Book of Abstracts

1st annual meeting of the MD-GAS COST Action

organized in the framework of the
COST Action CA18212 "Molecular Dynamics in the GAS phase"

18th - 21st February 2020
Caen, France

About MD-GAS

Emerging highly advanced ion-beam traps and storage rings combined with synchrotrons, X-ray facilities, and high performance computers offer completely new ways to study Molecular Dynamics in the GAS phase (MD-GAS). Cryogenic traps and rings will allow studies of decay and reaction processes involving molecular ions in well-defined conformations and in single or narrow ranges of quantum states.

The MD-GAS COST Action aims to further develop and fully exploit the exceptional potential of the above range of tools to unravel the connection between the initial energy transfer in interactions between isolated molecules or clusters and photons, electrons, or heavy particles (ions, atoms, molecules) and the related molecular dynamics in unexplored time domains ranging from sub-femtoseconds to minutes and hours.

Furthermore, the Action aims to identify reaction mechanisms and routes that lead to the growth of new molecular species, clusters and aerosols. The new knowledge will be important for fundamental atomic and molecular physics, chemical physics, and for applications in radiation therapy and -damage on the nanoscale, astrochemistry, astrobiology, atmospheric science, and climate research.

The MD-GAS COST Action is organized in three Working groups:

- New high-performance instrumentation and experimental methods to study gas phase molecular dynamics at ion-beam storage rings and traps, at synchrotrons and X-ray facilities;
- Survival and destruction of molecules following their processing by heavy particles, electrons, or photons;
- Charge-, energy flow, and molecular growth processes in intermolecular and intra-cluster reactions.

Organisation

Chair

Alicja Domaracka

Scientific committee

Paola Bolognesi	Italy
Sergio Díaz-Tendero	Spain
Alicja Domaracka	France
Marta Łabuda	Poland
Thomas Schlathölter	Netherlands
Sanja Tosić	Serbia
Henning Zettergren	Sweden

Local organising committee

Suvasthika Indrajith
Chiara Nicolafrancesco
Patrick Rousseau

Thursday 20th February 2020

09:00-09:20	*Inter- and intra-molecular interactions in uracil clusters studied by XPS*	J. Chiarinelli
09:20-09:40	*Fragmentation dynamics of ionized highly excited furan molecules: a combined theoretical and experimental approach*	E. Erdmann
09:40-10:00	*High radiative cooling rates of small clusters*	P. Ferrari
10:00-10:20	*The stability of the smallest carbon cluster dianion:* C_7^{2-}	P. Najeeb
10:20-11:00	Coffee break	
11:00-11:30	Working Group 3 Kick off Meeting - M. Alcamí	
11:30-12:00	*Ion-collision induced reactivity in molecular clusters*	P. Rousseau
12:00-12:30	*Gas-phase molecules through the lens of time-resolved photoelectron spectroscopy*	A. Ponzi
12:30-13:00	*Interaction of low energy electrons with biomolecules and clusters of biomolecules*	J. Kocisek
13:00-14:30	Lunch at the GANIL restaurant	
14:30-15:00	*Highly charged helium nanodroplets*	M. Gatchell
15:00-15:30	*Creation and destruction of chemical species in liquids treated by atmospheric pressure plasmas - from gas phase chemistry to bulk liquid*	N. Skoro
15:30-16:00	*Resonant Inelastic X-ray scattering of chloromethanes*	M. Zitnik
16:00-16:30	*Elastic electron scattering on molecules in the gas phase in the middle energy range*	J. Maljković
16:30-17:30	Coffee break	
16:30-17:30	*Laboratory visit*	
19:00-21:30	Conference diner - Café Mancel, le Château Ducal, Caen	

Abstracts of presentations

ELASTIC ELECTRON SCATTERING ON MOLECULES IN THE GAS PHASE AT MEDIUM ENERGY RANGE

J. B. Maljković[(a)1], J. Vuković[(b)], B. Predojević[(b)] B. P. Marinković[(a)]

[(a)] *Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[(b)] *Faculty of Science, University of Banja Luka, Mladena Stojanovića 2, 78000 Banja Luka, Republic of Srpska, Bosnia and Herzegovina*

We have investigated elastic electron scattering in the medium energy range from molecules in the gas phase. The measurements of the elastic differential cross sections (DCS) are performed with a cross electron-target beam apparatus UGRA [1], settled in the Institute of physics in Belgrade. Relative DCSs were normalized to the absolute scale according to points obtained using a relative flow technique. For this procedure Ar was used as a reference gas [2]. We have performed measurements for elastic electron scattering on different molecules, including anaesthetics [3], and absolute DCS for elastic electron scattering on sevoflurane at 300 eV is presented in Figure 1.

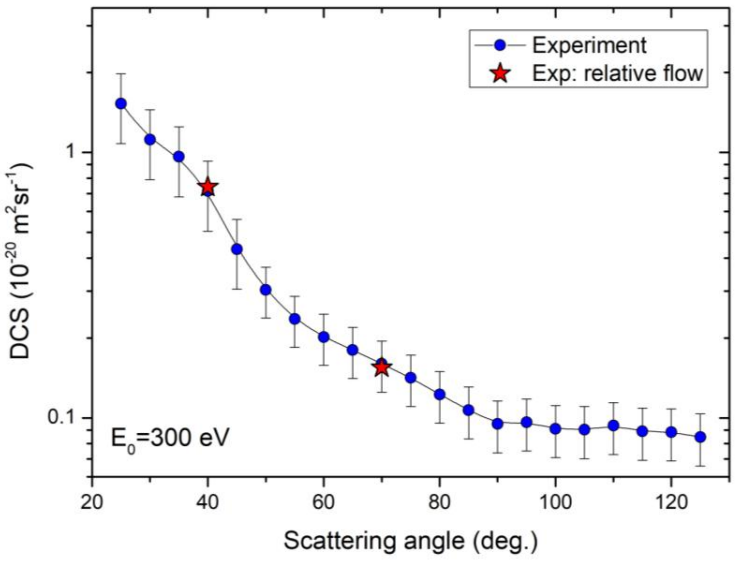

Figure 1: Angular dependence of the DCSs for elastic electron scattering from sevoflurane at 300 eV. Circles represent absolute experimental differential cross sections; stars represent absolute values obtained by relative flow method.

References

[1] A. R. Milosavljević, S. Mandžukov, D. Šević, I. Čadež, and B. P. Marinković, *J. Phys. B*, **39**, 609, (2006)

[2] M. Lj. Ranković, J. B. Maljković, K. Tökési and B. P. Marinković, *Eur. Phys. J. D* **72**, 30, (2018).

[3] J. B. Maljković, A. R. Milosavljević, Z. Pešić, F. Blanco, G. García, D. Šević and B. P. Marinković, Publ. Astron. Obs., 89, 33, (2010).

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Presentation

The 1st annual meeting of the COST Action CA18212 "Molecular Dynamics in the GAS phase" – MD-GAS – will be held in Caen (France) from Tuesday February the 18th 2020 to Friday February the 21st 2020.

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2. Survival and destruction of molecules following their processing by heavy particles, electrons, or photons;
3. Charge-, energy flow, and molecular growth processes in intermolecular and intracluster reactions.

Important dates

Registration deadline:
31/01/2020

Abstract submission deadline:
31/01/2020

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Program

Timetable

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Program > Speakers

Name	Institution	Title
Lorenzo Avaldi	CNR-ISM, Rome (Italy)	*Results and challenges of photofragmentation of molecules of biological interest*
Daniela Ascenzi	Università di Trento, Trento (Italy)	*Ion-molecule reactions of astrochemical and atmospheric interest*
Bogdan Calin	Center for Advanced Laser Technologies, Ilfov (Romania)	*Ultrafast laser fabrication of ion microtraps via multiphoton processing technologies*
Alessandra Candian	University of Amsterdam, Amsterdam (Netherlands)	*The importance of* H *(and* D*) scrambling in astronomically relevant hydrocarbon species*
Eduardo Carrascosa	École polytechnique fédérale de Lausanne, Lausanne (Switzerland)	*Unravelling isomer-specific shape and photochemistry of complex molecular ions*
Jacopo Chiarinelli	Università Roma Tre, CNR-ISM, Rome (Italy)	Synchrotron-based study of biomolecules and biomolecular clusters
Charles Desfrançois	Université Paris 13, Villetaneuse (France)	*IRMPD spectroscopy and quantum chemistry calculations on metal-ligand cluster ions*
Ewa Erdmann	Gdansk University of Technology, Gdansk (Poland)	*Fragmentation dynamics of ionized highly excited furan molecules: a combined theoretical and experimental approach*
Piero Ferrari	KU Leuven, Leuven (Belgium)	*High radiative cooling rates of small clusters*
Michael Gatchell	University of Innsbruck, Innsbruck (Austria)	*Highly charged helium nanodroplets*
Elisabeth Gruber	Aarhus University, Aarhus (Denmark)	*Excited-state lifetime measurements of stored chromophore ions*
Oded Heber	Weizmann Institute of Science, Rehovot (Israel)	*Electrostatic Ion Beam Trap: A versatile tool for studying gas phase molecular dynamics*
Ekaterina Iordanova	Bulgarian Academy of Sciences, Sofia (Bulgaria)	*Laser induced fabrication of three dimensional nanoparticle structures by femtosecond laser pulses*
Christine Joblin	CNRS, Institut de Recherche en Astrophysique et Planétologie, Toulouse (France)	*Identification and physical chemical processes of carbonaceous molecules in the ISM*
Jaroslav Kocisek	J. Heyrovsky Institute of Physical Chemistry, Prague (Czech Republic)	*Interaction of low energy electrons with biomolecules and clusters of biomolecules*
Janina Kopyra	Siedlce University of Natural Sciences and Humanities, Siedlce (Poland)	*Electron induced processes in biologically relevant molecules*
Holger Kreckel	MPIK, Heidelberg (Germany)	*Heavy ion storage rings: from magnetic to electrostatic and from room temperature to cryogenic*
Sylvain Maclot	KTH, Stockholm (Sweden)	*Dissociation dynamics of the diamondoid adamantane upon photoionization by XUV femtosecond pulses*
Jelena Maljkovic	Institute of Physics, Belgrade (Serbia)	*Elastic electron scattering on molecules in the gas phase in the middle energy range*

Emilio Martínez-Núñez	Universidad de Santiago de Compostela, Santiago de Compostela (Spain)	*Automated discovery of chemical reaction mechanisms*
Elisabetta Micelotta	Univeristy of Helsinki, Helsinki (Finland)	*Supernovae as "dust factories": grain composition, identifications, mechanism of formation and destruction*
Aleksandar Milosavljevic	Synchrotron SOLEIL, Saint-Aubin (France)	*X-ray photoelectron spectroscopy of nanocrystals for solar cells absorbers isolated in vacuo*
Chiara Nicolafrancesco	Normandie université, Caen (France)	*Energetic processing of biomolecular systems*
Steen B. Nielsen	Aarhus University, Aarhus (Denmark)	*Action and luminescence spectroscopy of biomolecular systems in the gas phase*
Alicia Palacios	Universidad Autónoma de Madrid, Madrid (Spain)	*Attosecond electron-nuclear dynamics in photoionized molecules*
Dariusz G. Piekarski	University of Munster, Munster (Germany)	*MD study on reversible folding of tetrakistriazole catalysts and their binding with anionic substrates*
Paula Pla	Universidad Autónoma de Madrid, Madrid (Spain)	*Stability and IR signatures of carbonaceous molecules*
Aurora Ponzi	Ruđer Bošković Institute, Zagreb (Croatia)	*Gas-phase molecules through the lens of time-resolved photoelectron spectroscopy*
Najeeb Punnakayathil	Stockholm University, Stockholm (Sweden)	*The stability of the smallest carbon cluster dianion:* C_7^{2-}
Patrick Rousseau	Normandie université, Caen (France)	*Ion-collision induced reactivity in molecular clusters*
Nikola Skoro	Institute of Physics, Belgrade (Serbia)	*Creation and destruction of chemical species in liquids treated by atmospheric pressure plasmas - from gas phase chemistry to bulk liquid*
Amanda Steber	DESY, Hamburg (Germany)	*Surveying fragmentation to aggregation of polycyclic aromatic hydrocarbons in multiple radiation environments*
Béla Sulik	MTA Institute for Nuclear Research (Atomki),Debrecen (Hungary)	*Ion-induced fragment emission from molecules: results, plans, new facilities*
Jelena Tamuliene	Vilnius University, Vilnius (Lithuania)	*High-energy ionizing radiation influence on the fragmentation of glutamine and valine*
Einar Uggerud	University of Oslo, Oslo (Norway)	*Proton mobility in water clusters*
Xavier Urbain	Université catholique de Louvain, Louvain (Belguim)	*Electron transfer and molecular ion formation in cation-anion reactions*
Matjaz Zitnik	Jozef Stefan Institute, Ljubljana (Slovenia)	*Resonant Inelastic X-ray scattering of chloromethanes*

ELASTIC ELECTRON SCATTERING ON THE MOLECULES IN THE GAS PHASE: aneasthetics, biomolecules, methane

Jelena Maljković

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