THE "FIRST MOLECULE": $He^{-}H^{+}$ AS A THEME TO STUDY CHEMICAL BONDING BY MOLECULAR MODELING

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ABSTRACT

In April 2019, it was reported [3] the detection (for the first time, in the interstellar space; previous detections were in the lab) of a species that is considered the very first molecule formed in the universe: $He^{-}H^{+}$(formed about only 100,000 years after the big bang). It was the beginning of chemical synthesis, and, of course, chemistry. In the present work it is reported as such chemical species can be employed as a very good theme to study chemical bonding by using molecular modeling. *[African Journal of Chemical Education—AJCE 10(1), January 2020]*

INTRODUCTION

As previously reported [1,2] molecular modeling can be a very powerful tool to be employed as a didactical/pedagogical resource, since it allows, for example, to study chemical bonding and chemical structure in an easy and ludic approach.

By molecular modeling, bond angles, lengths and energies can be "measured", and the student can "feel" such properties and not just having to believe the data that appears in the textbooks. Of course, different theoretical approach can provide different results and to discuss such differences and to decide what approach is reliable for a given system, also enlarge so much the quality of the chemical learning.

In April 2019, it was reported [3] the detection (for the first time, in the interstellar space; previous detections were in the lab) of a species that is considered the very first molecule formed in the universe: He-H^+(formed about only 100,000 years after the big bang). It was the beginning of chemical synthesis, and, of course, chemistry. In the early Universe, the reaction $He + H^+ \rightarrow HeH^+ + h\nu$ dominates HeH^+ formation [3].

In the present work it is reported as such chemical species can be employed as a very good theme to study chemical bonding by using molecular modeling.

METHODOLOGY

H-H, H-H^+ and He-H^+ were modeled at Hartree-Fock G-311 + G** level of theory. The obtained results were employed to illustrate the use of molecular modeling as a didactical tool to enhance the understanding of the chemical bond formation and properties.

RESULTS AND DISCUSSION

The obtained results are summarized in Table 1.

Table 1: Molecular modeling results.

Species	Bond length/pm	Löwdin Bond order	E_{homo}/eV	E_{lumo}/eV	Dipole moment/D	Electrostatic charge
$He\text{-}H^+$	78	0.35	-44.33	-7.23	0.7	He (0.318) H (0.682)
$H\text{-}H^+$	105	0.11	-30.08	-7.62	0.0	H(0.5) H(0.5)
H-H	74	0.51	-16.22	4.55	0.0	H(0.0) H(0.0)

The reliability of the chosen theoretical approach can be verified by using H_2 molecule as "standard": the H-H bond dissociation energy: 4.52 eV [4] is in very good agreement to the calculated lumo energy: 4.55 eV.

$He\text{-}H^+$ and the hydrogen molecule (H-H) have some similarities: two bonded atoms, a system with two nucleus and two electrons. As can be verified, the calculated bond lengths are very close. However, the negative lumo energy calculated to $He\text{-}H^+$ shows that such species is "avid" to receive electrons (what explain its high reactivity).

The calculated infrared spectrum to $He\text{-}H^+$ is shown in Figure 1. A single band at 3195 cm^{-1} (due to the He-H bond stretching vibration mode) is verified. The same band is also Raman active (Figure 2). In the same spectral range, H_2 does not exhibit any calculated IR band, in agreement with an experimental value of 4161.16 cm^{-1} to the H-H stretching mode [5].

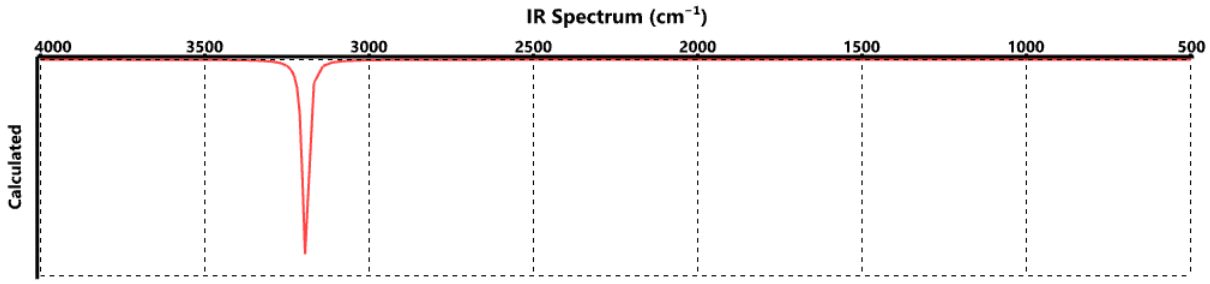

Fig. 1. Calculated infrared spectrum to He-H^+

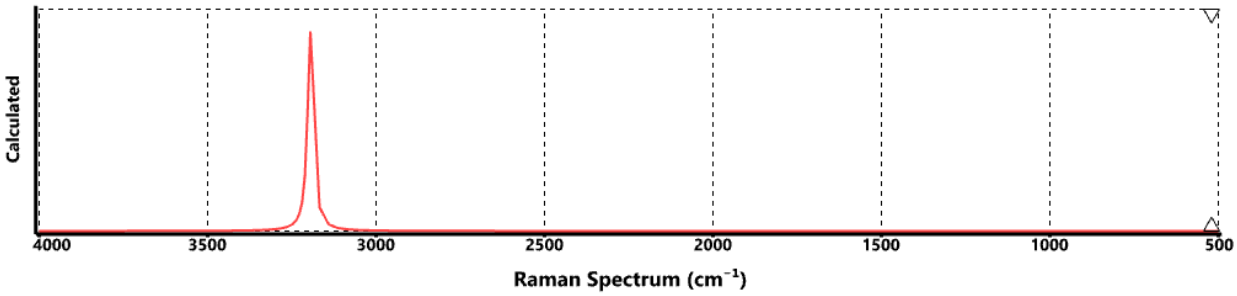

Fig. 2. Calculated Raman spectrum to He-H^+

Hence, He-H^+ and H-H can be easily differentiated by using such calculated spectroscopic data.

Furthermore, if He-H^+ has a vibrational mode active simultaneously in IR and Raman, it means that it has not an inversion centre, in agreement with the point group for which it belongs (C_{iv}). It can also be concluded that such vibration changes its dipole moment (IR) and polarizability (Raman).

The fact that in He-H^+ the larger positive (electrostatic) charge is on the hydrogen atom is in agreement with a larger electronegativity to He (4.16) than to H (2.30) in up to date Pauling scale values [6].

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