based on all of the 230 space groups

Calculates and display molecular orbitals: total electron density and frontier orbitals (HOMO, LUMO)

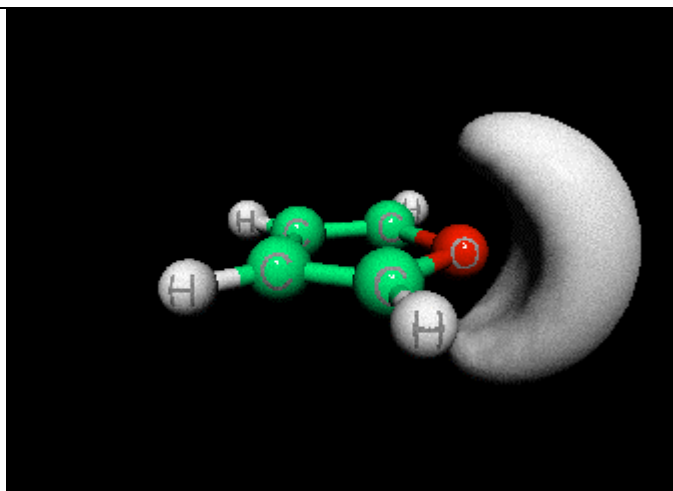
Displays electron spin density

Displays the electrostatic potential

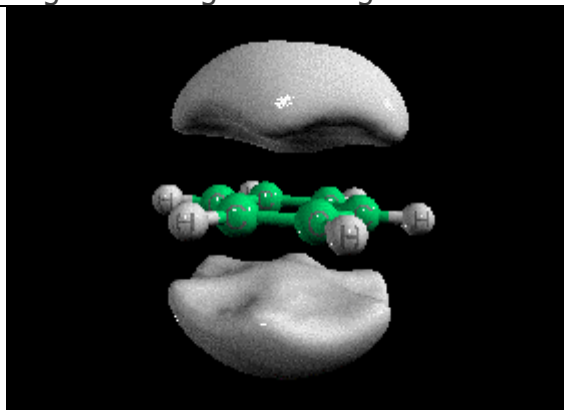
Calculates del Re, Huckel and Extended Huckel atomic charges



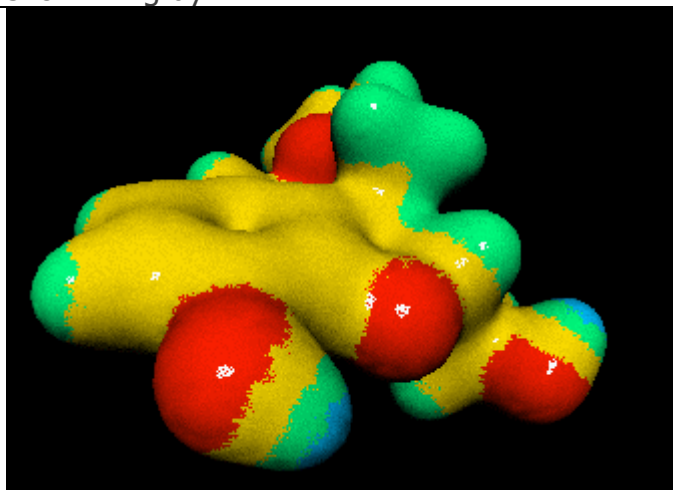
Methane: Electrostatic potential surface of methane. Regions of negative charge are shown in gray.



**Furan:** Electrostatic potential surface of furan. Regions of negative charge are shown in gray.



**Benzene:** Electrostatic potential surface of benzene. Regions of negative charge are shown in gray.



**Morphine:** Total electron density surface is shown. Regions of negative charge are red while regions of positive charge are blue.