MO 24: Molecular Spectroscopy I

Time: Thursday 11:00–12:45 Location: P 204

Invited Talk MO 24.1 Thu 11:00 P 204

Electronic Spectra of Doped Diamondoid Cations — •Parker Crandall, Ronja Schramm, Sebastian Völz, Domenik Schleier, and Otto Dopfer — Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstraße 36, Berlin, Germany

Pre-solar nanodiamonds grains have been found in significant abundance in primitive carbonaceous chondrites, suggesting a possible interstellar origin. Their presence raises the question of whether aliphatic (sp^3-hybridized), diamond-like hydrocarbons can form and survive in the harsh conditions of the interstellar medium. Diamondoid cations represent compelling spectroscopic targets. Not only are diamondoids the smallest molecular units of bulk diamond, but their cations are relatively stable and have electronic transitions that lie in the visible range, making them potential candidates as carriers of the diffuse interstellar bands. While our previous work focused on bare and functionalized derivatives, we present our recently measured spectra of N-, O-, and S-doped (cage-modified) diamondoid cations, measured in the gas-phase using either a photoelectron spectrometer, a cryogenically cooled ion trap coupled to a tandem mass spectrometer, or both. These results are further supported by quantum chemical calculations and can provide critical reference data for astronomical searches in the pursuit of a broader understanding of the chemical inventory of the interstellar medium.

MO 24.2 Thu 11:30 P 204

The first excited state of OH^+He — •Nima-Noah Nahvi and Otto Dopfer — Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The OH^+He dimer serves as a simple system to study the weak interaction of helium with open-shell cations, relevant to microscopic superfluidity and astrochemistry. In this work, we investigate the first excited state of OH^+He using a combined spectroscopic and computational approach. Quantum chemical calculations suggest that the transition into this state exhibits an unusual proton transfer to the helium atom ($OH^+ \cdots He \rightarrow O \cdots H^+He$). To prove this, we generate OH^+He inside a cryogenic quadrupole ion trap (10 K) and irradiate the clusters with tunable UV laser light to induce photodissociation. By detecting the dissociation fragments with a time-of-flight mass spectrometer, we obtain an optical action spectrum and are able to directly observe the proton transfer. Calculated potential energy surfaces of the ground and excited state at the coupled cluster level support our interpretation. In addition, we numerically calculate the vibrational wavefunctions, which give insights into the spectrum and the vibrational dynamics of the dissociation process into HeH^+.

MO 24.3 Thu 11:45 P 204

Towards Light-Shift Spectroscopy of RbYb near the D1 line of Rb — •Céline Castor — Institut für Experimentalphysik, Heinrich-Heine-Universität Düsseldorf

Ultracold dipolar molecules constitute a promising system for the investigation of topics like ultracold chemistry, novel interactions in quantum gases, precision measurements and quantum information.

Here we report on experiments in our apparatus for the production of ultracold RbYb molecules. In our former setup photoassociation experiments near the D1 line of Rb were conducted. Our current setup constitutes an improvement of our old apparatus, where the interactions in RbYb and possible routes to molecule production have already been studied extensively, including two-photon photoassociation spectroscopy near the Yb intercombination line.

A major goal is the efficient production of ground state RbYb molecules. We employ optical dipole traps to transport individually cooled samples of Rb and Yb from their separate production chambers to a dedicated science chamber. Combining our results on photoassociation spectroscopy near the Rb D1 line and the Yb intercombination line, we present a conceptual approach for studying stronger bound states in the excited molecular potential $^2\Pi_{1/2}$ using light-shift spectroscopy.

MO 24.4 Thu 12:00 P 204

Shedding Light on $(SiC)^+_{1,2}$: First Laboratory Spectra Obtained by Electronic Photodissociation — •Kai Pollow, Alexander Breier, and Otto Dopfer — Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstraße 36, Berlin, Germany

Silicon carbide ions ($Si_nC_m^+$) are expected in carbon-rich circumstellar environments such as those around asymptotic giant branch stars[1,2]. Several small neutral Si_nC_m species are known in the interstellar medium[3], but their cations remain unidentified due to missing spectroscopic data[4]. Spectra of $Si_nC_m^+$ are therefore essential for assessing their role in ion–molecule chemistry and silicon carbide dust formation.

We present the first laboratory spectra of $(SiC)^+_{1,2}$, recorded via vibronic photodissociation of mass-selected ions in a quadrupole/time-of-flight tandem mass spectrometer with a laser vaporization source[4]. The spectra exhibit clear vibrational structure, and the derived parameters agree with quantum-chemical predictions.

References:
[1] T. Chen et al., Mon. Not. R. Astron. Soc. 509, 5231 (2022).
[2] M. C. McCarthy et al., J. Mol. Spectrosc. 356, 7 (2019).
[3] S. Massalkhi et al., Astron. Astrophys. 611, A29 (2018).
[4] M. Förstel et al., J. Mol. Spectrosc. 377, 111427 (2021).

MO 24.5 Thu 12:15 P 204

Orbital-Resolved Bond-Breaking Asymmetry in the Strong-Field Dissociative Double Ionization Channel ($N_2^+ + O^+$) of N_2O — •Feras Afaneh — Physics Department, Faculty of Science, Hashemite University, P.O.Box 330127, Zarqa 13133, JORDAN

The dissociative double ionization of nitrous oxide (N_2O), induced by short-pulse polarized laser fields, was investigated using the COLTRIMS technique. Focusing on the dissociative channel ($N_2^+ + O^+$), we extracted both the molecular-frame photoelectron angular distributions and the ion sum-momentum distributions. Orientation-dependent ionization rates, analyzed across distinct kinetic energy release (KER) regimes, revealed contributions from multiple molecular orbitals. These results reveal a pronounced asymmetry in bond breaking relative to the instantaneous laser field vector, arising from the interplay between orbital geometry and electron localization-assisted enhanced ionization in stretched molecular configurations under strong-field conditions.

MO 24.6 Thu 12:30 P 204

Photoelectron Spectroscopy and dissociative photoionization of nitrogen heterocycles — •Domenik Schleier[1], Jordy Bouwman[2], Helgi Hrodmarsson[3], Andras Boedi[4], Patrick Hemberger[4], and Otto Dopfer[1] — [1]Institut für Physik und Astronomie, TU Berlin, Germany — [2]Department of Chemistry, CU Boulder, USA — [3]Laboratoire Inter-Universitaire des Systèmes Atmosphérique, Paris, France — [4]Paul-Scherrer-Institute, Villigen, Switzerland

Polycyclic aromatic hydrocarbons (PAHs) and their nitrogen-containing counterparts (PANHs) are ubiquitous in extraterrestrial environments ranging from planetary atmospheres to the interstellar medium. However, only large PA(N)Hs survive the extreme conditions, whereas smaller ones are destroyed. In this work, three nitrogen-containing PANH isomers of C8H6N2 composition have been studied by mass-selected threshold photoelectron spectroscopy and dissociative photoionization in a double imaging photoelectron photoion coincidence (i2PEPICO) apparatus at the VUV beamline of the Swiss Light Source. The experimental findings are supported by quantum chemical calculations and energy-dependent unimolecular dissociation rates for each channel were calculated as a function of internal energy based on RRKM statistical rate theory. The isomers show characteristic dissociation pathways that lead to the elimination of HCN, N2 and H fragments depending on the relative nitrogen position.