Ion-molecule collisions

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Ionisation and fragmentation of small molecules of biological and/or astrophysical interest by charged particle impact

2006-2008

Mechanisms leading to the formation of negative ions in collisions involving molecules of biological and/or astrophysical interest (ANIONCOL)

2012-2015

Collision-induced formation of highly reactive radicals from molecules in the gas phase 2017-2019 (running)

Partners

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Collisions of ions with atoms or molecules is essential for plasma physics, or for modeling the chemical changes in astrophysical environments and living matter. We study collision processes like:

(a few keV) O⁺ + H₂O \rightarrow O + H₂O²⁺ + e⁻ \downarrow H⁺ + OH⁺

Fundamental aspects:

Structure, dynamics

we measure the energy and angular distribution of the fragments

or or $O^+ + H_2O \rightarrow O^+ + \underline{H^-} + OH^+$ $OH^+ + Ar \rightarrow O^+ + \underline{H^-} + Ar^+$

Anions may start further reactions in the environment

Experimental setup (ARIBE, GANIL, France)

Measurement: energy & angular distributions of the emitted particles



- Ion beam from the ECR source
- Effusive atomic or molecular jet
- Electrostatic spectrometer: *E*/*q*
- Rotatable ring for the selection of angle

(The observation angle is defined with respect to the beam direction)

New experimental setup (Atomki, Debrecen)

Field free time of flight (TOF) of the fragments Especially suitable for low energy (0.1-1 eV) fragments



History: First fragmentation studies (2006-2009)

Coulomb explosion of small molecules –

angular and energy distribution of the fragments

- Juhász Z, <u>Sulik B</u>, Frémont F, Hajaji A, Chesnel JY, *Anisotropic ion emission in the fragmentation of small molecules by highly charged ion impact*, NUCLEAR INSTRUMENTS & METHODS B 267, 326-329. (2009)
- Juhász Z, Chesnel J -Y, Frémont F, Hajaji A, <u>Sulik B, Coulomb explosion and binary encounter</u> processes in collisions between slow ions and small molecules of biological interest, AIP Conf. Proc. 1080, (2009) 118,

Collisionally excited states of molecular projectiles -> new findings



FIG. 1. (Color online) Cross sections for emission of negatively charged particles at different observation angles. (a) 7-keV OH⁺ + Ar collisions. (b) 7-keV OH⁺ + acetone collisions. The curves represent electron emission, while the color-shaded peaks represent H⁻ emission. H⁻ ions emitted from OH⁺ projectiles are observed in the peak at about 300–400 eV. H⁻ emission from the acetone target results in a second peak, which appears at ~1100 eV at 30° and merges with the other peak at 60°. The multiplication factors on the right side are used only for graphical reasons.



H^{emission} from the projectile

 New proposal
 ANIONCOL project (2012-2015)



ANIONCOL: Experimental results: double-differential cross section for anions and cations

Anion spectra look quite similar to cation spectra at each angle! – Statistical model of charge state distribution

Anions can be formed in hard binary collisions.

Soft collisions (at large impact parameter) produce more ions than hard collisions.



J.-Y. Chesnel, Z. Juhász, E. Lattouf, J. A. Tanis, B. A. Huber, E. Bene, S. T. S. Kovács, P. Herczku, A. Méry, J.-C. Poully, J. Rangama and B. Sulik, Phys. Rev. A 91 (2015) 060701(R).

ANIONCOL results (2012-2015):

- Negative ion production is a general process in keV energy molecular collisions.
- For H-bearing molecules, H⁻ production follows statistical rules.
- Low energy anions are emitted in many-body processes, where excited transiens states are important.
- Juhász Zoltán, Sulik Béla, Rangama Jimmy, Bene Erika, Sorgunlu-Frankland Burcu, Frémont François, Chesnel Jean-Yves, Formation of negative hydrogen ions in 7-keV OH^{+}+Ar and OH^{+}+acetone collisions: A general process for H-bearing molecular species, PHYSICAL REVIEW A 87, 032718. 5 p. (2013)
- Lattouf E, Juhasz Z, Chesnel J -Y, Kovacs S T S, Bene E, Herczku P, Huber B A, Mery A, Poully J -C, Rangama J, Sulik B, Formation of anions and cations via a binary-encounter process in OH+ + Ar collisions: The role of dissociative excitation and statistical aspects, PHYSICAL REVIEW A 89, 062721 (2014)
- Chesnel J -Y, Juhasz Z, Lattouf E, Tanis J A, Huber B A, Bene E, Kovacs S T S, Herczku P, Mery A, Poully J -C, Rangama J, <u>Sulik B</u>, <u>Anion</u> emission from water molecules colliding with positive ions: Identification of binary and many-body processes</u>, PHYSICAL REVIEW A 91. 060701 (2015)

The running collaboration (2017-2019)

• New experimental directions: COLTRIMS,

Time of flight spectroscopy (developments),DebrecenHigher impact energies (0.5-1 MeV).Debrecen

Caen

- Fundamentally important collison systems, e.g., O²⁺ +H₂
- Theoretical developments: Classical Monte-Carlo simulations Caen
 Statistical model for the emission of all fragments Debrecen
 External collaborators in theory Madrid

Preliminary results of TOF measurement

At low fragment energy, TOF results agree with the theory; at high energy, the spectrometer results



Investigated/planned collision systems

O ⁿ⁺ +O ₂	Gas removal from Jupiter's moon Europa (escape energy 0.49 eV)	
$N^{n+}+N_2$	Titan	
O ⁿ⁺ +CO	Comets	
O ²⁺ +H ₂	Theory	
O ⁺ +H ₂ O	Radiobiology	

H⁺ +H₂O, +CH₄, N₂, freon at MeV by VDG generator Radiobiology, Atmospheric science

Beyond the scientific achievments, these bilateral collaboration projects have been extremely useful for

- Educating PhD students in both sides
- Establishing new collaborations in a European scale (Infrastructure initiatives, e.g., ITS-LEIF, COST Actions, inter-academic collaborations, e.g., CNRS-MTA, etc.)

Thank you for your attention,

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