# The New View of comet coma processes after Rosetta; The Importance of Electrons



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# The new view of comet coma processes after Rosetta: The importance

# of electrons

### Comenius University; Bratislava, Slovakia, May 24 to 26 2017 Hotel Sorea Regia, Bratislava

#### Wednesday May 24;

19.30 Arrive Social function welcome

| Thursday May   | Thursday May 25;  |  |  |  |
|----------------|---|--|--|--|
| Session 1      | Data from the Rosetta mission   |  |  |  |
| 09.00 to 09.45 | Opening and Introductory talk   |  |  |  |
|                | Rosetta observations of electron impact dissociative emission in the coma |  |  |  |
|                | of 67P  |  |  |  |
|                | Dennis Bodewits, University of Maryland, USA                              |  |  |  |
| 09.45 to 10.30 | The organics on the nucleus of 67P as revealed by COSAC                   |  |  |  |
|                | Jan Bredehöft, University of Bremen, Germany                              |  |  |  |
| 10.30 to 11.00 | Coffee  |  |  |  |
| 11.00 to 11.45 | Ground based observations of 67P  |  |  |  |
|                | Colin Snodgrass, The Open University, UK                                  |  |  |  |
| 11.45 to 12.30 | Observations of two CMEs inside the 67P comet coma and upstream of the    |  |  |  |
|                | comet   |  |  |  |
|                | Annie Wellbrock, University College London, UK                            |  |  |  |
| 12.30 to 13.00 | Electron-impact ionization and excitation around comet 67P                |  |  |  |
|                | Kevin Heritier, Imperial College London                                   |  |  |  |
| 13.00 to 14.00 | Lunch   |  |  |  |
| 14.00 to 14.45 | Observing Electron Impact Excitation of Cometary Comae from the Ground    |  |  |  |
|                | Alan Fitzsimmons, Queens University of Benast, UK                         |  |  |  |
| Session 2      | Electron collision processes in cometary environments                     |  |  |  |
| 14.45 to 15.30 | Review of relevant electron processes for comets                          |  |  |  |
|                | Nigel Mason, The Open University, UK                                      |  |  |  |
| 15.30 to 16.15 | Electron/molecular cation collisions in comet comas from reactional       |  |  |  |
|                | mechanisms to rate coefficients   |  |  |  |
|                | Ioan Schneider, University of le Havre, France                            |  |  |  |
| 16.15 to 16.45 | Tea   |  |  |  |
| 16 45 to 17 30 | Electron Induced emission spectra of molecules in the UV-Vis range        |  |  |  |
| 10.45 to 17.50 | Štefan Mateičík, Comenius University, Bratislava, Slovakia                |  |  |  |
| 17.30 to 18.00 | Electron Collision cross section and resonant states in HNCO              |  |  |  |
|                | Juraj Fedor, J Heyrovsky Institute of Physical Chemistry, Prague          |  |  |  |
| 17.30 to 18.00 | Electron-CO vibrational-resolved cross sections                           |  |  |  |
|                | Vincenzo Laporta, University of le Havre, France                          |  |  |  |
| 10.00          |   |  |  |  |
| 19.00          | worksnop ainner   |  |  |  |

# Friday May 26;

| <u>Session 3</u> |   |
|------------------|---|
| 09.00 to 09.45   | Electron and ion driven processes is cold clusters  |
|                  | Paul Scheier, University of Innsbruck   |
| 09.45 to 10.30;  | Electron attachment to astrophysically relevant molecules   |
| ,                | Thomas Field, Queen's University of Belfast, UK   |
| 10.30 to 11.00   | Coffee  |
| 11.00 to 11.30   | Reactive collisions of electrons with CO and $H_2^+$ in cometary coma   |
|                  | Youssef Moulane, University of le Havre, France   |
| 11.30 to 12.00   | Electron Impact Excitation data for H <sub>2</sub> O, N <sub>2</sub> O and H <sub>2</sub> S triatomic molecules |
|                  | Bratislav Marinković, Institute of Physics Belgrade, Serbia   |
| 12.00 to 12.30   | Low energy electron attachment to aminoacetonitrile and cyanamide   |
|                  | Stefan Denifl, University of Innsbruck  |
| 12.30 to 13.00   | Electronic excitation and neutral dissociation of ground and metastable   |
|                  | states of oxygen molecule and electron impact ionisation of metastable  |
|                  | states  |
|                  | James Hamilton, University College London and Quantemol ltd, UK   |
|                  |   |

13.00 to 14.00 Lunch

**Break out Session** 14.00 to 15.45 D Data needs

15.45 to 16.15 Tea

16.15 Lab tours

#### **Reactive collisions of electrons with CO<sup>+</sup> and H<sub>2</sub><sup>+</sup> in cometary coma**

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In order to improve our understanding of the kinetics of the cometary coma, a theoretical study of the major reactive collisions in these environments is nowadays needed. In the collisional inner cometary coma, the production of various species in ground state, but also in several excited states, is partly due to inelastic collisions between the thermal electrons and the molecular ions, namely the dissociative recombination (DR)/dissociation and vibrational excitation (VE)/de-excitation (VdE) [1]. The aim of our work is to reveal the importance of these reactive collisions, focusing on CO + and H2 + . The DR of CO + is expected to be a major source of excited C(1D) atoms [2], whose emission has been detected in the Hale–Bopp comet [3]. We have computed the DR and the VE/VdE cross sections using a method based on Multichannel Quantum Defect Theory (MQDT) [4-7] and eventually the corresponding Maxwell rate coefficients. We will present their variation with the cometocentric using an electron temperature profile inferred from the observations of the Giotto Neutral Mass Spectrometer on Halley's coma [8].

[1] Larsson, M., Geppert, W. D., & Nyman, G. 2012, Reports on Progress in Physics, 75, 066901

- [2] Raghuram, S., Bhardwaj, A., & Galand, M. 2016, ApJ, 818, 102
- [3] Oliversen R J, Doane N, Scherb F, Harris W M and Morgenthaler J P 2002, ApJ. 581 770-5
- [4] Epée Epée M. D., Mezei J. Z., Motapon O., Pop N., Schneider I. F., 2016, MNRAS, 455, 276

[5] J. Zs. Mezei et al, 2015, Plasma Sources Science and Technology, 24, 035005

[6] Schneider I. F., invited talk to this meeting

[7] Moulane et al 2017, article in preparation

[8] Eberhardt, P. & Krankowsky, D. 1995, A&A, 295, 795

#### Electron Impact Excitation data for H20, N20 and H2S triatomic molecules

#### Bratislav Marinkovic

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Triatomic molecules that have been investigated by electron collisions in Laboratory for Atomic Collision Processes at the Institute of Physics Belgrade comprise several different classes of such molecules: C2v symmetry molecules H<sub>2</sub>O, D<sub>2</sub>O and H<sub>2</sub>S [1]; linear C $\infty v$ molecule N<sub>2</sub>O [2]; D $\infty$ h molecules NO<sub>2</sub>, CO2 and CS<sub>2</sub> [3] and Cs molecule SO<sub>2</sub> [4]. The excitation processes have been studied by electron energy loss spectroscopy and threshold electron spectroscopy (when residual electron energy is close to zero). For some of the excited states the angular behaviour has been investigated and these states are characterised by differential cross sections. The main advantage of electron spectroscopy over synchrotron radiation or other types of optical spectroscopy is that the optically forbidden states are more pronounced in electron spectra. Another type of distinct features in electron spectra are resonances, i.e. peaks that arise from temporary negative ions formed in the process of collision. To fully model electron scattering process, one needs to know energy loss spectrum and the energy and angular behaviour of cross sections  $DCS(\varepsilon,\theta)$ . Energy loss spectra and DCSs for H<sub>2</sub>O, H<sub>2</sub>S and N<sub>2</sub>O molecules will be presented.

[1] D. S. Belić and M. Kurepa, Fizika, 17 (1985) 117; B. Marinković Thesis (1985); N. Lj. Durić, et al. Int. J. Mass Spectr. Ion Proc. 83 (1988) R7; Gy. Vikor and M. Kurepa, J. Serb. Chem. Soc. 60 (1995) 199; J. Jureta EPJD 32 (2005) 319.

[2] D. Cubić Thesis (1985); B. Marinković Thesis (1985); B. Marinković et al. J. Phys. B 19 (1986) 2365; 32 (1999) 1949; D Cubric et al., J. Phys. B 19 (1986) 4225.

[3] D. S. Cvejanović et al. J. Phys. B 18 (1985) 2541; D Lukić et al. Int. J. Mass Spectr. 205 (2001) 1.

[4] I. Čadež et al. J. Phys. D: Appl. Phys. 16 (1983) 305.

#### Low energy electron attachment to aminoacetonitrile and cyanamide

#### Stefan Denifl University of Innsbruck

Aminoacetonitrile as well as cyanamide are relevant molecules in interstellar chemistry and the chemical evolution of life. In the present study we investigated electron attachment to these compounds in the gas phase. Ion yields of formed anions were studied as function of the initial electron energy and resonance energies for the most abundant fragment anions were determined. No long-lived parent anion was observed for both compounds.

#### <u>Electronic excitation and neutral dissociation of ground and metastable states of oxygen</u> <u>molecule and electron impact ionisation of metastable states</u>

James Hamilton University College London and Quantemol ltd, UK

Molecular oxygen was recently detected in the coma of comet 67P by Bieler et al. (2015). Despite the ubiquity of oxygen in the universe many holes still persist in the data we have of molecular oxygen. A 2016 "Workshop on Oxygen Plasma Kinetics"[1] specifically identified a dearth in the data regarding the role of metastable states and electron impact cross sections for dissociation and electronic excitation. The radiative lifetime of the first metastable state of  $O_2$ ,  $O_2(a \ ^1\Delta_g)$ , has a lifetime of over 1 hour, see, for instance, Newman *et al.* (1999) and Miller *et al.* (2001), and is therefore very influential in any system containing  $O_2$ . According to selection rules excitation of  $O_2$  by photon impact from ground to metastable states is forbidden and therefore the creation of these states in a system is an electronic phenomenon. In this talk cross sections are presented and discussed for electron impact dissociation with and electronic (super)excitation of ground state  $O_2$ ,  $O_2(X \ ^3\Sigma^+{}_g)$ , along with metastable states of  $O_2$ ,  $O_2(a \ ^1\Delta_g)$  and  $O_2(b \ ^1\Sigma^+{}_g)$ . Quenching and electron impact ionisation cross sections of the metastable states are also presented.

Bieler, A. et al. Nature 526, 678–681 (2015) Newman, S. M. et al. J.J. Chem.Phys. ,110, 10749 (1999) Miller, H. C. et al. J. Quant. Spectrosc. Radiat. Transfer, 69, 305 (2001) [1] http://langmuir.raunvis.hi.is/~tumi/wox.html

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