

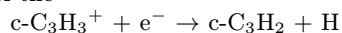
A Quantum Chemical Study of the Dissociative Recombination of $C_3H_3^+$ The Formation of Interstellar C_3H_2

Talbi D.

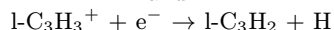
Laboratoire d'Etudes Théorique des milieux extrêmes, Muséum National d'Histoire Naturelle,
57 rue Cuvier, Case Postale 52, 75231 Paris cedex 05, FRANCE
email: talbi@mnhn.fr

Abstract. Quantum chemical calculations: Talbi & all (1993), Talbi & Ellinger (1998), Hickman & all (2005) have proven to be extremely useful for the understanding of electronic dissociative recombination processes (hereafter DR). Such processes may occur by direct and/or indirect mechanism; while the former involves a direct transition from the ionic state to the final neutral dissociative state, the second one is a two step process involving the formation of a vibrationally (rotationally) excited state of the neutral molecule. For this last case, either autoionization takes place or the state obtained after binding of the electron relaxes to lower energy states, leading if they have a dissociative character, to fragmentation of the molecule. Understanding such processes requires the knowledge of the potential energy surfaces governing the corresponding mechanism i.e. the potential energy surfaces of the ionic, excited and dissociative states of the parent neutral molecule. The difficulty in treating such problems resides in, first of all, the description of excited and dissociative states along the dissociative coordinate. This is not a trivial task because, very often, the nature of the states changes along such channels; carefully designed wavefunctions are thus necessary to follow those transformations. But the difficulty is also in the even handed treatment required for all the states involved in the mechanism. State of the art ab-initio quantum chemical methods are needed for a quantitative study of this kind of processes. To illustrate this matter, a quantum chemical investigation undertaken on the DR of the ion thought to be the source of the ubiquitous linear and cyclic C_3H_2 in diffuse and dense clouds : the $C_3H_3^+$ ion, will be presented

Our quantum chemical study of the



and



processes shows that while, for the first process, there is an efficient curve crossing (i.e for $v=0$) between the ionic state of $c-C_3H_3^+$ and the corresponding repulsive state leading to the formation of $c-C_3H_2$, for the second process, the crossing between the ionic and the repulsive curve (leading to the $l-C_3H_2 + H$ fragments) of $l-C_3H_3^+$, occurs for an excited vibrational state of the ion. It can therefore be suggested that the DR of $C_3H_3^+$ in its ground vibrational state, should be more efficient for the cyclic isomer than for the linear one.

This result will be presented in relation to the available experimental data (Abouelaziz & all (1993), Nigel & Babcock (2005)), and will be discussed within the astrophysical context.

Keywords. astrochemistry, molecular processes, ISM: molecules, ISM: abundances, etc.

References

- Abouelaziz, H., Gomet J.C., Pasquerault D. Rowe B.R. & Mitchell, J.B.A. 1993, *J. Chem. Phys.* 98, 1
Hickman, A.P., Miles, R.D., Hayden, C. & Talbi, D. 2005, *Astron. Astrophys.* in press

Nigel, G.A. & Babcock, L.M. 2005, *J. of Phys. Conference Series* 4 38, 49

Talbi, D. & Ellinger, Y. 1998, *Chem. Phys. Letters* 288, 155

Talbi, D., Hickman A.P., Pauzat, F. Ellinger, Y. & Berthier, G. 1989, *Astrophys. J.* 339, 231