HYBRID ORBITALS NOTATION: SOME MISCONCEPTIONS IN AN UNDERGRADUATE BASIC CHEMISTRY COURSE

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ABSTRACT

This work reports a study performed involving 26 students of an undergraduate basic chemistry course class at Federal University of Rio Grande do Norte, Brazil. The study was performed in order to evaluate the misconceptions about hybridization that students bring from high school courses and how to overcame such misconceptions. Methane, ammonia and water molecules were employed as examples. The equation was introduced in order to promote a most profound and mature interpretation of the hybridization notation. The sp4 and sp$^{2.3}$ water hybrid orbitals were used to illustrate the interpretation that can be given to the n value. In the same direction, a graphic "paint analogy" was employed to give a proper interpretation to the n value. *[African Journal of Chemical Education—AJCE 7(1), January 2017]*

INTRODUCTION

Despite some criticism [1], atomic hybrid orbitals still have a role to perform in chemistry [2], in both research and teaching. In high school chemistry courses, hybridization it is a theme that is a little confusing to most of the students. In undergraduate chemistry courses (general chemistry), such theme is introduced a second time, with no different approaches. Note that, in Brazil, the general chemistry textbooks are translated, generally, from American editions, from several authors (James Brady, Peter Atkins, Theodore Brown, etc.) and, in such textbooks, the subject hybridization is presented in a similar manner as it is presented in high school chemistry textbooks of Brazilian authors.

In such texts (both, high school and college chemistry), an interpretation to the notation sp^3 is that it represents four hybrid orbitals, made by the “mixing” of one s and three p orbitals. That is, the subscript 3 represents the number of p orbitals involved in the hybridization. However, this is a misinterpretation. For example, if the previous interpretation was right, the hybridization of nitrogen (in ammonia), and oxygen (in water), must be sp3 too, but this is not the case.

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METHODOLOGY

The study was conducted along the first semester of 2016 with 26 students of an undergraduate basic chemistry class at Federal University of Rio Grande do Norte, Brazil. The subject hybridization was introduced as part of the chemical bond study, specifically the covalent bond type (employing the valence bond theory). The subject was introduced, as classically done, by considering the hybridization of carbon, in methane (CH4, sp^3).

First, it was verified that to all students, hybridization was understood as a physical phenomenon. It was necessary to explain/clarify that hybridization is, in fact, a post facto manipulation of the atomic orbitals wave functions, in order to obtain “suitable” combinations (hybrid wavefunctions, associated with hybrid orbitals) that can, in the methane case, for example, account to the number of formed bonds, as well as the molecular geometry.

As a first approach to promote a most profound and mature interpretation of the hybridization notation, it was asked to the students what was the hybridizations of carbon (in methane), nitrogen (in ammonia) and oxygen (in water).

Repeating what they have learned in the high school textbooks (and what it is presented in many college basic chemistry textbooks, too), they stated that, in all three cases, the central atom exhibited a sp3 hybridization.

The three considered molecules where chosen taking into account that carbon, nitrogen and oxygen have increasing atomic numbers (6, 7 and 8, respectively), and that, in all three molecules, there is a total of four electrons pairs around the central atom. So, for the three considered molecules, four hybrid orbitals are employed, all of them been “constructed” from one s and three p atomic orbitals (2s and 2p orbitals).

However, as is known, a sp3 hybridization is associated with a tetrahedral geometry/angle (109.5°). So, the challenge presented to the students was: if in ammonia the bond angle is 107° and in water the bond angle is 104.5°, how the hybridization could be of the sp3 type?

Two thirds of the students have so employed the valence shell electrons pair repulsion (VSEPR) theory in order to explain the "deviations" shown by ammonia and water in relation to the 109.5° tetrahedral angle, arguing that the hybridization in such molecules are, anyway, sp3.

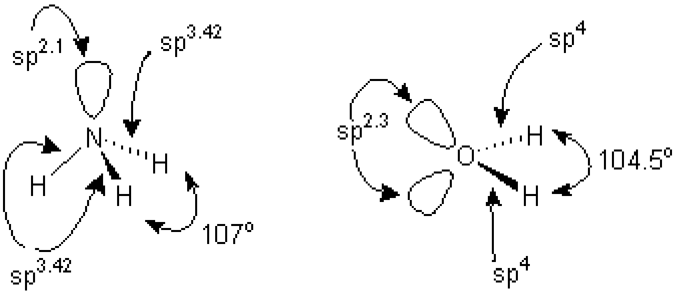

Figure 1. Hybrid orbitals to ammonia (left) and water (right) molecules (reproduced from: http://courses.chem.psu.edu/chem210/mol-gallery/hybridization/hybrids.html).

At this point, the following formula was introduced to the students:

$$n = \lambda^2 = -1/\cos\theta \qquad (1)$$

in which θ is the angle between the hybrid orbitals. This formula provides the n value in sp^n hybrids orbitals.

It must be emphasized here that, despite the fact that this equation comes from a higher level chemistry, there is no reason to, in an undergraduate course, to present and use this equation and its consequences to the interpretation of hybridization, providing, in a freshman chemistry course, a most profound and mature analysis of the chemical bond theories than that previously presented in high school chemistry courses/textbooks. In order words, the undergraduate basic chemistry courses must not be a simple "repetition" and "reinforcement" of the high school teaching and (unfortunately) misunderstandings, misconceptions and misinterpretations of chemistry concepts and theories.

If the bond angles 109.5º, 120º and 180º are applied in the previous equation, the calculated n values are 3, 2 and 1, respectively, providing the sp3, sp2 and sp well known hybrid orbitals (tetrahedral, trigonal planar and linear molecular geometry, respectively), for which the value of n really coincides with the number of p orbitals involved in the hybridizations.

However, in water, for example, the two orbitals involved in the O-H bonds exhibits a sp4 hybridization. So, how them (students) explain that? In ammonia, the 107º bond angle provides a sp3.42 hybridization to the orbitals involved in the N-H bond formation.

All students gets very surprised with this results, not only to the fact that a number higher than 3 was obtained, but also to the fact that, as shown to ammonia, a not integer n value can be obtained. At this point, the following formula was presented:

$$\cos\alpha = -1/(m.n)^{0.5} \qquad (2)$$

that provides the angle (α) between two hybrid orbitals: spm and spn. It can be verified that, when m =n, if m = 3, 2 or 1, the calculated values to α will be, of course, 109.5º, 120º and 180º. The hybridization to all orbitals in ammonia and water are shown in Figure 1.

RESULTS AND DISCUSSION

Since the bond angles are reliable and well stablished experimental data, the maxima that "against facts there are no arguments", was used in order to convince the students that the calculated values were correct and then, that a new physical explanation/interpretation must be provided to the n value in sp^n hybrid orbitals.

It must be stated here that convince the students to change the high school interpretation of the value of n in sp^n hybrid orbitals as the number of p orbitals employed in the hybridization, was not an easy task. It was possible to perceive that many students “accept” what the teacher is saying, but are not “really convinced”.

Such resistance to new ideas or new interpretations of “old” ideas is not an exclusive feature of the freshman student profile. Instead, it is a recurrent fact in science. However, taking into account that the “new” ideas considered here, are, in fact, an established chemical model, the “resistance” must be overcame, in order to achieve a really undergraduate level teaching/learning process.

The apparent difficulty, in the present study, was related with the counterintuitive nature of the obtained results: how could three 3 p orbitals give raise to sp4 hybrid orbitals? However, the counterintuitive nature of this result is consequence, of course, of the misinterpretation employed in the high school courses/textbooks and (unfortunately) reinforced in many undergraduate courses and textbooks.

In CH4, NH3 and H2O there are only three p orbitals involved in the hybridization. So, the superscript on p must be associated with another meaning: it is related with the percentage of p character (that is, the “contribution” of the three p orbitals) of the hybrid orbitals. So, a sp3 orbital has (1/4)x 100 = 25% of s-character and 75% of p character. In water, the hybrid orbitals involved in the O-H bond has (1/5) x 100 = 20% of s character and 80% of p character. On the other hand, the orbitals associated with the electron lone pair have (1/3.3)x 100 = 30.3% of s character and 69.7% of p character. So, one s orbital and three p orbitals could be combined in any proportion, in order to produce hybrid orbitals.

An analogy that was employed in the classroom and well received for all students was to compare the pure s and p orbitals with cans of paint: the s orbital is a can of black paint and the three p orbitals are three cans of white paint. In the sp3 hybridization (CH4, for example), the four resulting cans of paint have all the same color (that is, the same proportion of black and white paints).

To water, the black paint (s orbital, in the analogy), and the white paint (p orbitals) where mixed in different proportions, resulting in two orbitals with minor s character (sp4) and two orbitals with higher s character (sp2.3). The graphic analogy employed in the classroom is shown in Figure 2. A similar graphic analogy was employed to illustrate the hybrid orbitals to ammonia.

The “paint analogy” was chosen taking into account that paint of different colors can be mixed in any proportion (like the pure orbitals to produce hybrid ones), but only certain proportions are able to produce certain resulting colors (such as only certain combination of pure orbitals can produce hybrid orbitals that accounts to the experimental bond numbers and geometry of a given molecule).

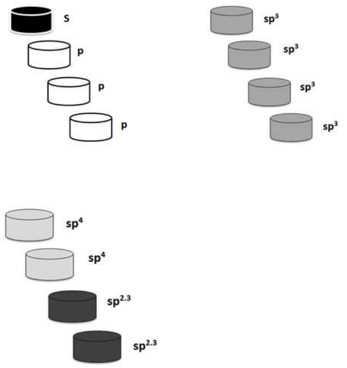

Figure 2. Graphic analogy employed in the classroom to illustrate the contribution of one s orbital and three p orbitals to the formation of four hybrid orbitals in methane (sp3) and water (sp4 and sp2.3)

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