EINSTEIN WAS HERE:
INTRODUCING RELATIVISTIC CHEMISTRY IN A BASIC CHEMISTRY COURSE

Robson Fernandes de Farias

Universidade Federal do Rio Grande do Norte, Caixa Postal 1664, 59078-970 Natal-RN, Brasil.
E-mail: robdefarias@yahoo.com.br

ABSTRACT

The presented work reports a study performed to introduce relativistic chemistry in basic (introductory) college chemistry classrooms. The study involved fifty students. It was verified that exploring the previous (high school) knowledge on special relativity, and introducing a simple equation, it is possible to explain the unexpected variations in covalent radius observed for groups 11, 12 and 18 heaviest elements. *[African Journal of Chemical Education—AJCE 8(1), January 2018]*

INTRODUCTION

Despite the fact that since the late 1920, special relativity [1] was "combined" (by Paul Dirac) with quantum mechanics, and, since that times, is well known that the properties of many elements and compounds can only be explained without taking into consideration the relativistic contributions [2.3], not only in general chemistry texts but even in inorganic chemistry texts used in many colleges and universities around the world, relativistic chemistry remains an ignored topic.

Every year, many chemistry students finish their undergraduate courses without any contact with relativistic chemistry. This was my personal case, twenty-five years ago.

It is worth nothing that the relativistic contributions to the chemical and physical properties of the elements (and hence, their compounds) is not a simple curiosity, relegated to a few elements. In fact, for something about 1/3 of the periodic table (for the heaviest elements) such contributions are paramount. It is not possible to provide a really correct explanation to many chemical facts (the liquid state of mercury at room temperature and the color of gold are very good examples) disregarding the relativistic contributions. For example, it was demonstrated that 1.7 to 1,8 V of the 2.13 V of the lead acid battery is because a relativistic contribution [4].

As will be seen in the examples considered in the present study, the so-called "periodic properties" exhibits "anomalies" that cannot be explained if the relativistic contributions are neglected. Nowadays, special relativity is presented even in high school physics books. So, the laymen college student is familiar with their equations.

This paper reported a study performed with fifty students of basic (introductory) college chemistry classrooms. The purpose was to introduce relativistic chemistry at this level of study and used it to explain the unexpected observed variations in properties such as covalent radius.

METHODOLOGY

Fifty students from two basic (introductory) college chemistry classrooms were involved. Of course, quantum chemistry and relativistic quantum chemistry are very complex subjects even for higher levels students. In the present study, a simplified exposition of the relativistic chemistry was performed, using the equations of special relativity such as they appear in high school physics books.

The covalent radius was the chosen property to be explored, since variation in the radius provokes a "domino effect" with consequences on so many other properties, such as ionic radius, lattice energy, ionization energy, electron affinity, redox potentials, frontier orbitals energy, and so on.

Elements from groups 11 and 12 were chosen and the students were provoked to explain the observed variations in the covalent radius of such elements. From special relativity, is known that, for a body (in our case, an electron) traveling at a speed not negligible (compared with the speed of light), a length contraction can be calculated by

$$L = L_0/\gamma; \text{ where } \gamma = 1/[1-(v^2/c^2)]^{1/2} \tag{1}$$

The velocity of the 1s electron is $\approx Z/137$, where Z is the atomic number [2] (the term $Z/137$ makes clear that relativistic effects matters only for heavy elements). Hence, the previous equation can be rewrite as

$$L = L_0/\gamma; \text{ where } \gamma = 1/[1-((Z/137)^2/c^2)]^{1/2} \tag{2}$$

In our case, L_0 is the covalent radius as expected by a simple extrapolation (see examples in the sequence) and L is the atomic radius calculated taking into account the relativistic

contribution. Of course, Eq. (2) represents a profound simplification of very complex theory/models but, nevertheless, it could provide useful results. The covalent radii employed here were taken from the Royal Society Periodic Table website [5].

RESULTS AND DISCUSSION

As a first task, it was proposed to the students to obtain an empirical equation relating covalent radius and atomic number. For Cu and Ag, the covalent radius (pm) are 122 and 136, respectively. By using this data, and the respective Z values, we found: $r = 0.778\,Z + 99.444$. Using this equation, a covalent radius for Au equal to 161 pm is calculated.

At this point, it must be noted that the "extrapolated" 161 pm radius is in agreement with the traditional explanation to the periodic properties: since gold is an element from 6th period, it has a larger number of filled electronic shells and, presumably, a larger covalent radius than Ag, as Ag has a larger covalent radius than Cu. This was the explanation provided by 100% of the students in an applied questionnaire. But this is not the case, and only the relativistic contraction can explain this.

At this point, it was proposed a new task: calculate γ value for gold and, using it, the "corrected" covalent radius and then, compare this new radius with the experimental value. The γ value for gold (Z = 79), calculated using Eq. (2) is 1.224. So, the "relativistic corrected" radius is 131.5 pm, is very good (+ 1.2%) agreement with the experimental value (130 pm) [5].

The same procedure was applied to group 12 elements: Zn (120 pm) and Cd (140) pm, providing the equation: $r = 1.111\,Z + 86.667$. The extrapolated covalent radius to Hg (Z = 80) is 176 pm, and the "corrected" value (γ value for mercury = 1.232) of 143 pm, is in good (+8.3%) agreement with the experimental value (132 pm).

This comparison between "extrapolated" and "relativistically corrected" covalent radius with the experimental values was a fundamental aspect of the work. That is, it is necessary to the student to verify that relativistic correction really provides better results, and such better results are the "proof" that the scientific method requires.

As a final task, the students have to apply the same previous procedure to the noble gases. The covalent radius (pm) to Ne (62), Ar (101), Kr (116) and Xe (136) leaves to the equation: $r = 1.485\ Z + 59.934$. Such an equation gives to Rn ($Z = 86$) a calculated radius of 187.6 pm. For radon, $\gamma = 1.285$ and the "corrected" radius is 146 pm, which is, exactly, the experimental value (!) [5].

This last example was chosen and used as a classroom task to the students to show that, even when the periodic trend is the expected (in this case, the covalent radius increases down the group), the covalent contribution matters.

REFERENCES

1. Einstein, A., Zur Elektrodynamik bewegter Körper, Annalen der Physik, 1905, 17, 891.
2. Leszczynski, J. (Ed.), Relativistic methods for chemists, Springer, New York, 2010.
3. Dyall, K.G., Faegri Jr., K., Introduction to relativistic quantum chemistry, Oxford University Press, Oxford, 2007.
4. Aruja, R. et al., Relativity and the lead-acid battery, Phys. Rev. Lett., 2011, 106, 018301.
5. http://www.rsc.org/periodic-table (accessed Jun 2017).