

SYLA 2: Laboratory Astrophysics

Time: Monday 16:30–18:30

Location: Audimax

Invited Talk

SYLA 2.1 Mon 16:30 Audimax
State-to-State Rate Coefficients for NH₃-NH₃ Collisions obtained from Pump-Probe Chirped-Pulse Experiments — ●CHRISTIAN P. ENDRES¹, PAOLA CASELLI¹, and STEPHAN SCHLEMMER² — ¹MPI für extraterrestrische Physik, Garching, Germany — ²Universität zu Köln, Köln, Germany

The kinetics of rotational inelastic NH₃-NH₃ collisions is studied using pump-probe experiments, which are carried out with a Ku-band waveguide chirped pulse Fourier transform microwave spectrometer by observing the ammonia inversion doublets in the ground vibrational state. The population of one ammonia inversion doublet of a single rotational state is altered by a resonant pump pulse. Due to collisions, the resulting deviation from thermal equilibrium propagates to other states and is interrogated by probe pulses as a function of the pump-probe delay time. The bandwidth of the spectrometer allows to probe the intensity of many inversion transitions within a single chirped pulse excitation (probe pulse) on sub-microsecond timescales as a function of the pump pulse conditions. State-to-state rates are obtained by simulations of all coupled states fitted to the temporal behavior of the complete pump probe experiments where many individual (J,K) rotational states are addressed step by step by separate pump pulse sequences.

SYLA 2.2 Mon 17:00 Audimax

Optical Absorption and Photodissociation Properties of Small Silicon-Containing Clusters - Si₃O₂⁺ — ●TAARNA STUDEMUND, MARKO FÖRSTEL, KAI POLLW, JULIAN VOSS, ROBERT G. RADLOFF, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstrasse 36, D-10623 Berlin

Interstellar dust consists to a significant fraction of μm-sized silicate particles. Origin and formation mechanisms of such dust, which can form solar systems, are still poorly understood. Si/O-containing molecules may be precursors to the larger silicate particles found. So far, only silicon monoxide (SiO) has been detected in the interstellar medium (ISM) [1]. Larger intermediates remain elusive but should exist if the larger grains are formed from the bottom up.

To understand the photodissociation and optical absorption behavior, structures, and energies of Si/O-containing molecules, we measure optical spectra of mass-selected Si_nO_m⁺ clusters and compare them to quantum chemical calculations. Our experimental setup is based on mass spectrometry and resonant laser photodissociation [2]. Initial data show competing fragmentation channels, their appearance energies and branching ratios. In addition, we present the first optical spectrum of Si₃O₂⁺. The results are discussed in an astrophysical context.

[1] R. Wilson et al, 1971, *Astrophys. J.* 167, L97.[2] M. Förstel et al, *Rev. Sci. Instrum.* 2017, 88, 123110.

SYLA 2.3 Mon 17:15 Audimax

The Optical Spectrum and Astrochemical Relevance of 1-Cyanoadamantane⁺ — ●PARKER CRANDALL, ROBERT RADLOFF, MARKO FÖRSTEL, and OTTO DOPFER — Technische Universität Berlin, Berlin, Germany

Astrochemical measurements have demonstrated similarities between the IR spectra of diamondoids and unidentified infrared emission (UIR) bands seen in the spectra of young stars with circumstellar disks.^[1,2] Due to their low ionization energy and open-shell character, it is also suggested that the radical cations of these molecules might be responsible for features in the well-known diffuse interstellar bands (DIBs).^[3] However, the optical spectra of these cations have not been measured experimentally until recently. Here, we present the first optical spectrum of the 1-cyanoadamantane cation (C₁₁H₁₅N⁺) and compare it to the recently reported spectrum of the adamantane radical cation.^[4] These spectra were recorded in the gas phase at 5 K using a cryogenic 22-pole ion trap. The experimental results are compared to time-dependent DFT calculations for interpretation. Geometric changes due to Jahn-Teller distortion and the astrophysical implications of these

ions will also be discussed.

[1] O. Guillois, et al., *Astrophys. J.*, 521, L133 (2009).[2] O. Pirali, et al., *Astrophys. J.*, 661, 919 (2007).[3] M. Steglich, et al., *Astrophys. J.*, 729, 91 (2011).[4] P. B. Crandall et al., *ApJL*, 900, L20 (2020).**Invited Talk**

SYLA 2.4 Mon 17:30 Audimax
A multifaceted approach to investigate the reactivity of PAHs under electrical discharge conditions — ●DONATELLA LORU¹, AMANDA L. STEBER^{1,2}, JOHANNES M. M. THUNNISSEN³, DANIEL B. RAP³, ALEXANDER K. LEMMENS^{3,4}, ANOUK M. RIJS⁵, and MELANIE SCHNELL^{1,6} — ¹Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, 22607 Hamburg, Germany — ²Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid, Spain — ³Radboud University, Institute of Molecules and Materials, FELIX Laboratory, Toernooiveld 7c, 6525 ED, Nijmegen, The Netherlands. — ⁴Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098 XH, Amsterdam, The Netherlands — ⁵Division of BioAnalytical Chemistry, AIMMS Amsterdam Institute of Molecular and Life Sciences, Vrije Universiteit Amsterdam, De Boelelaan 1108, 1081 HV Amsterdam, The Netherlands — ⁶Institute of Physical Chemistry, Christian-Albrechts-Universität zu Kiel, Max-Eyth-Straße 1, 24118 Kiel, Germany

Polycyclic aromatic hydrocarbons (PAHs) are a class of molecules whose presence in the interstellar medium (ISM) has been established via the aromatic infrared bands (AIBs), mid-IR emissions (3 – 20 μm) detected in several interstellar objects. The ubiquitous nature of the AIBs suggests that PAHs are widely spread in the ISM and, as such, they are expected to play an important role in interstellar physics and chemistry. Despite their importance, little is known about the reactivity of PAHs under the harsh energetic conditions of the ISM. To explore the reactivity of PAHs under laboratory conditions, we coupled an electrical discharge nozzle with spectroscopic techniques. Under plasma conditions, PAHs are expected to undergo fragmentation processes and/or recombination chemistry. The species formed are then detected via their mass and their IR signature by IR-UV ion dip spectroscopy, and via their microwave signature by broadband rotational spectroscopy.

Here, we present our results obtained from the electrical discharge experiments on the PAHs naphthalene (C₁₀H₈) and phenanthrene (C₁₄H₁₀) with acetonitrile (CH₃CN). The different sensitivity of the two spectroscopic techniques revealed an interesting diversity in the resulting species from the electrical discharge experiments of the two investigated PAHs.

Invited Talk

SYLA 2.5 Mon 18:00 Audimax
Exploring the Femtosecond Dynamics of Polycyclic Aromatic Hydrocarbons Using XUV FEL Pulses — ●JASON LEE^{1,2}, DENIS TIKHONOV^{1,3}, BASTIAN MANSCHWETUS¹, and MELANIE SCHNELL^{1,3} — ¹Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany. — ²The Chemistry Research Laboratory, University of Oxford, Oxford, United Kingdom. — ³Institute of Physical Chemistry, Christian-Albrechts-Universität zu Kiel, Kiel, Germany.

Satellite infrared measurements show signatures of aromatic vibrations in practically every corner of the universe, attributed to polycyclic aromatic hydrocarbons (PAHs) in the interstellar medium (ISM). These PAHs account for up to 20% of carbon in space and have long been proposed as carriers of the Diffuse Interstellar Bands and Unidentified Infrared Bands.

Given their abundance, PAHs have been the subject of laboratory experiments for many decades, exploring their interaction with a wide range of photon energies. Our experiments utilise XUV pulses at 30.3 nm (40.9 eV) from the Free-Electron-Laser FLASH at DESY, Hamburg to replicate some of the harsh radiation of the ISM. The femtosecond laser pulses allow us to investigate the ultrafast relaxation and fragmentation of PAHs. Combining the ion time-of-flight data, ion imaging data and electron imaging data provides a detailed insight into the various molecular processes occurring after the initial photoionisation.