Topological Study of the H_3^{++} Molecular System: H_3^{++} as a Cornerstone for Building Molecules during the Big Bang

by

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Abstract

The present study is devoted to the possibility that tri-atomic molecules were formed during or shortly after the Big Bang. For this purpose we consider the ordinary H_3^+ and H_3 molecular systems and the primitive tri-atomic molecular system, H_3^{++}, which, as is shown, behaves differently. The study is carried out by comparing the topological features of these systems as they are reflected through their non-adiabatic coupling terms. Although H_3^{++} is not known to exist as a molecule, we found that it behaves as such at intermediate distances. However this illusion breaks down as its asymptotic region is reached. Our study indicates that whereas H_3^+ and H_3 dissociate smoothly, the H_3^{++} does not seem to do so. Nevertheless, the fact that H_3^{++} is capable of living as a molecule on *borrowed* time enables it to catch an electron and form a molecule via the reaction $H_3^{++} + e \rightarrow H_3^+$ that may dissociate properly:

$$H_3^+ \rightarrow \begin{cases} H^+ + H_2 \\ H + H_2^+ \end{cases}$$

Thus, the two unique features acquired by H_3^{++}, namely, that it is the most primitive system formed by three protons and *one* electron and topologically, still remain for an instant a molecule, may make it the sole candidate for becoming the *cornerstone* for creating the molecules.