

# Excitation and fragmentation in high velocity $C_nN^+$ - He collisions

T.Mahajan<sup>†</sup>, T.Id Barkach<sup>\*</sup>, N.F.Aguirre<sup>‡</sup>, M.Alcami<sup>‡</sup>, M.Bonnin<sup>†</sup>, M.Chabot<sup>\*</sup>, S.Diaz-Tendero<sup>‡</sup>, F.Geslin<sup>\*</sup>, T.Hamelin<sup>\*</sup>, F.Hammache<sup>\*</sup>, C.Illescas<sup>‡</sup>, A.Jallat<sup>\*</sup>, A.Jorge<sup>‡</sup>, T.Launoy<sup>§</sup>, T.K.C.Le<sup>†</sup>, A.LePadellec<sup>‡</sup>, F.Martin<sup>‡</sup>, A.Meyer<sup>\*</sup>, L.Perrot<sup>\*</sup>, T.Pino<sup>†</sup>, B.Pons<sup>#</sup>, N. de Séréville<sup>\*</sup>, K.Béroff<sup>†1</sup>

<sup>†</sup>Institut des Sciences Moléculaires d'Orsay, CNRS- Univ.Paris-Sud F-91406 Orsay, France

<sup>\*</sup>Institut de Physique Nucléaire d'Orsay, CNRS- Univ.Paris-Sud F-91405 Orsay, France

<sup>‡</sup>Departamento de Química Universidad Autónoma de Madrid, 28049 Madrid, Spain

<sup>§</sup>Laboratoire de Chimie Quantique et Photophysique Univ Libre de Bruxelles, CP160/09 1050 Bruxelles, Belgium

<sup>†</sup>Institut de Recherche en Astrophysique et Planétologie, CNRS-INP Univ. Toulouse 3 F-31028 Toulouse, France

<sup>#</sup>CELIA Univ.Bordeaux CNRS UMR 5107 CEA 351 Cours de la Libération, 33405 Talence, France

**Synopsis:** We will present measurements and modeling for two aspects of the  $C_nN^+$  - He collisions ( $n=1-3$ ,  $v=2.25$  a.u) : cross sections for electronic excitation processes and fragmentation branching ratios for the excited and ionized  $C_nN^{q+}$  molecules produced in the collision ( $q=-1,0,1,2-5$ ).

The study of molecule-atom collisions is a difficult topic, both from the experimental and theoretical point of views. In the high velocity regime, mostly small molecular systems have been studied [1]. On the other hand, the so-called Independent Atom and Electron (IAE) model was applied recently with reasonable success to  $C_n^+-He$ , Ar systems with state of the art CTMC and SCAOCC P(b) probabilities [2]. We will test this approach again in this work.

Fragmentation of the excited molecular system is another topic of interest. In high velocity collisions ( $\tau_{coll}\sim 10^{-16}$ s) it occurs well after the excitation and can be treated separately. The MMMC approach and its new more general version M3C [3] is dedicated to treatment of statistical fragmentation. The systems studied here belong typically to this class of fragmentation [4]. We will ultimately compare our experimental fragmentation branching ratios (BR) to predictions of this statistical approach.

Experiments have been performed at the Tandem accelerator in Orsay with beams of  $C_nN^+$  molecular ions ( $n=1-3$ ) of constant velocity  $v=2.25$  a.u colliding with helium atoms. The setup is identical to the one described in [5] (see also Jallat et al, this conference). Briefly the setup allows to reconstruct, from fragments complete collection and identification in charge and mass, the charge  $q$  of the projectile after the collision, signature of the process. An example is given in Table 1 for the case of double electron capture ( $q=-1$ ) in the  $C_2N^+$  - He collision where contribution of various channels to the  $\{C_2N^-\}$  production is reported.

We will present two types of results. First experimental cross sections for various electronic processes will be presented and compared to predictions of the IAE + CTMC calculations. These calculations will use structure calculations for  $C_nN^+$  systems that we performed. Second, fragmentation BR for  $C_nN^{q+}$  species with  $q=-1,0,1,2,3-5$  will be presented. In addition to the fundamental aspects discussed before, these BR are also of interest in astrochemistry as already pointed out [6]. Note than  $C_nN$  species, on their neutral and anionic forms, have been detected in interstellar medium [7] and planetary atmospheres [8].

**Table 1** Measured fragmentation BR of  $\{C_2N^-\}$  species produced by double electron capture in the collision  $C_2N^+$  - He ( $v=2.25$  a.u).

| Channel       | Exp. BR     | Error |
|---------------|-------------|-------|
| $C_2N^-$      | 0.40        | 0.04  |
| $CN^- + C$    | 0.51        | 0.06  |
| $C^- + CN$    | 0.07        | 0.02  |
| $C_2^- + N$   | $\leq 0.01$ |       |
| $C^- + C + N$ | 0.020       | 0.012 |

## References

- [1] H.Luna et al PRA 93, 052705 2016
- [2] G.Labaigt et al JPB 48, 075201 2015
- [3] N.F. Aguirre et al JCTC to appear 2017
- [4] G. Martinet et al 93, 063401 2004
- [5] T. Launoy et al PRA 95, 022711 2017
- [6] M. Chabot et al ApJ 771 :90 2013
- [7] M.Agundez et al Chem.Tev 113, 8710 2013
- [8] V.Vuitton et al Planet. Space Sc. 57, 1558 2009

<sup>1</sup>E-mail: [karine.beroff@u-psud.fr](mailto:karine.beroff@u-psud.fr)