

Accepted Manuscript

Influence of a graphene surface on the first steps of the hydrogenation of a coronene molecule

S. Morisset, N. Rougeau, D. Teillet-Billy

PII: S0009-2614(17)30436-0

DOI: <http://dx.doi.org/10.1016/j.cplett.2017.05.004>

Reference: CPLETT 34793

To appear in: *Chemical Physics Letters*

Received Date: 14 March 2017

Accepted Date: 2 May 2017

Please cite this article as: S. Morisset, N. Rougeau, D. Teillet-Billy, Influence of a graphene surface on the first steps of the hydrogenation of a coronene molecule, *Chemical Physics Letters* (2017), doi: <http://dx.doi.org/10.1016/j.cplett.2017.05.004>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Influence of a graphene surface on the first steps of the hydrogenation of a coronene molecule

S. Morisset*, N. Rougeau, D. Teillet-Billy

Institut des Sciences Moléculaires d'Orsay, ISMO, CNRS, Université Paris-Sud, Université Paris Saclay, F-91405 Orsay, France

Abstract

The first steps of the hydrogenation of a coronene molecule deposited on a graphene surface is investigated using Density Functional Theory including a van Der Waals functional. Binding energies and geometries are calculated. The role of the surface is determined by comparing hydrogenation reactions in the gas phase and on the surface. The radical product of the H with a closed-shell system is more stable on the surface. The closed-shell product of the H with a radical species is more stable in the gas phase. This can be interpreted in terms of electronic and geometrical properties of these hydrogenated species.

1. Introduction

The presence of Polycyclic Aromatic Hydrocarbons (PAH) in the InterStellar Medium (ISM) has been suggested many years ago [1, 2, 3]. PAHs can be seen as large molecules or as small grains. They may represent 5 to 10 % of the carbon in the ISM [4]. Neutral PAHs are thought to exist as gas phase species [5] and condensed on interstellar dust grains [6]. In the ISM, numerous infrared bands are generally assigned to PAHs and related species [7] but they have not been attributed to particular species.

Molecular hydrogen is the most abundant molecule in the ISM. H_2 plays an important role in the chemistry of the ISM. The H_2 formation is catalysed by silicated or carbonaceous dust grains. H_2 can be formed on small grains or PAHs [8]. The H_2 formation in the photodissociation regions proceeds through an Eley-Rideal mechanism [9]: a H atom coming from the gas phase can abstract a H atom from the superhydrogenated PAHs to form H_2 .

Therefore, the study of the hydrogenation of PAH is essential for understanding H_2 formation.

*Corresponding author

Email address: `sabine.morisset@u-psud.fr` (S. Morisset)

Download English Version:

<https://daneshyari.com/en/article/5378082>

Download Persian Version:

<https://daneshyari.com/article/5378082>

[Daneshyari.com](https://daneshyari.com)