Organic Chemistry - Exercise 1

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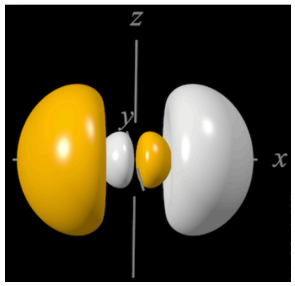
1. The Schrödinger equation is a central element to describe quantum-mechanical systems.
   a. Paraphrase briefly in your own words what the Schrödinger equation is and what it describes!

      The Schrödinger equation is a differential equation that describes the allowed stationary states of an electron in the field of atomic nucleus.

   b. What is an atomic orbital and how is it graphically represented?

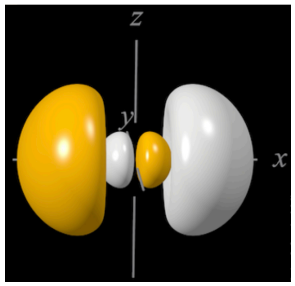
      An atomic orbital describes the shape of the allowed stationary state ψ of an electron in space. The shape of the atomic orbital is represented with a contour surface enclosing the probability density $|\psi|^2$ = const.

2. The image below shows an atomic orbital at time $t = t_0$.
   a. What is the name of the orbital that is shown, if you have the additional information that this orbital contains at least one electron in a chlorine atom?



      This orbital has a shape of 3p orbital, and since it is aligned with x-axis, this is $3p_x$ atomic orbital.

   b. Draw schematically how this orbital would look at time $t = t_0$ +2 s.



      The Schrödinger equation is time-independent, meaning that the orbital shape does not change with time.

   c. Give the two sets of all four quantum numbers for the two electrons that could possibly occupy in this orbital in a chlorine atom.

      $n = 3; l = 1; m_l = -1; m_s = +1/2$

      $n = 3; l = 1; m_l = -1; m_s = -1/2$

d. What is the value of the wavefunction ψ in the point of intersection of all three axes in this case (x = y = z = 0) and what is the physical meaning of that?

If we follow the orbital along the x axis (from right to left), we can see that around zero, the sign of the ψ function changes from negative to positive (yellow to white), which means that the value of the ψ function must be 0, as ψ is a continuous function. That means that the probability of finding an electron in that point is 0.

3. The electron configuration of an atom describes the distribution of electrons onto atomic orbitals.

   a. What are the electronic configurations of carbon, nitrogen, oxygen, phosphorus and argon in their respective ground state?

   C: $1s^2\ 2s^2\ 2p^2$

   N: $1s^2\ 2s^2\ 2p^3$

   O: $1s^2\ 2s^2\ 2p^4$

   P: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$

   Ar: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$

   b. With the help of the previous question, explain what the elements belonging to the 2nd period of the periodic table have in common.

   All elements in the same period have the same number of electron shells (2 in this case); another correct answer would be to say: they have the same valence shell (outer-most, at least partially filled shell).

   c. In a similar way, explain what the elements belonging to the 15th group (main group V) of the periodic table have in common.

   All elements in the same group have the same number of electrons in their valence shell (5 in this case).

   d. According to their respective electronic configuration in the ground state, what is the maximum number of atoms that carbon, nitrogen and oxygen can bond to? Why?

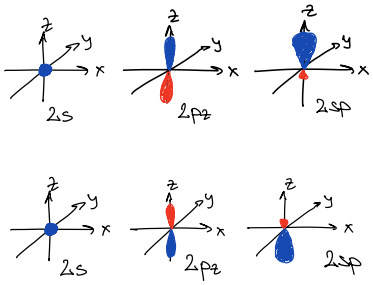
   All the atoms from the second period have to obey the octet rule: a completely filled valence shell can accommodate a maximum number of eight electrons or four electron pairs; so carbon can bond to maximum 4 other atoms, nitrogen to 3 other atoms and oxygen to 2 other atoms, if each partner brings one additional electron.

4. Hybrid orbitals are obtained by linear combination of atomic orbitals.

   a. How many orbitals can be obtained when one 2s and one 2pz atomic orbitals are combined? Give their name.

   When two atomic orbitals are combined, two new hybridized orbitals can be obtained – 2sp.

   b. Schematically draw the starting atomic orbitals and the final hybridized orbitals.



Reading Suggestions:

Clayden, Greeves, Warren, Wothers, *Oxford University Press*, **2001**.

Organic Chemistry, John McMurry, *Thomson Brooks/Cole*, **2008**.

Chimie Organique, Les Grands Principes, John McMurry, *Dunod Editeur*, **2009**.

Chimie Organique, Paul Arnaud, *Dunod Editeur*, **2009**.