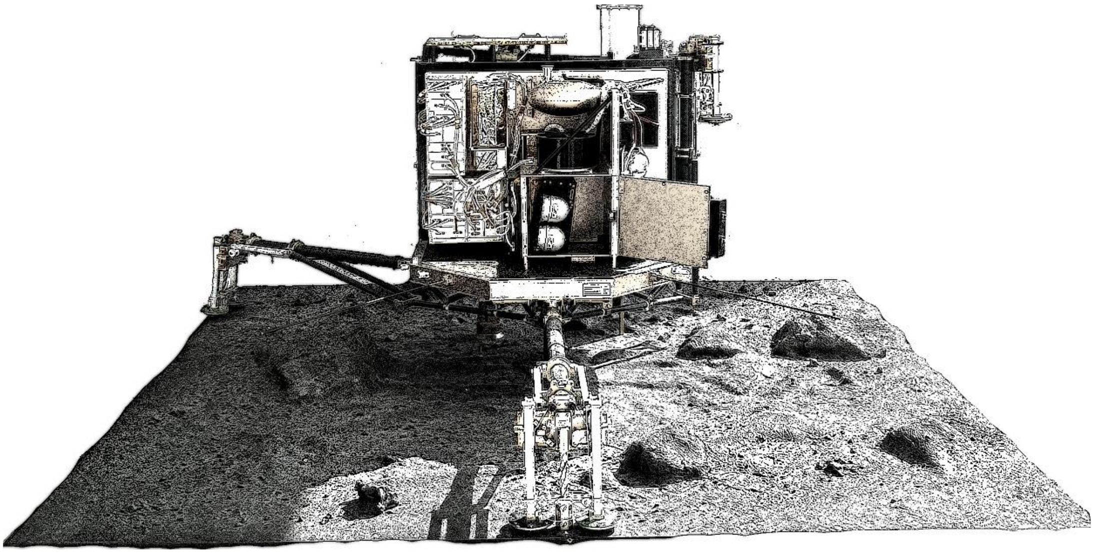
The New View of comet coma processes after Rosetta: The Importance of Electrons



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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 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 Belfast, 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 **Štefan Matejčík**, 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
19.00	***Workshop dinner***

Friday May 26;

Session 3

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_2O, N_2O and H_2S 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	Data needs
15.45 to 16.15	***Tea***
16.15	**Lab tours**

Rosetta observations of electron impact dissociative emission in the coma of 67P

Dennis Bodewits
University of Maryland in College Park.

Rosetta orbited comet 67P between August 2014 and September 2016, exploring a regime not accessible before: the inner coma of a medium-activity comet at a large range of heliocentric distances. The Wide Angle Camera (WAC) of the OSIRIS instrument on board the Rosetta spacecraft was equipped with several narrowband filters that are centered on the emission lines and bands of various molecules and ions. Our observations allowed us to study changes in the physical environment of the inner coma with respect to heliocentric distance and at a broad range of activity levels. I will present the results of our observations and review the status of cross sections needed for further interpretation of electron impact reactions in cometary atmospheres.

The organics on the nucleus of 67P as revealed by COSAC

Jan Hendrik Bredehöft
University of Bremen, Institute for Applied and Physical Chemistry

In November 2014 the ROSETTA spacecraft successfully deployed its lander Philae to the surface of comet 67P/Churyumov-Gerasimenko[1]. In the following 63 hours, the 10 instruments on-board provided a wealth of ground-truth data of the composition and properties of the comet nucleus. Among the instruments, the COmetary Sampling and Composition (COSAC)[2] instrument took mass spectra of the gas phase evolved from the dust that the landing kicked up[3]. In these spectra, 16 small organic molecules have been identified, some of which had not previously been seen in comets. The complexity and richness of the identified chemistry is shown in the various inter-relations between the molecules found on the nucleus. They are not arbitrary organic molecules but a large family of related species that are formed in reactions with one another.

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[2] Goesmann F et al. (2007) Space Science Reviews 128:257-280.
[3] Goesmann F et al. (2015) Science 349(6247):aab0689.

Ground based observations of 67P

Colin Snodgrass
School of Physical Sciences, The Open University, UK

I will present a summary of observations of comet 67P, and in particular gas observations. I'll discuss the potential influence of electron impact chemistry on these observations. I will also discuss observations of other comets, and how electron interactions influence these.

Observations of two CMEs inside the 67P comet coma and upstream of the comet

Annie Wellbrock
University College London, UK

We use a radiation environment monitor on-board Rosetta to identify Solar Energetic Particle (SEP) events arriving at 67P in order to study the effects on the conditions deep inside the comet coma. We also use the identified SEP events to find other associated solar transient events such as Coronal Mass Ejections (CMEs) or Corotating Interaction Regions (CIRs). In this presentation we show March & April 2015 observations of the effects of two CMEs on the plasma conditions inside the comet coma using the Rosetta Plasma Consortium. We also identify these CMEs upstream of the comet using the STEREO and MESSENGER missions. We highlight the significance of changing conditions in the comet coma as a result of solar transient events which can remove neutrals, increase ionisation rates and cause dust charging.

Electron-impact ionization and excitation around comet 67P

K.L. Heritier[1], M. Galand[1], P. Henri[2], A. Eriksson[3], E. Odelstad[3], K. Altwegg[4], A. Beth[1], T.W. Broiles[5], J. Burch[5], C. Carr[1], E. Cupido[1], K.-H. Glassmeier[6], H. Nilsson[7], I. Richter[6], M. Rubin[4], X. Valličres[1], E. Vigren[3]
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[7]*Swedish Institute of Space Physics, Kiruna, Sweden.*

The Rosetta spacecraft escorted comet 67P for two years and assessed the evolution of the cometary coma throughout a wide range of heliocentric distances. In-situ measurements by the Rosetta instruments gave us a unique opportunity to assess the local electron population and its interaction with the neutral coma. The neutral number density was continuously measured by Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA)/Cometary Pressure Sensor (COPS). The suprathermal electron fluxes were measured with Rosetta Plasma Consortium (RPC)/Ion and Electron Sensor (IES), corrected in energy to take in account the negative spacecraft potential measured by RPC/Langmuir Probe (LAP). The suprathermal electron flux can be used to compute ionization and dissociative excitation rates through electron-impact with cometary neutrals. Another source of ionization is the solar Extreme UltraViolet (EUV) radiation. Both ionization rates are implemented into a ionospheric model to estimate the total number of cometary ions as a function of the cometocentric distance. The results present excellent agreement with the in-situ measurements of electron densities performed by RPC/Mutual Impedance Probe (MIP), cross calibrated with RPC/LAP. During most of Rosetta's escort phase, electron-impact ionization is the dominant ionization source and is enhanced over the winter hemisphere. As the solar activity has decreased since the beginning of the mission in 2014, the relative importance of photo-ionization has decreased as well. However, at low heliocentric distances (<1.5 AU), photo-ionization seems to be the most dominant ionizing source, in particular through the perihelion period, from July to September 2015.

Observing Electron Impact Excitation of Cometary Comae from the Ground.

Alan Fitzsimmons
Queens University of Belfast, UK

One of the many highlights of the Rosetta mission was the discovery of the important role of electron impacts in the excitation of cometary gases. Feldman et al. (2015) and Bodewits et al. (2016) found that the near-nucleus brightness distribution of various atomic and molecular species was only explainable by electron impact dissociation. At the same time, it is clear that the vast majority of Earth-based comet observations are consistent with normal photodissociation models coupled with simple photon scattering. We have made commenced some ad-hoc calculations of electron-impact dissociation models of comae brightness distributions, to assess whether ground-based detection of this process is feasible. We will present initial findings at this meeting.

Review of relevant electron processes for comets

Nigel Mason
School of Physical Sciences, The Open University, UK

The role of electron processes in cometary processes has been highlighted by results from the Rosetta mission but what is the status of our knowledge of relevant electron interactions with atoms molecules and ions prevalent in cometary atmospheres? What is the status of our knowledge of electron interactions with the ices on the cometary body and how they may fashion local chemistry and molecular synthesis? In this talk I will present an overview of our knowledge of such processes and how such knowledge may be expanded, both through experiment and theory, such that physical and chemical models of cometary systems may be developed. 'Grand challenges' facing both the cometary and electron scattering communities will be suggested with the aim to provide debate in this workshop.

Electron/molecular cation collisions in comet comas from reactional mechanisms to rate coefficients

Ioan Schneider
University of le Havre, France

Electron-driven reactions induced on molecular positive ions contribute to the chemical kinetics of the comet comas. We will outline the multichannel aspect of these reactive collisions and the role of the super-excited states in the dynamics of the dissociative recombination and of the ro-vibrational excitation. Cross sections and rate coefficients for H_2^+, CO^+, CH^+, OH^+ and other systems will we be shown and compared with experimental data, and the role of the excited target states for the kinetics will be demonstrated.

Electron Induced emission spectra of the molecules in the UV-VIS range

M. Ďurian, J. Országh and Š. Matejčík
Comenius University Bratislava, Faculty of Mathematics, Physics, and Informatics, Department of Experimental Physics, Mlynská dolina F-2, 842 48 Bratislava, Slovakia

The fundamental data regarding the electron – molecule interactions are of vital interest in several fields of science such as plasma physics, astrophysics, radiation chemistry, etc. The Electron Induced Fluorescence technique is a suitable instrument which can be applied to explore such processes as electronic excitation and dissociative excitation of molecules as well as other electron interactions associated with emission of photons (electron ionisation). We are going to present this technique and several examples of electron molecule interactions of potential interest for the astrophysical community.

Electron collision cross sections and resonant states in HNCO

Juraj Fedor
J Heyrovsky Institute of Physical Chemistry, Prague

Isocyanic acid, HNCO, is the simplest molecule containing all four basic chemical elements of life. It is abundant in interstellar space and has been detected in coma of 67P/Churyumov–Gerasimenko by the Rosetta mission. We present absolute cross sections for the dissociative electron attachment to this molecule and amend them by theoretical characterization of resonant states using the regularized-analytical continuation method. A unique interplay of two distinct dissociation processes is observed.

Electron-CO vibrational-resolved cross sections

Vincenzo Laporta
University of le Havre, France

Ab initio calculations of vibrational-resolved cross sections and rate coefficients for electron-CO scattering will be presented based on the R-matrix method. In particular, the processes of vibrational excitation, dissociative attachment and dissociative excitation will be discussed. Apart from vibration also rotation will be take into account. These cross sections are useful in kinetic modelling of CO-containing plasmas.

Electron and ion driven processes in cold clusters

M. Kuhn, J. Postler, L. Kranabetter, M. Rastogi, P. Martini, N. Gitzl, O. Echt, D.K. Bohme, S. Krasnokutski and P. Scheier
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Pickup of atoms and molecules into superfluid helium nanodroplets provides a versatile method to form complexes and clusters that represent laboratory analogs of dust particles in comets

and in cold interstellar clouds[1]. The low isothermal temperature of 0.37K and the enormous cooling rate of the helium matrix lead to the formation of isomeric structures that may be far off the global energetic minimum due to the lack of annealing processes and thus to targets that can hardly be formed by other methods in laboratories. However, in the cold interstellar medium we expect that the binding energy of a molecule, attaching to a cluster, is also released via black body radiation before the next molecule arrives which also quenches annealing.
Electron irradiation of doped helium nanodroplets leads to the formation of positively[2] and negatively[3] charged product ions that subsequently are investigated utilizing mass spectrometry and optical spectroscopy. Both electron and ion driven processes trigger complex ion-molecule reactions and the formation of new molecular species can be investigated[4].
Finally, ions tagged with helium atoms are perfect targets for messenger type spectroscopy which can be utilized to determine absorption lines of ionic species that may be carriers for diffuse interstellar bands[5].
Acknowledgement: This work was supported by the FWF (Projects P26635, W1259, I978-N20, P19073, L633) and the COST action CM1401

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5. Kuhn, M., et al., Atomically Resolved Phase Transition of Fullerene Cations Solvated in Helium Droplets. Nature Communications 2016, 7, 13550.

Electron attachment to astrophysically relevant molecules

Tom Field
Centre for Plasma Physics, School of Maths and Physics, Queen's University Belfast, UK

Experiments to investigate electron attachment to astrophysically relevant molecules will be considered. Many linear carbon chain molecules have been detected in space and the results of experiments to investigate electron attachment to two such molecules will be presented; HCCCN [1] and NCCCCN [2]. Negative ion formation is observed in the interaction of low energy electrons (<10 eV) with both of these molecules. Results of relevant theoretical calculations of electron attachment will be considered along with conclusions regarding the formation of negative ions in the interstellar medium and the role of radiative electron

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[3] Thomas J. Millar, Catherine Walsh, and Thomas A. Field. Negative Ions in Space. Chemical Reviews, 117 (2017) 1765–1795

Reactive collisions of electrons with CO^+ and H_2^+ 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].

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[5] J. Zs. Mezei et al, 2015, Plasma Sources Science and Technology, 24, 035005
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Electron Impact Excitation data for H_20, N_20 and H_2S triatomic molecules

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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_2O, D_2O and H_2S [1]; linear C∞v molecule N_2O [2]; D∞h molecules NO_2, CO2 and CS_2 [3] and Cs molecule SO_2 [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(ε,θ). Energy loss spectra and DCSs for H_2O, H_2S and N_2O molecules will be presented.

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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.

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

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)
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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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