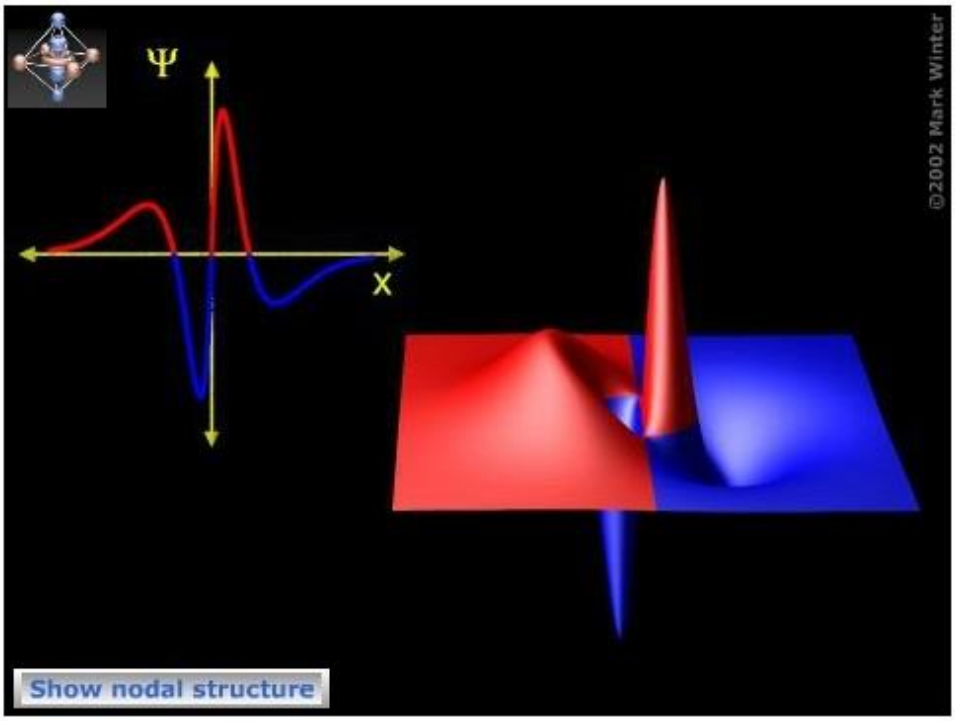
Atomic orbitals: 3*p* wave function



Schematic plot of the 3p_x wave function ψ_{3p_x}. *Note the line plot*

Atomic orbitals: 3*p* equations

The symbols used in the following are:

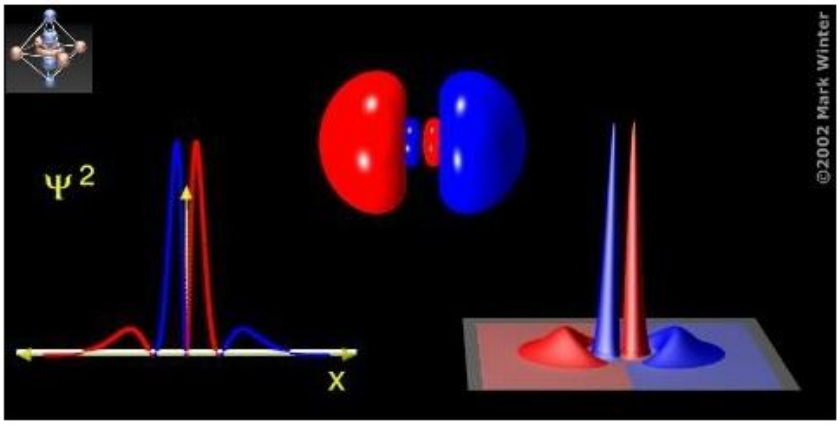
- r = radius expressed in atomic units (1 Bohr radius = 52.9 pm)
- π = 3.14159 approximately
- e = 2.71828 approximately
- Z = effective nuclear charge for that orbital in that atom.
- $\rho = 2Zr/n$ where n is the principal quantum number (3 for the 3*p* orbitals)

Table of equations for the 3*p* orbital.

Function	Equation
Radial wave function, R_{3p_x}	$= (1/9\sqrt{6}) \times \rho(4 - \rho) \times Z^{3/2} \times e^{-\rho/2}$
Angular wave function, Y_{3p_x}	$= \sqrt{(3)}x/r \times (1/4\pi)^{1/2}$
Wave function, ψ_{3p_x}	$= R_{3p_x} \times Y_{3p_x}$
Electron density	$= \psi_{3p_x}^2$
Radial distribution function	$= r^2 R_{3p_x}^2$

The radial equation for the $3p_x$, $3p_y$, and $3p_z$ orbitals is the same in each case. The angular functions are the same but substitute y and z as appropriate in the formula for Y_{3p_x} given above. Substitute similarly for the wave equations ψ_{3p_y} and ψ_{3p_z}.

Atomic orbitals: 3*p* electron density

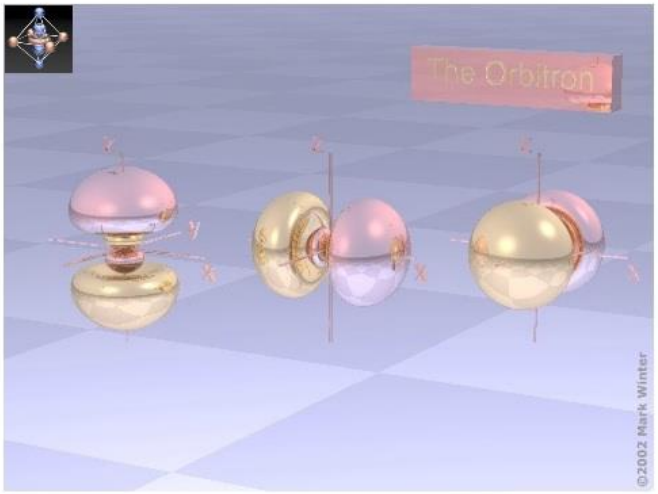


Schematic plot of the 3p$_x$ electron density function $\psi_{3p_x}^2$. *Blue represents negative values for the wave functions and red represents positive values.*

The "surface" of the orbital represents points for which the electron density for that orbital is the same - an *isosurface*. By choosing different values of electron density, denoted by the bar moving up and down on the line plot or by the moving plane on the surface plot, then the size of the three-dimensional plot changes. This plot also shows that the magnitude of the electron density for the inner lobes is high so that if we choose a high threshold value (when the bar is high), then we only see the inner lobes in the three-dimensional plot. Only by moving the bar down sufficiently far does the main outer lobe become visible.

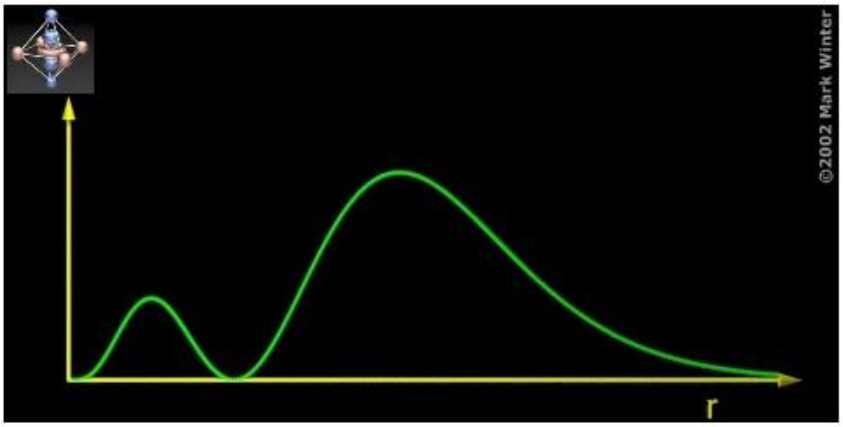
The plot above is labelled for the 3p_x orbital but the form of the plots for the 3p_y and 3p_z orbitals is similar, differing only in orientation.

Atomic orbitals: 3p



The shape of the three 3p orbitals. *From left to right: 3p$_z$, 3p$_x$, and 3p$_y$. For each, the gold zones are where the wave functions have negative values and the copper zones denote positive values.*

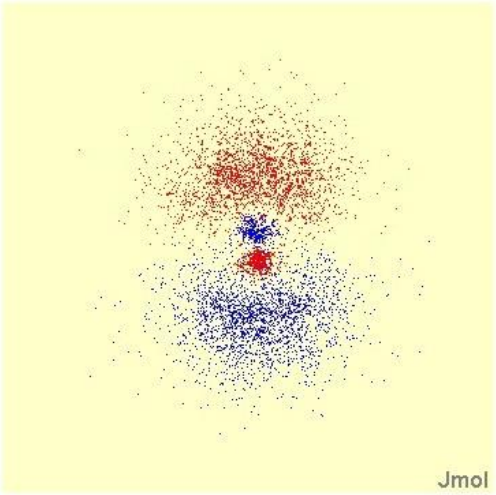
Atomic orbitals: 3*p* radial distribution function



Schematic plot of the 3p radial distribution function $r^2R_{3p}^2$ *(*R_{3p} *= radial wave function).*

For 3*p*-orbitals, the radial distribution function is related to the product obtained by multiplying the square of the radial wave function R_{3p} by r^2. By definition, it is independent of direction.

Atomic orbitals: 3*p* electron density



"Dot-density" plot of the 3p$_x$ electron density function $\psi_{3p_x}^2$***.***
Blue represents negative values for the wave functions and red represents positive values.

This page displays the electron density of a 3*p* orbital as a "dot-density" diagram. High density of dots in a region denotes high electron density.

The form of the plots for the $3p_x$, $3p_y$ and $3p_z$ orbitals is similar, differing only in orientation.

Die Adresse der Seite ist:
http://winter.group.shef.ac.uk/orbitron/AOs/1s/index.html