Program of International online seminar
“Origin and evolution of molecules in our Galaxy”
21 April 2021, 10.00 am (GMT+4)

Chair – **Marsel Zagidullin**; Moderator – **Eugeny Fomin**.

10.00 - 10.05	**Opening Remarks. Valery Azyazov** (Lebedev Physical Institute, Samara Branch, Samara University, Samara, Russia)
10.05 - 10.50	**Ralf I. Kaiser** (University of Hawaii at Manoa, Honolulu, USA) *Exploiting Tunable Vacuum Ultraviolet Light to Unravel the Synthesis of Complex Organic Molecules in Interstellar and Solar System Ices*
10.50 - 11.35	**Naoki Watanabe** (Institute of Low Temperature Science, Hokkaido University, Japan) *Monitoring of OH radicals on ice surface under astrochemical conditions*
11.35 - 11.45	**Break**
11.45 - 12.30	**Dmitri Wiebe** (Institute of Astronomy of the RAS, Moscow, Russia) *Complex Organic Molecules in Space*
12.30-13.00	**Sergei Kalenskii** (Lebedev Physical Institute, Moscow, Russia) *Spectral scan of the region of massive star formation W51e in the 4-mm wave range*
13.00-13.30	**Nonna Molevich** (Lebedev Physical Institute, Samara Branch, Samara University, Samara, Russia) *Traveling gasdynamic structures in isentropically unstable PDRs of the interstellar medium*
13.30-13.35	**Closing Remarks. Marsel Zagidullin** (Lebedev Physical Institute, Samara Branch, Samara University, Samara, Russia)

Join a Zoom meeting
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Conference ID: 889 0344 1468
Access code: 623637

The link will be available 20 minutes before the start of the workshop.

Exploiting Tunable Vacuum Ultraviolet Light to Unravel the Synthesis of Complex Organic Molecules in Interstellar and Solar System Ices

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Kuiper Belt Objects (KBOs) – small planetary bodies orbiting the sun beyond Neptune - emerged in their critical role to understand the chemical evolution of the Solar System and how the molecular precursors to life formed and came together to create environments such as on early Earth. This talk presents novel developments in the understanding of the formation of key classes of biorelevant molecules central to the Origins of Life in ices of Kuiper Belt Objects (KBOs) – and those related to the interstellar medium - exploring cutting edge low temperature surface science experiments exploiting soft photo ionization with tunable vacuum ultraviolet light coupled with a time of flight mass spectrometric, isomer selective product detection (PI-ReTOF-MS). By probing specific structural isomers without their degradation (fragment-free), the incorporation of tunable vacuum ultraviolet photoionization allows for a critical understanding of reaction mechanisms that exist in extraterrestrial ices compared to traditional methods thus eliminating the significant gap between observational and laboratory data that existed for the last decades thus defining the first inventory of (biorelevant) molecules, which forms the nucleus for evolution of life in our Solar System billions of years ago. Considering that Kuiper Belts have been observed around stars like Vega outside our Solar System as well, this knowledge can be transferred to extrasolar planetary systems thus revolutionizing our understanding of the origin of cosmic life as we know it and eventually revealing the molecular birthplace of life. Since cometary matter (at least partially) originated from the molecular cloud, which provided the molecular feedstock for our Solar System, these investigations also expose how ubiquitous astrobiologically relevant molecules such as glycolaldehyde can be synthesized on ice coated interstellar grains at 10 K via a cosmic-ray initiated non-equilibrium chemistry. With the commission of the Atacama Large Millimeter/Submillimeter Array (ALMA), the detection of more complex organic molecules in space will continue to grow – including biorelevant molecules connected to the Origins of Life theme - and an understanding of these data will rely on future advances in hard core physical chemistry laboratory experiments ultimately revealing the level of complexity of astrobiologically relevant molecules which can be synthesized in our Universe.

A. M. Turner, R. I. Kaiser, Exploiting Photoionization Reflectron Time-of-Flight Mass Spectrometry to Explore Molecular Mass Growth Processes to Complex Organic Molecules in Interstellar and Solar System Ice Analogs , Acc. Chem. Res., 53, 2791-2805 (2020).

N. F. Kleimeier, A. K. Eckhardt, P. R. Schreiner, R. I. Kaiser, Interstellar Formation of Biorelevant Pyruvic Acid ($CH_3COCOOH$), Chem, 6, 1-11 (2020).

A. Eckhardt, A. Bergantini, S. Singh, P.R. Schreiner & R.I. Kaiser Formation of Glyoxylic Acid in Interstellar Ices: A Key Entry Point for Prebiotic Chemistry, Angewandte Chemie Int. Ed. 58, 17, 5663-5667, (2019).

M. J. Abplanalp, R. Frigge, R. I. Kaiser, Low-temperature synthesis of polycyclic aromatic hydrocarbons in Titan's surface ices and on airless bodies, Science Advances, 5, eaaw5841 (2019).

Monitoring of OH radicals on ice surface under astrochemical conditions

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The surface of cosmic ice dust grains is known as the birth place of various interstellar molecules in a very cold region in space, so-called a molecular cloud. Because the temperatures of ice grains are typically as low as 10 K in molecular clouds, radical reactions having little barriers and tunneling reactions play dominant roles in molecular formation on the surface. Since the beginning of 2000s, tunneling reactions on the ice surface have been studied experimentally fairly well [1]. In contrast, because of intrinsic experimental difficulty in detecting radicals, little is known about the behaviors of radicals on the ice surface. On cosmic ice grains, hydroxyl (OH) radical is considered to be one of most abundant adsorbates. The OH radicals can be easily produced by photolysis of water ice and reaction of hydrogen and oxygen atoms. Recently, we have developed the method to monitor the OH radical on ice at very low temperatures, which can open a new phase of research on physicochemical processes of radicals. My presentation will consist of two topics: description of the OH detection method and information of OH adsorption sites [2]; clarifying a proton-hole transfer in ice using that method [3,4].

[1] e.g. N. Watanabe, A. Kouchi, Prog. Surf. Sci. 83, 439 (2008); T. Hama, N. Watanabe, Chem Rev. 113, 8783 (2013).
[2] A. Miyazaki, N. Watanabe *et al.*, Phys. Rev. A. 102, 052822, (2020).
[3] N. Watanabe *et al.*, Chem. Phys. Lett. 737, 136820 (2019).
[4] K. Kitajima *et al.*, J. Phys. Chem. Lett. 12, 704 (2021)

Complex Organic Molecules in Space

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One of the greatest discoveries in physics and chemistry of the interstellar medium of the last decades is the large abundance of various organic molecules in molecular clouds and circumstellar material. Having started with formaldehyde in late 1960ies, the interstellar organic inventory now comprises compounds, consisting of more than 10 atoms, which include alcohols, sugars, and aromatic species. I will present an overview of observational data that currently form a basis for our understanding of chemical processes accompanying the process of star and planet formation and discuss the organics cosmic life cycle.

M. Ohishi, Prebiotic Complex Organic Molecules in Space, in Astrobiology, A. Yamagishi et al. (eds.), Springer, 11–21 (2019)

A. Fuente, D. G. Navarro, P. Caselli, M. Gerin et al., Gas phase Elemental abundances in Molecular cloudS (GEMS) I. The prototypical dark cloud TMC 1, A&A, 624, A105 (2019)

J. K. Jørgensen, A. Belloche, R. T. Garrod, Astrochemistry During the Formation of Stars, Annu. Rev. Astron. Astrophys., 58, 727–778 (2020)

Spectral scan of the region of massive star formation W51e in the 4-mm wave range

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Spectral survey of the region of massive star formation W51 at 68--87 GHz has yielded detections of 88 molecules and their isotopic species, from simple diatomic or triatomic molecules, such as SiO, SO, SO2 up to complex organic compounds, such as CH3OCH3, CH3COCH3, and C2H5OOCH. Many lines that are absent from the Lovas list of molecular lines observed in space were detected, and most of these were identified. A significant number of detected molecules are typical for hot cores. These include the neutral molecules CH3OCHO, C2H5OH, CH3COCH3 etc, which are currently believed to exist in the gas phase only in hot cores and shock-heated gas. In addition, vibrationally excited SiO, C4H, HCN, l-C3H, HCCCN, CH3CN, CH3OH, and SO2 lines with upper-level temperatures of several hundred Kelvin were found. Such lines can arise only in hot gas with temperatures of the order of a few x 100 K or higher. Apart from neutral molecules, molecular ions HCO+, HCS+, and their isotopologues are also detected. Individual lines of some observed molecules are too weak to be detected, and these molecules were found by stacking many lines. Although this method made it possible to detect several molecules already known in space no new cosmic molecule have been found. No new molecule have been found by means of spectral line stacking using the results of spectral surveys of other hot cores. This is in contrast with the success of this method for discovering new molecules in a dark cloud TMC-1. We argue that spectral surveys at lower frequencies (10--30 GHz) may be more successful in the case of hot cores.

S.V. Kalenskii, L.E.B. Johansson, Spectral survey of the star-forming region W51 e1/e2 at 3 mm, Astron. Rep 54, 1084.

C. Goddi, A. Ginsburg, Q. Zhang, Hot ammonia around young O-type stars III. High-mass star formation and hot core activity in W51 Main, A&A 589, 44 (2016).

R.A. Loomis, A.M. Burkhardt, C.N. Shingledecker, et al., An investigation of spectral line stacking techniques and application to the detection of HC11N, Nature Astronomy, 5, 188 (2021).