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Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares

Conferencia: Chemical Reaction Dynamics: Unimolecular Dissociation at Different Time Scales

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16/04/15

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Aula de Seminarios do CIQUS

12:15 h

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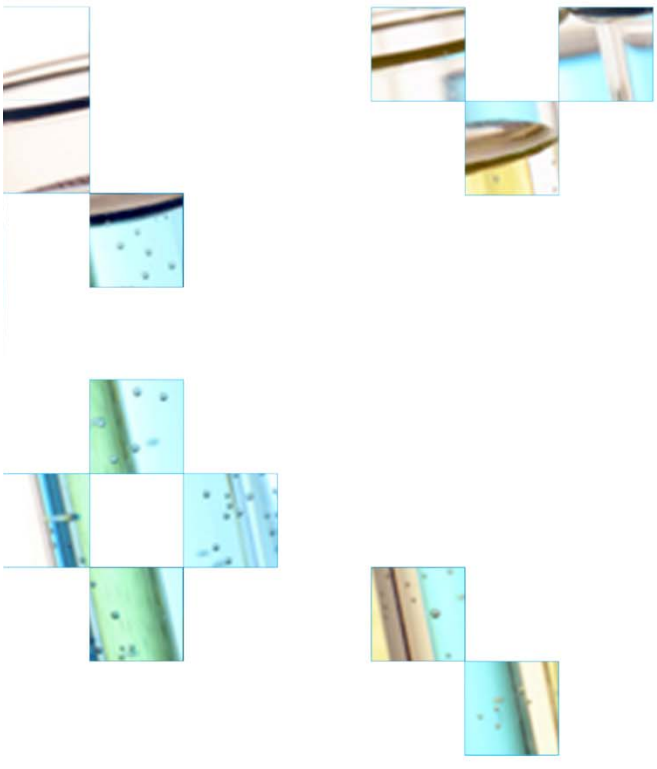

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Chemical Reaction Dynamics: Unimolecular Dissociation at Different Time Scales

In this seminar I shall present how chemical dynamics can explain reactivity in gas phase of different systems from relatively small to large biomolecules.

First, by coupling chemical dynamics simulations with RRKM theory, it was possible to understand the complex gas phase reactivity of different molecular ions. As a prototypical example, I will discuss the collision induced dissociation (CID) of complexes formed by Ca^{2+} or Sr^{2+} with formamide. There are, as expected, many similarities between the reactivity exhibited by Sr^{2+} and Ca^{2+} complexes [1,2]. Some of these similarities and differences could be rationalized by analyzing the topology of the respective potential energy surfaces (PESs) through the use of density functional theory calculations. On the contrary other observations cannot be understood from the PES.

One example is the loss of formamide observed as a dominant process which is not possible to explain in terms of the topology of the PES, and which can arise from non-statistical processes. Hence we have carried out a kinetic analysis of the processes by using a RRKM formalism [3] as well as chemical dynamics simulations of ion-Ar collisions to mimic collision induced dissociation (CID) experiments[4]. In particular from dynamics we were able to: (1) understand the formation of high energy products observed in experiments formed on short time scales (< 2 ps); (2) use the energy transfer distributions obtained in chemical dynamics in the RRKM equations to obtain products on longer time-scales (ns and μs).

The combination of both non-statistical and statistical reaction mechanisms at different time-scales lead to the full understanding of CID experiments and of the difference between the two systems. This approach will give some theoretical basis to set up a strategy to obtain theoretical tandem mass spectrometry spectra that will be useful to better resolve analytical identification of complex systems, like peptides and carbohydrates.

References

1) A. Eizaguirre, O. Mó, M. Yáñez, J.-Y. Salpin, Phys. Chem. Chem. Phys. 13, 18409 (2011)
2) A. Eizaguirre, O. Mó, M. Yáñez, J.-Y. Salpin, J. Tortajada, J. Org. Biomol. Chem. 10, 7552 (2012)
3) A.Martin-Somer, M.-P.Gaigeot, M.Yanez and R.Spezia. Phys. Chem. Chem. Phys. 16, 14813-14825 (2014).
4) A.Martin-Somer, M.Yanez, M.-P.Gaigeot and R.Spezia. J. Phys. Chem. A 118, 10882-10893 (2014).

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Professional Preparation

2000	Laurea (M.S.), Chemistry, Università di Roma "La Sapienza", Italy
2004	Ph.D., Chemistry, Università di Roma "La Sapienza", Italy
2004-2005	Postdoctoral Fellow, Ecole Normale Supérieure, Paris, France
2005-2006	Postdoctoral Fellow, Université d'Evry-Val-d'Essonne, France
2012	Habilitation, Université d'Evry-Val-d'Essonne, France

Academic/Professional Appointments

2006-2010	Junior (CR2) CNRS researcher in Theoretical Physical Chemistry, LAMBE UMR8587, Université d'Evry-Val-d'Essonne, France
2009	Visiting Scientist, HPC-Europa fellowship, Department of Physics, Università di Roma "La Sapienza", Italy.
2009	Visiting Scientist, Texas Tech University, USA.
2010	Visiting Scientist, University of Minnesota, USA.
2011	Visiting Scientist, Korea National University of Education, Korea.
2010-present	Senior (CR1) CNRS researcher in Theoretical Physical Chemistry, LAMBE UMR 8587, Université d'Evry-Val-d'Essonne

Synergistic Activities

• Co-head of the team "Interactions in complex molecular assemblies: theory and simulations", LAMBE, Université d'Evry-Val-d'Essonne (6 permanent researchers).
• PI of the young researchers ANR project 'ACtinoids and LAnthanoids SOLVation" involving 6 permanent researchers from Evry, ENS-Paris, CEA and Université de Nice. (January 2011 – August 2014).
• Responsible of seminars of the UMR 8587 LAMBE, Université d'Evry-Val-d'Essonne.
• PI of the project "Dissociation mechanisms of oligosaccharides in gas phase from molecular dynamics" supported by LABEX CHARMMMAT (2013-2014).
• PI of the ANR-NSF project (with W.L.Hase PI for NSF) DynBioReact, involving 8 permanent researchers from Evry and Texas Tech University (January 2015 – …).