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Towards new potential strategies for biosignatures detection: correlating the physico-chemistry and complexity of amino acids from deep space

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Abstract

Amino acids are high priority targets in the search for life elsewhere in the Universe. However, the wide range of amino acids from abiotic synthesis as revealed from meteoritic findings suggest that amino acids are not unambiguous indicators of life. More fundamental concepts as complexity of molecules are recently being proposed for new strategies for biosignatures detection. Here we present a study, based on quantum chemistry modelling, of the possible link between spectroscopic quantities, a complexity measure, a chirality descriptor and H-bonding network properties for amino acids of the isoleucine series, found in Antarctic meteorites, which are either involved in protein synthesis, featured in human plasma, or external to our biosphere.

1. Introduction

With the observation of liquid water and active geology on the Jupiter's moon Europa and Saturn's moon Enceladus, water ice in the shallow subsurface of Mars, and the expected increase in the number of observed exoplanets, planetary exploration is making fundamental steps in the search for life beyond Earth [1]. However, current strategies for biosignatures detection can be affected by the underlying assumption that life elsewhere in the Universe would be based on a chemistry similar to the terrestrial one.
Being the building units of proteins, amino acids are high priority targets in the search for biosignatures. However, meteoritic samples exhibit a large set of amino acids, most of them unknown to our biosphere [2,3], suggesting that amino acids are not unambiguous indicators of life. Recently, concepts as "complexity" are being proposed for the development of new strategies for biosignatures detection, with no assumption on the underlying biology [4,5].

1.1 Selected amino acids and Computational approach

We analyze the properties of the α-amino acids from the isoleucine series [2-amino3-methylpentanoic acid, CH_3CH_2-$CH(CH_3)$-$CH(NH_2)$-COOH]. Isoleucine contains two chiral C atoms and exists as two distinct compounds based on the spatial orientation of the substituents at those C atoms. The isomer with absolute configuration S at both carbons is the α-amino acids L-isoleucine (L-Ile), used for the proteins synthesis. Its enantiomer is D-isoleucine, and its diasteroimer is D-alloisoleucine (D-allo, with opposite chirality only at one C atom), both not found in living organisms. The enantiomer of the latter is L-alloisoleucine, not involved in protein synthesis but featured in plants and human plasma.
Structural and electronic properties have been calculated with Density Functional Theory (DFT) and employing also higher methods to obtain more accurate ionization potential (IP) and electron affinity (EA) for the gas phase molecules and their forms as extracted from the solids. A complexity measure (from Lopez-Ruiz, Mancini, Calbet [6], C_{LMC}) based on the Shannon entropy of the electronic distribution (a general measure of randomness of the distribution) and on the disequilibrium of the distribution (quantifying the departure from uniformity), H-bond properties and a chirality index (Continuous Chirality Measure, CCM measuring the distance from the closest achiral object), have been calculated.

2. Results

The results show that for L-isoleucine and D-alloisoleucine, the forms extracted from the condensed phase (Fig. 1b,c and Fig. 1e,f), which are more similar to the ones acquired in a liquid

fisiological solution, have lower gap (distance in energy between occupied and uncopied states, determining reactivity, polarizability and spectroscopic properties) with respect to the gas phase molecules (Fig. 1a and Fig. 1b) and that their complexity is higher (see Fig. 2). Complexity is not always correlated in a straightforward manner to the chirality index. L-isoleucine exhibits slightly higher complexity and acquires a higher chirality degree upon condensation when averaging over forms A and B in the condensate. In the context of molecular configurations, entropy is the degree of symmetry (in an ensemble of molecular configurations or in relation to the electronic distribution) and information is the degree of non symmetry. On the basis of order/entropy arguments, L-isoleucine would allow to store more information than D-alloisoleucine, despite a simpler H-bond pattern.

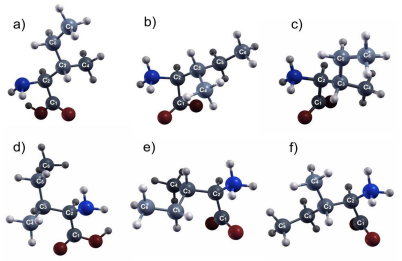

Figure 1: a) L-isoleucine in the gas phase; b) and c) forms of L-isoleucine in the condensed phase; d) D-alloisoleucine in the gas phase; e) and f) forms of D-alloisoleucine in the condensed phase

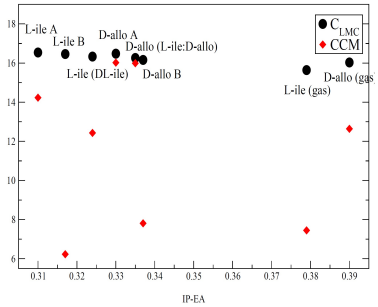

Figure 2: Complexity C_{LMC} and Chirality CCM vs the gap values for L-isoleucine and D-allosioleucine in the condensed and gas phase (a.u. are used).

3. Summary and Conclusions

The results show intriguing correlations among properties of the (few) amino acids here considered and might serve to design new strategies for biosignatures detection, allowing for a mean to score known and unknown amino acids on a universal complexity, electronic, bonding properties scale. A threshold might be identified in the relationship entropy/disorder and electronic properties, expressing propensity for charge transfer, beyond which complex molecules are unlikely to support the development of a full biological machinery. At fixed computational effort, this approach can be used for a large groups of molecules, also for those for which spectroscopic lines are not known.

Acknowledgements

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