

Looking for prebiotic species in space: a theoretical study of molecular structures of interest for the origin of life

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Abstract. The simplest possible species containing the peptide bond, $\text{NH}_2\text{-CH=O}$, was identified in space more than thirty years ago (Rubin *et al.* (1971)). About the same time, a precursor of the peptide bond, HNCO , was also identified (Snyder *et al.* (1972)) and later confirmed (Brown (1981)) in the interstellar medium (ISM). The same molecule has been recently observed in the comets Hyakutake (Lis *et al.* (1997)) and Hale-Bopp (Lis *et al.* (1998)). More elaborate material, including the 20 aminoacids present in living organisms (Cooper *et al.* (1992)), has only been found associated with solids, namely in the meteorites collected on Earth, not in the ISM.

Before designing complex chemical models for astrobiology, we considered the two following questions: *i*) what is the relative stability of the peptide bond compared to other types of bonds? *ii*) what is the relative stability of aminoacids compared to other possible isomers?

In order to be able to perform calculations at the same level of theory for all compounds, whatever the size, we employed a unique approach based on the B3LYP formulation of density functional theory (DFT). Vibrational frequencies have been calculated for asserting the nature of the stationary points and evaluation of zero-point energy corrections.

A systematic investigation of the structure and relative stability of all the isomers that may possibly form in the six atom system $[\text{C}, 3\text{H}, \text{N}, \text{O}]$ has been carried out. The most stable compound is formamide, $\text{NH}_2\text{-CH=O}$, i.e. the one with the peptide bond. The same study was done for the systems where one of the heavy atoms C, N or O is replaced by its second row analogue. From this comprehensive study it can be concluded that the species containing the peptide type of linkage are the most stable, namely: $\text{NH}_2\text{-SiH=O}$ and $\text{NH}_2\text{-CH=S}$. The exception is $\text{CH}_3\text{-P=O}$ that is more stable than $\text{PH}_2\text{-CH=O}$.

The same type of study has been performed on glycine, that is the simplest α aminoacid that has been identified in chondrites of the CM and CI types. All possible isomers of prebiotic interest have been considered. The calculation of the energies of formation showed that glycine is not the most stable compound of the family. This results holds for alanine with respect to its isomers.

From the present numerical simulations, it can be deduced that the peptide bond is particularly stable and may be more general than originally thought; it is coherent with observation of formamide in various objects and may explain why other isomers have not yet been observed. It has also been shown that glycine and alanine are not the most stable compounds of their families, which may explain why glycine has not yet been found in the ISM.

Keywords. astrochemistry, astrobiology, molecular data, ISM: molecules

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