

ORBITAL.EXE

Robert M. Hanson
Dept. of Chemistry
St. Olaf College
Northfield, MN 55057
507-546-3107
hansonr@stolaf.edu
1/18/02

Abstract

ORBITAL.EXE is a Visual Basic 4.0 program that runs under Microsoft Windows 95 or later. It allows for the production of probability-based three-dimensional representations of the atomic orbitals of the hydrogen atom and other single-electron systems. Unlike traditional representations of orbitals, which depict a surface containing a fixed percentage of the electron density, the orbitals created by ORBITAL.EXE depict the electron density itself, using dots of various spatial density and color. The orbitals are produced using a Monte Carlo technique and saved as Chime XYZ files. These files are suitable for uploading to web sites and are indexed by name and by energy. They are displayed automatically using the default browser, provided it has the Chime plug-in installed.

Orbitals may be visualized using several different options, including slices along the xy , yz , or xz planes and 1st quadrant-only sections. Colors can be selected to emphasize probability or the sign of the wavefunction. Any orbital up through principal quantum number $n=20$ for nuclear charge Z up to 120 may be displayed and may involve from 625 to 320,000 points. As the orbital is produced, the progress of the Monte Carlo calculation can be monitored in the form of a developing histogram of number of "hits" vs. radius. This histogram can be compared to a plot of theoretical radial probability either in three-dimensional space or in the selected planes.

Quantum numbers n , l , and m may be selected either by direct entry or by pointing to orbitals on an energy level diagram. In addition, the hydrogen atom emission spectrum can be displayed. The correlation between lines on the emission spectrum and transitions between energy states can be easily correlated.

Accompanying the program is an HTML help file that discusses the Monte Carlo method, presents program options, and provides the context in which the program is used at St. Olaf College (a second-semester laboratory experiment relating to atomic spectroscopy).