



Chemistry in Titan's ionosphere : towards a realistic ion-neutral coupled model

S. Plessis (1,2), N. Carrasco (3), P. Pernot (1,2)

(1) Laboratoire de Chimie Physique, CNRS, UMR 8000, Orsay, F-91405, (2) Université Paris-Sud 11, Orsay, F-91405, (3) Service d'Aéronomie, CNRS, IPSL, Université de Versailles Saint Quentin, BP 3, Verrières le Buisson, F-91371

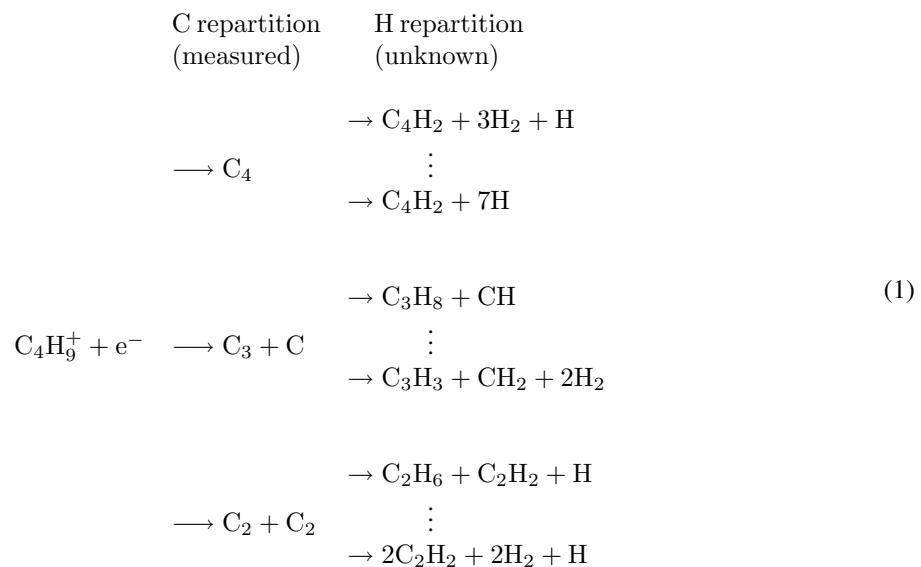
Modelling the chemical composition of Titan's ionosphere is a very challenging issue. Latest works perform either inversion of CASSINI's INMS mass spectra (neutral[1] or ion[2]), or design coupled ion-neutral chemistry models[3].

Coupling ionic and neutral chemistry has been reported to be an essential feature of accurate modelling[3]. Electron Dissociative Recombination (EDR), where free electrons recombine with positive ions to produce neutral species, is a key component of ion-neutral coupling. There is a major difficulty in EDR modelling: for heavy ions, the distribution of neutral products is incompletely characterized by experiments. For instance, for some hydrocarbon ions only the carbon repartition is measured, leaving the hydrogen repartition and thus the exact neutral species identity unknown[4]. This precludes reliable deterministic modelling of this process and of ion-neutral coupling.

We propose a novel stochastic description of the EDR chemical reactions which enables efficient representation and simulation of the partial experimental knowledge.

The description of products distribution in multi-pathways reactions is based on branching ratios, which should sum to unity. The keystone of our approach is the design of a probability density function accounting for all available informations and physical constrains. This is done by Dirichlet modelling which enables one to sample random variables whose sum is constant[5]. The specifics of EDR partial uncertainty call for a hierachiral Dirichlet representation, which generalizes our previous work[5].

We present results on the importance of ion-neutral coupling based on our stochastic model.



References

- [1] J. Cui, R.V. Yelle, V. Vuitton, J.H. Waite Jr., W.T. Kasprzak, D.A. Gell, H.B. Niemann, I.C.F. Müller-Wodarg, N. Borggren, G.G. Fletcher, E.L. Patrick, E. Raaen, and B.A. Magee. Analysis of Titan's neutral upper atmosphere from Cassini ion neutral mass spectrometer measurements. *Icarus*, In Press, Accepted Manuscript:–, 2008.
- [2] V. Vuitton, R. V. Yelle, and M.J. McEwan. Ion chemistry and N-containing molecules in Titan's upper atmosphere. *Icarus*, 191:722–742, 2007.
- [3] V. De La Haye, J.H. Waite Jr., T.E. Cravens, I.P. Robertson, and S. Lebonnois. Coupled ion and neutral rotating model of Titan's upper atmosphere. *Icarus*, 197(1):110 – 136, 2008.
- [4] J. B. A. Mitchell, C. Rebrion-Rowe, J. L. Le Garrec, G. Angelova, H. Bluhme, K. Seiersen, and L. H. Andersen. Branching ratios for the dissociative recombination of hydrocarbon ions. I: The cases of $C_4H_9^+$ and $C_4H_5^+$. *International Journal of Mass Spectrometry*, 227(2):273–279, June 2003.
- [5] N. Carrasco and P. Pernot. Modeling of branching ratio uncertainty in chemical networks by Dirichlet distributions. *Journal of Physical Chemistry A*, 11(18):3507–3512, 2007.