Theoretical Study of Hydrogenation Reactions of Amino Acids Precursors in the Interstellar Medium: An Analysis Based on the Reaction Force

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Based on the experimentally determined network of hydrogenation processes of hydrogen cyanide (HCN) into methylamine (CH_3NH_2)[1], in this research we study the mechanisms of hydrogenation of precursors needed in the amino acids formation reactions that takes place in the interstellar medium. Using high level ab-initio calculations and theoretical descriptors of the electronic and structural activity taking place during a chemical reaction, a detailed characterization of the mechanisms involved in the different steps of the hydrogenation are provided.

The study is based upon the reaction force analysis[2,3] and takes advantage of the partition of the reaction coordinate into reaction regions where different mechanisms might be taking place. The reaction mechanisms are elucidated through the characterization of the evolution along the intrinsic reaction coordinate of various structural and electronic properties. The reaction electronic flux[4] is used to characterize the electronic activity that drives the reactions. Characterization of transition states, the physical nature of potential energy barriers and the specific interactions driving the reaction mechanisms are produced.

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1. Theule P., Borget F., Mispelaer F., Danger G., Duvernay F., Guillemin J. C., Chiavassa T. A&A 534, A64 (2011).
2. Toro-Labbé, A. J. Phys. Chem. A 103, 4398 (1999).
3. Gutiérrez-Oliva S., Díaz S., Toro-Labbé A., Lane P., Murray J. S., Politzer P. Mol. Phys. 112, 349 (2014).
4. Cortés-Arriagada D., Gutiérrez-Oliva S., Herrera B., Soto K., Toro-Labbé A. J. Chem. Phys. 141, 134701 (2014).