TA07

10:54 – 11:09

EXPLOITING TUNABLE VACUUM ULTRAVIOLET PHOTOIONIZATION COMBINED WITH REFLECTRON TIME-OF-FLIGHT MASS SPECTROMETRY FOR THE ISOMER-SPECIFIC DETECTION OF COMPLEX ORGANIC MOLECULES FORMED VIA INTERACTION OF IONIZING RADIATION WITH MIXED ASTROPHYSICAL ICE ANALOGUES

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Over 200 molecules have been detected in the interstellar medium (ISM) with close to one third considered to be complex organic molecules (COMs), molecules containing six or more atoms. Gas-phase reaction networks of ion-molecule and neutral-neutral reactions have aided in the understanding of the evolution of the interstellar medium (ISM). However, these models fail to explain the synthesis of ubiquitous COMs with predicted abundances several orders of magnitude lower compared to observations in the ISM, such as in Sagittarius B2. Over the last decades astrophysical laboratory simulation experiments have shown that some of these COMs are formed via interaction of ionizing radiation within simple ices deposited on interstellar dust particles at 10 K (H₂O, CH₃OH, CO, CO₂, CH₄, NH₃). After processing the ice temperature programmed desorption was utilized to sublime the ice along with its newly formed products for analysis with single photon vacuum ultraviolet ionization coupled with a reflectron time-of-flight mass spectrometer (PI-ReTOF-MS). The use of PI-ReTOF-MS allows for the selective ionization and identification of structural isomers of COMs. Here, we report that the key COMs propynal (HCCCHO) and cyclopropenone (c-C₃H₂O), which have both been detected in the ISM, can be synthesized within interstellar ices containing carbon monoxide (CO) and acetylene (C₂H₂) at temperatures as low as 5 K. This is accomplished via non-equilibrium chemistry induced by the energetic electrons simulating those produced by galactic cosmic rays penetrating interstellar ices. Furthermore, cyclic COMs may act as tracers for non-equilibrium chemical processes at 10 K involving electronically excited reactants such as acetylene in excited triplet state(s). The incorporation of solid state data from these experiments, such as yield, branching ratio, and chemical and temperature conditions, into astrochemical models accounting for non-equilibrium has been shown to greatly improve predicted abundances.

TA08

11:12 – 11:27

THE MILLIMETERWAVE SPECTRUM OF SUCCINONITRILE

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Only two dinitriles, the protonated cyanogen NCCNH⁺ and one isocyanonitrile, NCNC have been detected in the interstellar medium (ISM) among about 200 other compounds, despite nitriles constitute almost 20% of the molecules observed in the interstellar medium. The lack of detections of dinitriles may be explained by the lack of accurate spectroscopic data on their rotational spectra since most of them do not present permanent dipole moment. Succinonitrile, NCCH₂CH₂CN is one of the simplest dinitriles and it could be a candidate molecule to be observed in the ISM. The rotational spectrum for succinonitrile has been previously observed in the 2-78 GHz frequency region by Jahn *et al.*,^a but these measurements were limited to the ground state. In this talk we report the study of succinonitrile and its low lying excited vibrational states using a newly built broadband Fourier transform millimeter wave spectrometer^b equipped with Q-band (31.5-50 GHz) and W-band (72-116 GHz) receivers, similar to those used in the radio-telescopes. The spectrometer is well suited for high resolution emission spectroscopy of molecules of astrophysical importance.

^aM. K. Jahn, J.-U. Grabow, P. D. Godfrey and D. McNaughton, *Phys.Chem.Chem.Phys.*, **2014**, 16, 2100.

^bJ. Cernicharo *et al.*, *A&A*, **2019**.

TA09

11:30 – 11:45

PHOTOPHYSICS AND ELECTRONIC STRUCTURE STUDIES OF PROTONATION OF QUINOLINE

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Study of the photophysics and electronic structure properties of quinoline and its derivatives have been the subject of considerable interest because of their commercial and pharmaceutical applications. Some of the quinoline derivatives have been found as a potential probes for measuring the polarity of microenvironment in chemical and biological systems. Diffuse interstellar bands in the emission spectrum of the interstellar medium, indicate the presence of quinoline and other small polycyclic aromatic nitrogen heterocycles, which readily dissociate under exposure to interstellar radiation. Since the quinoline ring is the basic fluorophor unit in all its derivatives, it is important to understand the change in dynamics and electronic structure of quinoline in presence some external perturbation. Being isoelectronic with naphthalene, these molecules provide useful comparisons for checking the electronic and vibrational state assignments, ionization potentials, and other properties of the parent hydrocarbon. In addition, these molecules possess nonbonding electrons which give rise to n-*Pi** states. The location and characterization of these states are of both theoretical and practical significance. Further, solvents have an important influence on the fluorescence property of N-heterocyclic compounds. Experimentally, Quinoline shows vibronic absorption spectrum and corresponding large Stoke shifted broad fluorescence emission spectrum having very low quantum yield and dual decay time, however protonated quinoline shows red shifted fluorescence spectrum with increase in quantum yield and fluorescence decay become mono-exponential. To understand the vibronic structure of electronic absorption spectra and photophysics of protonation of quinoline, both vibronic and electronic structure studies of quinoline (Q) and protonated quinoline (QH⁺) were carried out along with vibrational calculations for absorption and fluorescence bands at B3LYP 6-311++G(d, p) level in ground and excited state by density functional methods (DFT) and (time-dependent density functional) TD-DFT methods respectively with the help of Gaussian 09 software. Normal mode mixing is taken into account by the Duschinsky transformation. The vibronic structure of strongly dipole-allowed transitions is calculated within the Franck–Condon approximation. Weakly dipole-allowed and dipole-forbidden transitions are treated within the Franck–Condon–Herzberg–Teller and Herzberg–Teller approximation, respectively. A good correlation between computational spectroscopic calculations and experiment results are found to understand the photo-physics of protonation of quinoline.