Continue

Parts of a wave function

Schrödinger equation solutions for atomic orbitals can be expressed in terms of spherical coordinates: r, θ, and ϕ. For a point (r, θ, ϕ), the variable r represents the distance from the center of the kernel, θ represents the angle on the positive z axis, and ϕ represents the angle on the positive x-axis in the xy-flat. Because atomic orbitals are described with a potential V independent of time, Schrödinger's equation can be solved using the variable separation technique, so that any wave function has the shape: $\Psi(r,\theta,\phi) = R(r) \, Y(\theta,\phi)$ where $R(r)$ is the radial wave function and $Y(\theta,\phi)$ is the angular wave function: $Y(\theta,\phi) = \Theta(\theta) \; \; \; \Phi(\phi)$ Each set of quantum numbers, (n), (l), (m_l), describes a different wave function. The radial wave function depends only on n and l, while the angular wave function depends only on l and m_l. So a particular orbital solution can be typed as: $\Psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r) \, Y_{l,m_l}(\theta,\phi)$ Where $n = 1, 2, 3, ...$) $l = 0, 1, ..., n-1$) $m_l = -l, ... , -2, -1, 0, +1, +2, ..., l$) A wave function node occurs at points where the wave function is zero and changes signs. The electron is zero likely to be placed in a node. Due to the separation of variables for an electronic orbital, the wave function will be zero when any of its component functions is zero. When $R(r)$ is zero, the node consists of a sphere. When $\Theta(\theta)$ is zero, the node consists of a cone with the z axis as the axis and apex at the source. In the special case $\Theta(\pi/2) = 0$, the cone is flattened to be the x-y plane. When $\Phi(\phi)$ is zero, the node consists of a plane through the z axis. The shape and extent of an orbital only depends on the square of the magnitude of the wave function. However, when considering how the union between atoms might take place, the signs of wave functions are important. As a general rule, a bond is stronger, i.e. it has less energy, when the orbitals of shared electrons have their wave functions positively match positive and negative to negative. Another way to express this is that the bond is stronger when the wave works constructively to interfere with each other. When orbital overlap so that the wave functions positively match negative, the bond will be weaker or cannot be formed at all. Radial waves are of the general form: $R(r) = N \; p_(r) \; e^{-kr}$) Where N is a positive normalization constant $p(r)$ is a polynomial to r (k) is a positive constant The exponential factor is always positive, so the nodes and sign of $R(r)$ depends on the behavior of $p(r)$. As the exponential factor has a negative to the exponent, $R(r)$ $R(r)$ approach 0 as r goes to infinity. Ψ^2 quantifies the probability that the electron is at a specific point. Probability distribution, $P(r)$ is the probability that the electron is at any point other than the r distance of the kernel. For any type of orbital, since $\Psi_{n,0,0}$ is separable into radial and angular components that are properly normalized, and an r radius sphere has area proportional to r^2, we have: $P(r) = r^2 R^2(r)$) The angular wave function $Y(\theta,\phi)$ does a lot to give an orbital badge its shape. $Y(\theta,\phi)$ is normalized so that the $Y^2(\theta,\phi)$ integral on the drive sphere is equal to one. In this case, $Y^2(\theta,\phi)$ serves as a probability function. The probability function can be interpreted as the probability that the electron is in the emission of rays from the source found at angles θ,ϕ of the axes. The probability function can also be interpreted as the probability distribution of the electron that is in position θ,ϕ in an r radius sphere, since it is r distance from the kernel. Angular wave functions for a hydrogen atom, $Y_{l,m_l}(\theta,\phi)$ are also wave function solutions in schrödinger equation for a rigid rotor made up of two bodies, for example a diatomic molecule. The simplest case to consider is the hydrogen atom, with a positively charged proton in the nucleus and only a negatively charged electron orbiting around the nucleus. It is important to understand the orbitals of hydrogen, not only because hydrogen is an important element, but also because they serve as building blocks for understanding the orbitals of other atoms. Hydrogen orbits correspond to $l=0$) and only allow $m_l = 0$). In this case, the solution for angular wave function, $Y_{0,0}(\theta,\phi)$ is a constant. As a result, wave functions $\Psi_{n,0,0}(r,\theta,\phi)$ depend only on r and orbital ones are all spherical in shape. Because $\Psi_{n,0,0}$ depends only on r, the electron probability distribution function: $\Psi^2_{n,0,0}(r,\theta,\phi) = \dfrac{1}{4\pi}R^2_{n,0}(r)$ $R(r)$), $R^2(r)$), $P(r)$) are followed by n = 1, 2 and 3. The function chart has been scaled several times along the vertical axis to allow easy comparison of its shapes and where they are zero, positive and negative. Vertical scales for different functions, either in or between diagrams, are not necessarily the same. In addition, a cross-section outline diagram is given for each of the three orbits. These outline diagrams indicate the physical shape and size of the orbitals and where the odds are concentrated. An electron will be in the most likely regions-10% 10% of the and it will be in the regions (including the most likely regions-10% 50% of the time. In all these outline diagrams, the x axis is horizontal, the z axis is vertical, and the y axis comes out of the chart. The actual orbital shape 3 dimensional is obtained by rotating the 2-dimensional cross section over the symmetry axis, which is shown as a line of blue dashes. Outline diagrams also indicate for regions that are separated by nodes, whether the wave function is positive (+) or negative (-) in that region. In order for the wave function to change sign, a node must be crossed. Orbital 2s Orbital 3s Orbital Diagrams, we see that orbital 1s has nodes, orbital 2 has a node, and orbital 3 has 2 nodes. Because for orbital s, $\Psi^2 = R^2(r)$), it is interesting to compare the graphs $R^2(r)$) and the graphs $P(r)$). Comparing the maximum values, in orbital 1s, the graph $R^2(r)$ shows that the most likely place for the electron is in the kernel, but the graph $P(r)$ shows that the most likely radius for the electron is a_0), the Bohr radius. Similarly, for the other orbitals, the only place where the electron is most likely to be in the nucleus, but the radius most likely for the electron in which it is found is outside the outer most external node. One thing that is not easily evident from these diagrams is that the average radius of orbitals 1, 2 and 3s is 1.5 a0, 6 a0 and 13.5 a0, forming ratios of 1:4:9. In other words, the average radius is proportional to n^2). Hydrogen p orbits correspond to l = 1 when n ? 2 and allow ml = -1, 0 or +1. The following diagrams describe the wave function per ml = 0. The angular wave function $Y_{1,0}(\theta,\phi = body\theta$ depends only on θ. Then the angular wave function displayed with a node in $\theta = \pi/2$). Radial waves and orbital outline diagrams for orbital p with n = 2 and 3 are: Orbital 2p Orbital 3p Orbitals As in the case of orbital s, the real 3-dimensional orbital p shape is obtained by rotating the 2-dimensional cross sections over the symmetry axis, which is shown as a line of blue dashes. Orbital P shows its distinctive timbre shape. The angular wave function creates a nodal plane (the horizontal line in the cross section diagram) in the x-y plane. In addition, the 3p radial wave function creates a spherical node (the circular node in the cross section diagram) to r = 6 a0. For $m_l = 0$), the symmetry axis is along the z axis. Wave functions per ml = +1 and -1 can be rendered in different ways. To facilitate calculation, they are often represented as real value functions. In this case, orbitals have the same shape and size as $m_l = 0$), except that they are oriented in a different direction: the symmetry axis is along the x axis with the nodal plane on the y-z plane or the is along the axis and with the nodal plane on the x-z plane. Orbital hydrogen correspond to l = 2 when n ? 3 and allow ml = -2, -1, 0, +1 or +2. There are two basic forms of orbital, depending on the shape of the angular wave function. The first shape of an orbital d corresponds to ml = 0. In this case, $Y_{2,0}(\theta,\phi)$ depends only on θ. The graphs of the angular wave function, and for $n = 3$), the radial wave function has no nodes. The second orbital form is illustrated by ml = +1 and n = 3. In this case, $Y_{2,1}(\theta,\phi)$ depends on both θ and ϕ, and can be displayed as a surface curve above and below a rectangular domain. As a result, diagrams separated by $Y_{2,1}(\theta,\phi)$ are displayed on the left and $Y^2_{2,1}(\theta,\phi)$ on the right. Orbital 3d, ml = 0: As in the case of orbital s and p, the real 3-dimensional orbital shape is obtained by rotating the 2-dimensional cross section over the symmetry axis, which is shown as a line of blue dashes. This first orbital shape shows a ring shape along the z axis, but is surrounded in the middle by a doughnut (corresponding to regions where the wave function is negative). The angular wave function creates nodes that are cones that open at about 54.7 degrees on the z axis. A n=3, the radial wave function has no nodes. Each of the four arms of the outline is rotated on its symmetry axis to produce the 3-dimensional shape. However, rotation is a non-standard rotation, producing only radial symmetry on the axis, not circular symmetry as was the case with other orbitals. This produces a double shape of dumbell, with nodes in the x-y plane and the y-z plane. Similar to orbits p, wave functions per ml=+2, -1 and -2 can be represented as real functions that have the same shape as by ml=+1, oriented in different directions. In two cases, the shape is re-oriented so that the symmetry axes are in the x-y plane or in the z-y plane. In both cases, symmetry axes are at 45 degrees in their axes of repethematic coordinates, as with ml=+1. For the third and final case, the orbital shape is re-oriented so that the symmetry axes are in the x-y plane, but it is also placed along the x and y axes. Hydrogenic atoms are atoms that have only one electron orbiting around the nucleus, although the nucleus may have more than one proton and one or more neutrons. In this case, the electron has the same shapes as the hydrogen atom, except that they are scaled by a factor of 1/Z. Z is the atomic the number of protons in the nucleus. Increasing the number of positively charged protons reduces the size of orbitals. Thus, the same hydrogen graphics above apply to hydrogen atoms, except that instead of expressing the radius in units of a0, the radius is expressed in units of a0/Z. Correspondingly, the values must be renormalized by a factor of (Z/a0)3/2. So a He+ atom has orbits that are the same shape but half the size of the corresponding hydrogen orbitals and a li2+ atom has orbitals that are the same shape, but a third the size of the corresponding hydrogen orbitals.

References Atkins, P., && of Paula, J. (2006). Physical Chemistry for Life Sciences. In 1997, the New York government was the first to do so. Ladd, M. (1998). Introduction to Physical Chemistry (3rd ed). Cambridge, United Kingdom: Cambridge University Press. McMahon, D. (2005). Demystified quantum mechanics. New York: McGraw-Hill Professional. Retrieved 19 December 2014. Physical Chemistry: A molecular approach. Sausalito, CA: University Science Books. Attributions of collaborators and attributions