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

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

[†] Institut des Sciences Moléculaires d'Orsay, CNRS- Univ.Paris-Sud F-91406 Orsay, France
[*]Institut de Physique Nucléaire d'Orsay, CNRS- Univ.Paris-Sud F-91405 Orsay, France
[¤]Departamento de Quimica Universidad Autonoma de Madrid, 28049 Madrid, Spain
[§]Laboratoire de Chimie Quantique et Photophysique Univ Libre de Bruxelles, CP160/09 1050 Bruxelles, Belgium
[‡]Institut de Recherche en Astrophysique et Planétologie, CNRS-INP Univ. Toulouse 3 F-31028 Toulouse, France
[#]CELIA Univ.Bordeaux CNRS UMR 5107 CEA 351 Cours de la Libération, 33405 Talence, France

We studied the collision between C_nN^+ molecules (n=1-3) and Helium atoms at high velocity (v=2.25 a.u). Cross sections for various electronic processes (excitation, ionization, electron capture) were measured as well as dissociation branching ratios of excited (ionized) molecules. Modeling of the collision within the IAE (Independent Atom and Electron) and CTMC (Classical Trajectory Monte Carlo) approaches is performed. Interpretation of dissociation branching ratios is in progress.

Experimental set-up and methods

AGAT set-up at the Tandem accelerator in Orsay

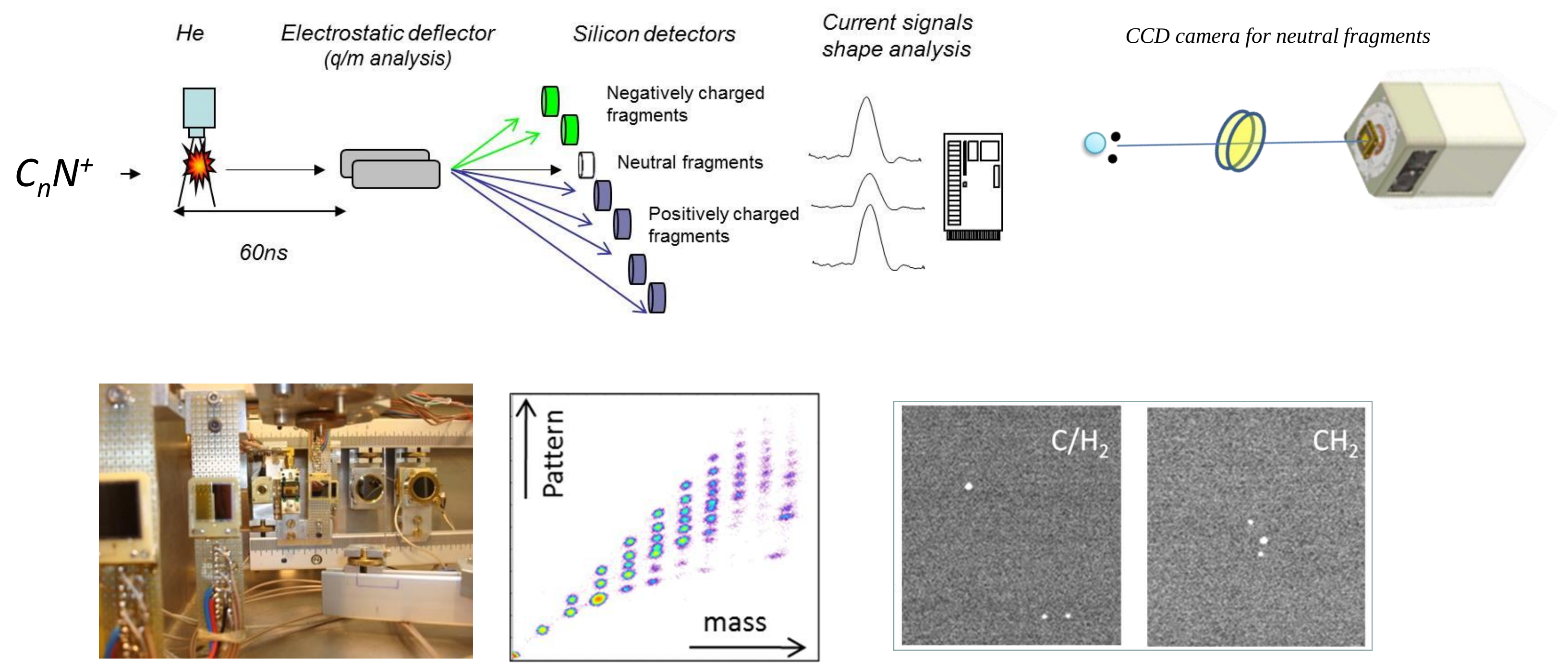


Figure 1: View of the detectors (left). Fragmentation resolution by current shape analysis (middle) or using an X-ray thinned CCD camera (right, illustration for CH_2 fragmentation)

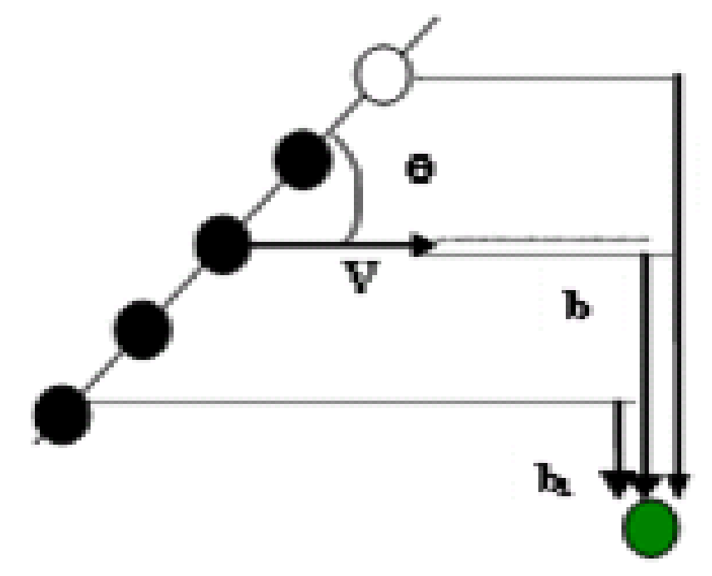
Collisions between v=2.25 a.u C_nN^+ projectiles and He target have been studied. Cross sections associated to a given electronic process are obtained by summing many channels. For instance single ionization cross section of C_2N^+ was derived by summing the nine relaxation channels of $\{C_2N\}^{++}$ whose relative probabilities (Branching Ratios BR) are presented in Table 1. The shape analysis, illustrated in Figure 1 (middle), was used for fragmentation resolution of neutrals but was not sufficient to separate some channels (for instance CN/C from C_2/N) because C and N have very close shapes. We then used a position sensitive detector, namely an X-ray thinned CCD camera, to resolve these cases [1]. There is an illustration of the fragmentation resolution with the camera in Figure 1 (right).

Channel	BR exp	Err abs BR
C_2N^{++}	0.082	4 e-3
CN^+/C^+ C_2^+/N^+ CN/C^{++} C_2/N^{++}	0.476 0.041 1.15 e-3 1.87 e-4	4.6 e-2 2 e-3 1.3 e-4 5.8 e-5
$C/\{CN^{++}\}$ $N/2C^+$ $C/N/C^{++}$ $2C/N^{++}$	0.216 0.174 7.7 e-3 1.25 e-3	3.3 e-2 1 e-2 3.9 e-4 9.3 e-5

Table 1: Relaxation channels of $\{C_2N\}^{++}$
with their measured Branching Ratio (BR exp)

Theoretical description of the collision

The independent atom and electron (IAE) model



$$P_{C_n^+\to C_n}(\mathbf{b}) = \sum_{i=1}^{n} P^{(1)}_{\text{capt}}(b_i) \times \prod_{i=1}^{n}\left(1 - P_{\text{ion}}(b_i)\right) \prod_{j\neq i}\left(1 - P_{\text{capt}}(b_j)\right) + \left[\sum_{i=1}^{n} P^{(2)}_{\text{capt}}(b_i) + \sum_{i=1}^{n}\sum_{j>i} 2P^{(1)}_{\text{capt}}(b_i)P^{(1)}_{\text{capt}}(b_j)\right] \times \left[\sum_{i=1}^{n} P^{(1)}_{\text{ion}}(b_i)\prod_{j\neq i}\left(1 - P_{\text{ion}}(b_j)\right)\right], \qquad (1)$$

Figure 2: Principle of the model (left) and derivation of the projectile neutralization probability (right)

Calculation of underlying atom(ion)-atom collision probabilities

Classical trajectory Monte Carlo (CTMC) calculations have been performed in the case of the C, C^+, N, N^+ -He collisions. For electron capture by the projectile, one active electron of He was placed in the field of two frozen model potentials optimized so as to reproduce binding energies and electron radial densities of the target and (projectile+electron) systems. For projectile ionization two types of calculations were performed : a first one, with a single active electron using the e-He potential of [2] (referred to as model V1), and a second one, with one active electron on both projectile and target (referred to as model 2e). In all cases 2s and 2p electrons of projectile were treated separately.

The atom (ion)-atom impact parameter probabilities

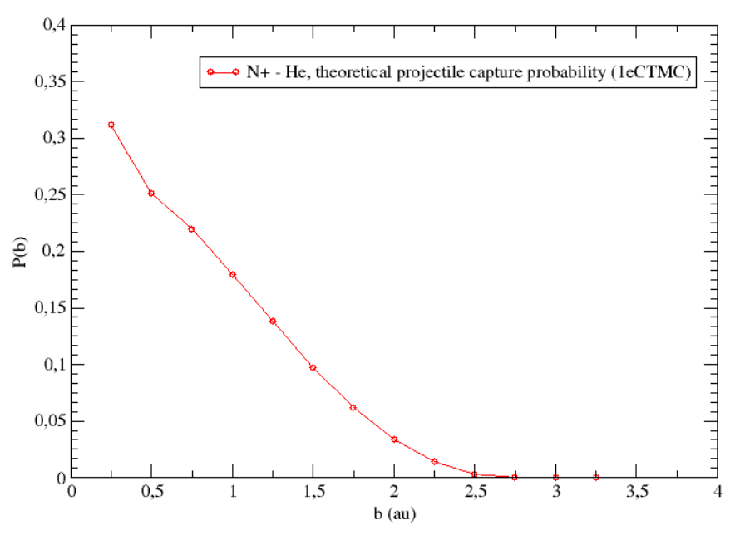


Figure 3: P(b) versus b for electron capture by N^+

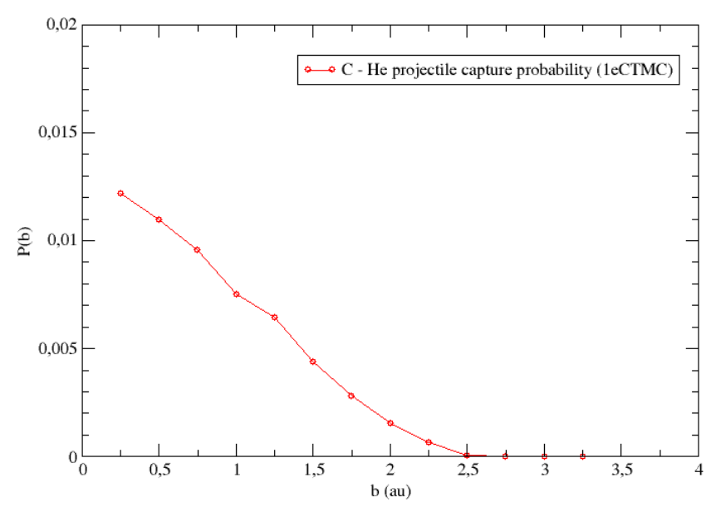


Figure 4: P(b) versus b for attachment of an electron on C

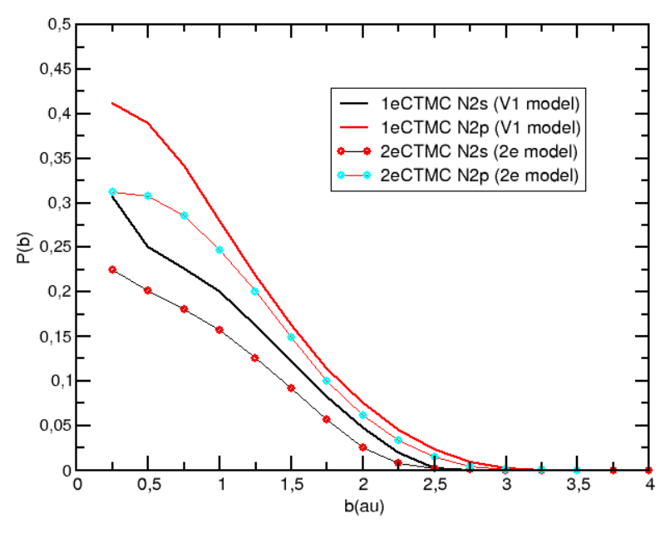


Figure 5: P(b) versus b for N 2s and N 2p ionization

Some results of CTMC calculations are shown in Figures 3-5. In Figure 3 electron capture by N^+ is shown. The probability is very close to the one obtained for electron capture by C^+. By contrast electron capture by a neutral projectile (*i.e.* attachment) is much smaller for the case of C (see Figure 4). Electron capture by N was not considered as N^- is not stable. In Figure 5 are shown the 2s and 2p ionization probabilities in N for the two types of calculations: 2e and V1. Results with V1 are always much higher than their 2e counterparts. Similar results were obtained for N^+, C and C^+.

Comparison between measured and calculated cross sections

Projectile Neutralization

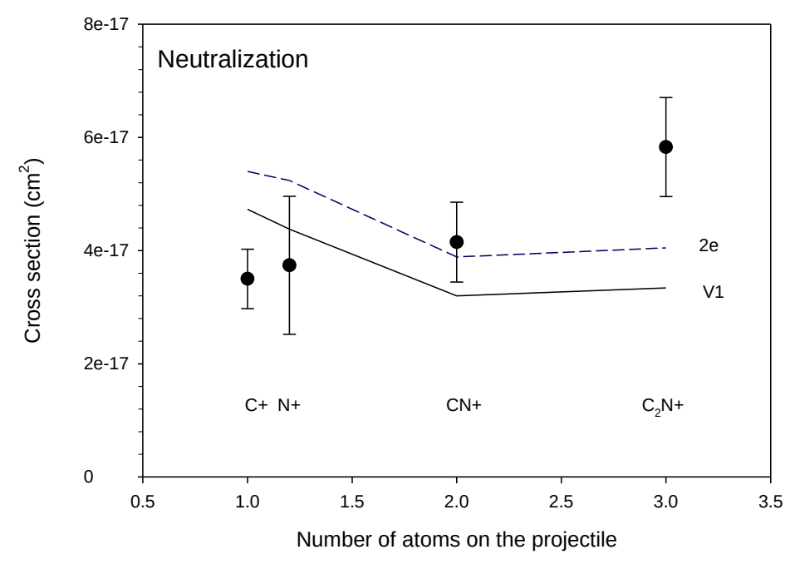


Figure 6: Measured and calculated neutralization cross sections in C^+, N^+, CN^+, C_2N^+ - He collisions. Projectile probabilities entering in the neutralization formula were calculated with the 2 model (broken line) and one electron V1 model (solid line).

Projectile Ionization

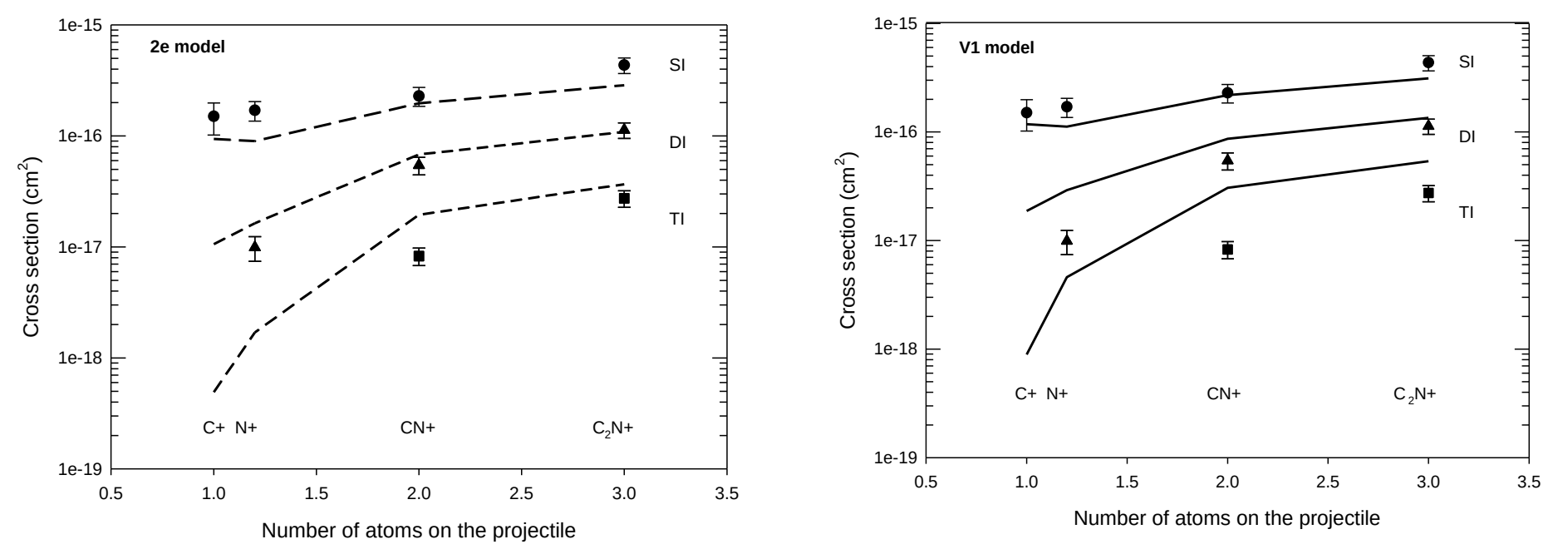


Figure 7: Measured and calculated projectile single, double and triple ionization cross sections in C^+, N^+, CN^+, C_2N^+ - He collisions. Projectile probabilities were calculated with the 2 electrons (2e) model (left) and one electron (V1) model (right).

Comparison between measured and calculated cross sections are shown in Figure 6 for neutralization and Figure 7 for projectile ionization. The agreement is pretty good with the 2e model.

Fragmentation Branching Ratios

channel	BR exp (err.abs)	Eform. (eV)	BR(Nf) (err.abs)
C2N	0.36 (0.02)	-	
CN/C	0.45 (0.02)	4.95	
C2/N	0.10 (0.01)	6.88	
C/C/N	0.09 (0.02)	12.98	
Σ Nf=2			0.55 (0.01)

Table 2: Measured fragmentation BR of C_2N

channel	BR exp (err.abs)	Eform. (eV)	BR(Nf) (err.abs)
CN/C+	0.218 (0.015)	6.48	
C/CN+	0.145 (0.007)	8.96	
C2/N+	0.025 (0.002)	11.76	
N/C2+	0.086 (0.004)	8.96	
C/C/N+	0.112 (0.005)	17.87	
C/N/C+	0.414 (0.03)	14.51	
Σ Nf=2			0.474 (0.028)
Σ Nf=3			0.526 (0.035)

Table 3: Measured fragmentation BR of C_2N^+

channel	BR exp	Err abs BR
C_2N^-	0.40	0.04
CN^-/C	0.51	0.06
C^-/CN	0.07	0.02
C_2^-/N	8 e-3	8 e-3
$C^-/C/N$	0.02	0.01
Σ Nf=2	0.59	0.09

Table 4: Measured fragmentation BR of C_2N^-

In Tables 2-4 are reported measured fragmentation BR for respectively neutral, singly charged and anionic C_2N. Whereas the branching ratios in number of fragments provide information on the energy deposit, BR of individual channels constitute stringent tests of statistical fragmentation theory such as the M3C one [3]. Theoretical work on theses systems is currently in progress, following previous work on carbon clusters [4] and hydrocarbon molecules [5].

[1] A.Jallat et al, this conference
[2] P.Valiron et al JPB (1979)
[3] N.Aguirre et al JCTC (2017)
[4] G.Martinet et al PRL (2004)
[5] to be submitted