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BOOK OF ABSTRACTS

Edited by: B. Stachová, P. Papp, Š. Matejčík

Table of Contents

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Numerical modeling of coplanar barrier discharge in air

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The coplanar barrier discharge is a non-equilibrium low-temperature plasma. The coplanar barrier discharge driven at atmospheric pressure is currently a well established, durable and robust technology (under the name diffuse coplanar surface barrier discharge, DCSBD) used in plasma activation treatment for multiple purposes.

The challenges in numerical simulation of such discharge lies in the modeling of the discharge itself and also of its complex interaction with dielectric surface. In [6] the ignition and propagation of surface streamer was studied and compared with experimental results using spatio-temporal distribution of electric field. The study of surface streamer propagation requires very fine mesh over large region of computational domain. That doesn't allow to study the whole discharge behavior on longer timescales. In this work we present the results using combination of coarser and finer mesh to better study events leading to the ignition of the surface streamer.

At low applied voltages the coplanar barrier discharge shows behavior close to the Townsend discharge. It is characterized by avalanches of electrons which are seeded from secondary emission by impact of ions on the dielectric surface at the cathode. The applied electric field is not disturbed by space charge effects.

When the applied voltage is increased the electron density in discharge volume is increasing in time and it eventually may lead to the avalanche to streamer transition. Such electron density increase may take a long time as it depends on the applied voltage. When the increase of electron density is slow, the accumulation of surface charge on dielectrics reduces the electric field in the discharge volume. And that prevents further increase of electron density.

For higher applied voltage the electron density in avalanche increases fast enough so that the avalanche to streamer transition appears before the electric field in the discharge volume is reduced by accumulated surface charge. Then the surface streamer ignites and propagates above dielectrics.

In conclusion it is observed that the surface streamer ignites and starts to propagate at lower applied voltages than in which improves the agreement with experimental measurements.

Antibacterial oxazoline thin films

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Polyoxazolines (POx) are a promising class of polymers that have attracted substantial attention recently due to their antibiofouling properties and good biocompatibility. Usually, POx are prepared by living-cationic ring opening polymerization, which is a lengthy wet process conducted in organic solvents. POx thin films are created in a subsequent step, which needs to be tailored for any particular types of substrates. Other possible polymerization techniques are photocoupling [6] and grafting, and both techniques require the premodification of substrates. So, the formation of polyoxazoline coatings using conventional methods is slow and a complex multistep procedure, which can be conducted only on a limited range of substrates. The difficulties of these conventional methods can be overcome via plasma polymerization. Plasma polymerization is known to be a suitable method for the deposition of many biomaterial coating.

In this contribution, a new way to produce plasma polymerized oxazoline-based films with antibiofouling properties and good biocompatibility is presented. The films were created via the plasma deposition from 2-methyl-2-oxazoline vapours in nitrogen atmospheric pressure dielectric barrier discharge. Diverse film properties were achieved by increasing the substrate temperature at the deposition. The physical, chemical and biological properties of plasma polymerized polyoxazoline films were studied by SEM, EDX, FTIR, antibacterial and cytocompatibility tests. After tuning of the deposition parameters, films having the capacity to resist bacterial biofilm formation were achieved. Deposited films also promote cell viability.

Effect of atmospheric pressure cold plasma on the qualitative characteristics of hazelnuts and peanuts

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The global consumption of edible nuts and kernels has an increasing tendency as a healthy snack in the form of fresh or dried nuts or as popular nut butter. The microbial contamination of nuts is serious problem due to raw form consumption. Predominant contamination on nuts are fungi, typically *Aspergillus* spp, *Penicilium* and *Fusarium* [2]. Fungi contamination in nuts is also related to mycotoxins, especially aflatoxins [3]. Several methods were studied for detoxification of nuts from mycotoxins and preventing contamination and inhibiting fungi, including cold low-pressure or atmospheric-pressure plasma [4], [5], [6].

In this study, the effect of low-temperature plasma (LTP) on antioxidant stability, and the possible impact on the ageing of selected nut samples, was investigated. LTP was generated in ambient air using Diffuse Coplanar Surface Barrier Discharge (DCSBD). Nuts are sources of polyphenols with antioxidant activity and unsaturated fatty acids, which are prone to oxidation. Based on FTIR analysis, no significant changes were detected on the surface of peanuts. In hazelnuts, moderate changes were recorded mainly in regions belonging to lipids. Changes inside the samples were not detected. At lower treatment time, a slight increase of polyphenol, flavonoid content and antioxidant activity was observed. With longer plasma treatment, the decrease of target parameters in the case of hazelnuts was measured; however, in peanuts, the increase compared to the initial concentration was noticed.

Acknowledgement

This work was supported by the Slovak Research and Development Agency under the contract No. APVV-21-0147.

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Electron induced fluorescence of neutral fragments of acetone

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Electron induced fluorescence of acetone was studied by optical emission spectroscopy. Acetone is the simplest ketone and it is an abundant compound of the interstellar medium. The emission spectrum following electron impact on acetone was studied in a crossed-beam experiment. The emission spectrum was measured in the wavelength range of 280 – 950 nm at 50 eV electron energy. There were no detected transitions in the region of 300 – 380 nm. The wavelength region of 445 – 900 nm consists of the lines of hydrogen's Balmer series H_α at 656.3 nm and H_β at 486 nm, and the Swan system of C2 ($d^3\Pi_g$–$a^3\Pi_u$) within 460 – 472 nm. The emission spectrum within the wavelengths of 370 - 445 nm is depicted in Figure 1. The emission band in the range of 415 – 445 nm corresponds to the radiation of CH ($A^2\Delta$–$X^2\Pi$) (v,v) fragment. Less intensive radiation of CH ($B^2\Sigma^-$–$X^2\Pi$) (0,0) fragment was identified within 386 – 402 nm. Several emission lines of hydrogen's Balmer series H_γ – H_η were detected throughout the spectrum as well.

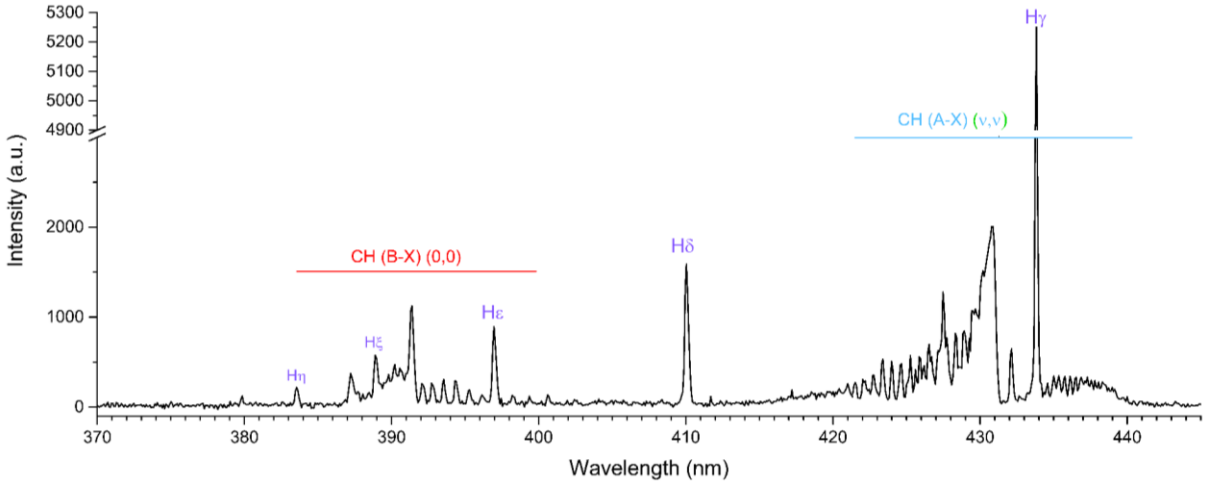

Fig. 1: The emission spectrum of acetone measured within 370 – 445 nm at 50 eV.

Acknowledgement

The presented research was partially supported by Slovak grant agency VEGA within the projects nr. 1/0489/21, by Slovak Research and Development Agency within projects nr. APVV-19-0386. This research has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 871149.

Clusters of $Co(CO)_3NO$ molecules formed in Ar gas: dissociative electron attachment

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The dissociative electron attachment to $Co(CO)_3NO$ clusters formed in an argon environment was studied. Our findings reveal that the ion yields of DEA products from clusters align closely with both gas-phase results [1,2] and cluster investigations conducted in helium nanodroplets [3]. Additionally, recent cluster experiments identified several core-excited resonances peaking above 4 eV, 6 eV, and approximately 10 eV, previously unreported in similar studies. The exclusive formation of the molecular ion from clusters is confirmed, indicating its relaxation process competing with the CO ligand loss in $[Co(CO)_3NO]^-$ at energies around ~0 eV, which has been validated as an exothermic process with CBS-QB3 calculations. We report new resonances for various ions known from the similar studies, including $[Co(CO)_2NO]^-$ above 4 eV, $[Co(CO)NO]^-$ close to 10 eV, $[Co(CO)_3]^-$ at 7 and 10 eV, and $[Co(CO)_2]^-$ at 7 eV. Using CBS-QB3, we evaluate the electron affinities of $Co(CO)_3NO$ and its fragments, and the bond dissociation energies in neutral $Co(CO)_3NO$ and anionic $[Co(CO)_3NO]^-$. This dataset enable us to predict ion-molecular fragment pairs observed in dimer-like clusters:

- $[Co(CO)_3NO]_2^-$, $[Co(CO)_3NO+Co(CO)_2NO]^-$, $[Co(CO)_2NO]_2^-$, $[Co(CO)_3NO+CoNO]^-$,
- $[Co(CO)_3NO+Co(CO)_3]^-$, $[Co(CO)_3NO+Co(CO)_2]^-$, $[Co(CO)_3NO+CoCO]^-$,$[Co(CO)_3NO+Co]^-$.

We offer theoretical explanations for resonances occurring at lower energies than is the expected threshold of the potential DEA fragment in the small ion clusters, involving the $[Co(CO)_2]^-$ or even $[Co(CO)_4]^-$ ion constituents for $[Co_2(CO)_{6...3}NO]^-$ clusters. The $[Co(CO)_4]^-$ is confirmed in this study as the product of DEA to $Co(CO)_3NO$ clusters, alongside the $[Co_2(CO)_5]^-$ variation. Due to the stoichiometry of $[Co(CO)_4]^-$ ion, as well as of various dimer-like $[Co_2(CO)_{1,2}(NO)_{1,2}]^-$ clusters measured in this study, the formation of the potential products is explained only by inelastic electron scattering, initiating neutral dissociation in one constituent followed by DEA to the neighboring molecule.

Acknowledgement

This work was supported by the Slovak Research and Development Agency APVV-19-0386 and the Slovak Grant Agency for Science (contract no. VEGA 1/0553/22).

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Electron induced excitation of CO

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Carbon monoxide is one of the dominant carbon bearing molecules in extra-terrestrial bodies such as comets or centaurs. Especially the $A^2\Pi - X^2\Sigma^+$ transition of CO^+ is prominent in emission spectra of the comet tails and is referred to as the Comet Tail system. The diagnostic of these cometary volatiles is a necessity for solar system formation models [1]. CO molecule is also present in interstellar gas clouds which are the precursors of star formation. It is also an important compound of planetary atmospheres, such as Mars or Venus. Tracking atmospheric CO on Mars is an effective method for exploring the oxidizing capacity of the Martian atmosphere [2].

Electron induced fluorescence of CO was studied in a crossed-beam experiment. The emission spectrum composed of neutral CO and CO^+ emission bands and atomic lines of C and O was measured at several electron energies ranging from 5 to 100 eV. The emission spectrum of CO in the wavelength range of 280 – 950 nm at 50 eV electron energy is depicted in Fig. 1. Excitation-emission functions for all identified transitions of the spectrum were measured as well.

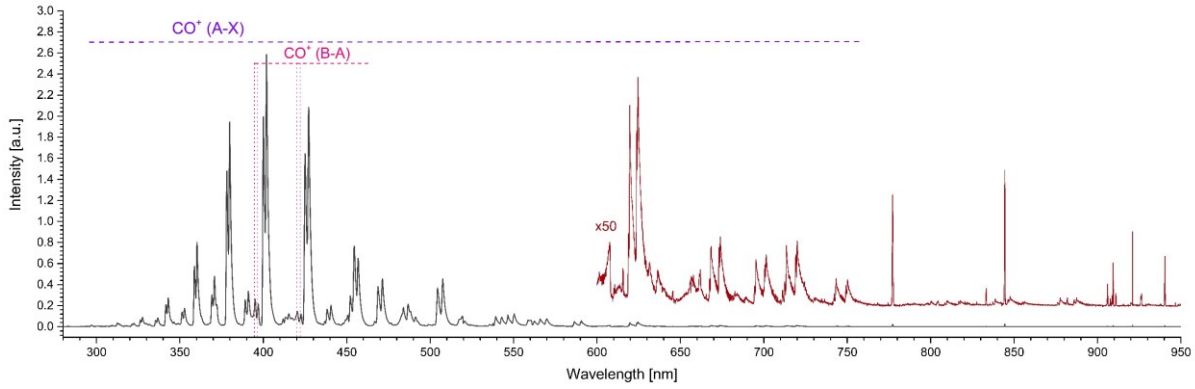

Fig. 1: The emission spectrum of CO measured by CCD camera at 50 eV.

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Effectiveness of two cold plasma sources on changes in the surface properties of plant seeds

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The application of cold plasma at atmospheric pressure (CAP) in the field of agriculture is a promising technology that has been confirmed by many scientific studies [1]. In our contribution, we present the results focused on plasma treatment of pea seeds. We used two different plasma sources based on dielectric barrier discharge: planar diffuse coplanar surface barrier discharge (DCSBD) [2] and multi-hollow surface dielectric barrier discharge (MSDBD) [3]. Both create cold plasma at atmospheric pressure in the ambient air, or in oxygen, nitrogen and their mixtures. We investigated different plasma treatment parameters and pea (*Pisum sativum* L.) was selected as a model seed. We focused on the use of suitable surface diagnostic methods to investigate changes on the surface of seeds after plasma treatment. The evaluation of changes in the physical and chemical surface properties of biological samples after plasma treatment is significantly more complex than in the case of inorganic, polymer or other samples. Established methods therefore require innovative approaches in determining the surface energy, elemental composition and chemical bonds, or surface morphology of biological samples. It is also interesting to observe the aging of the surface treatment of biological samples.

Acknowledgement

This work was supported by the Slovak Research and Development Agency under the contract No. APVV-21-0147.

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Microporous polypropylene membranes grafted by acrylic acid for the use in alkaline water electrolysis cells

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Connection of alkaline water electrolysers with intermittent renewable energy sources like wind power or photovoltaics in power-to-gas applications sets high requirements on inter-electrode separator. The desired properties are mainly high conductivity of current-carrying OH^- ions and low permeability of molecular hydrogen and oxygen to suppress mutual contamination of these gases. These properties can only be achieved with good wettability of the separator by aqueous alkaline electrolyte (usually 30 wt.% KOH) [1]. Nowadays, microporous separators are made of a composite of polymer, which gives them toughness, and ceramic filler, which is evenly dispersed in the material and gives the membranes wettability. However, to achieve the necessary wettability, a high amount of the ceramic filler is required, which reduces the mechanical strength [2]. In this work, wettability of polypropylene microporous membranes was achieved by plasma-initiated graft polymerization of acrylic acid. Membranes were activated in a low-pressure capacitively-coupled radiofrequency discharge in argon or oxygen. To compare the long term stability of grafted membranes activated by argon and oxygen plasmas, aging tests in 30 wt.% KOH aqueous electrolyte were conducted. In addition, the membranes were characterized as separators in alkaline water electrolysis cell in terms of electrical resistance and diffusion flux of hydrogen through membranes. The results of aging tests indicate that membranes grafted after argon plasma activation exhibit better stability over time than membranes grafted after oxygen plasma activation. Results of electrical resistance and diffusion flux of hydrogen through membranes show that with higher grafting degree the values for both parameters are lower.

Acknowledgement

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Low energy electron attachment by halogenated silanes

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Silanes and their halogenated derivatives are highly versatile materials employed across a broad spectrum of applications. These applications encompass roles as adhesion promoters, coupling agents, crosslinking agents, dispersing agents, and surface modifiers. These compounds are of particular interest due to their involvement in crucial industrial processes such as the decomposition of silane in low-pressure plasmas and the reduction of chlorosilanes by hydrogen in plasmas. These processes play a fundamental role in silicon manufacturing and silicon film deposition.

The aim of the work reported here was to study the kinetics of thermal electron attachment to some halogenated silane in carbon dioxide buffer gas using the pulsed Townsend method.

Employing the Pulsed Townsend technique, we conducted measurements of rate coefficients, denoted as k (T), utilizing thermal conditions within the temperature interval of 298–378 K. The investigated molecules include hexachlorodisilane (Si_2Cl_6), (difluoromethyl)trimethylsilane $(CH_3)_3SiCHF_2$. The corresponding rate coefficients at 298 K are equal to $(2.17\pm0.04)\times10^{-9}$ cm^3s^{-1} and $(2.01\pm0.09)\times10^{-10}$ cm^3s^{-1}, for Si_2Cl_6 and $(CH_3)_3SiCHF_2$ respectively.

Acknowledgement

The project is co-financed by the Polish National Agency for Academic Exchange, by the Slovak Research and Development Agency bilateral contract no. SK-PL-21-0025 and the Slovak Grant Agency for Science contract no. VEGA 1/0552/22.

Deposition of functional coatings using atmospheric pressure plasma polymerization

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Plasma polymerization (PP) is a method by which thin, functional, polymer-like coatings are deposited using a plasma source. Compared to conventional chemical polymerization, this technique offers a more environmentally friendly approach, as it doesn't require solvents or catalysts to facilitate the polymerization process.

Characteristics of the deposited layers are affected by parameters such as exposure time, substrate and monomer properties, temperature, input power and many more. By adjusting these parameters, it is possible to produce layers with a desired functionality (e.g. hydrophobic/hydrophilic, anti-corrosive, etc.). However, this adaptability poses a challenge for the reproducibility of PP experiments, as slight variations in uncontrolled parameters can influence the resulting layer properties. While substantial research has been conducted in the field of PP, it remains unclear which factors are the most critical in the layer formation process.

Our research is dedicated to investigating and optimizing PP of hexamethyldisiloxane (HMDSO) using a Diffuse Coplanar Surface Barrier Discharge (DCSBD) operating at atmospheric pressure, with the aim of creating functional layers on various substrates, building upon our previous works [1,2]. We have examined the prepared layers through various surface diagnostic techniques, including WCA, ATR-FTIR and SEM. The layer preparation process has undergone multiple modifications aimed at enhancing both reproducibility of the experiments and functionality of the prepared layers.

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Memory effect in palladium microdischarges

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The statistical relationships between electrical discharge parameters of the pulsed vacuum breakdown at different microgaps are reported. The main focus of this study is on the entire breakdown evolution process, including a comparison of the conditioning of the full and semi-virgin electrodes, and an investigation of the memory effect between successful breakdowns. The experiments were performed in the sphere-to-plane geometry using palladium electrodes with the gap spacing ranging from 500 nm up to 10 μm. The gap was energized using a pulsed voltage with a ramp speed of 10^7 kV/s.

Results and conclusion

The conditioning process is necessary for obtaining the proper measurement of vacuum breakdown for microdischarges. During the conditioning process, the surface oxide layer, residual gases, and other contaminants are cleaned through successive breakdowns. Figure 1 shows the conditioning process of both virgin electrodes. It is evident that the breakdown voltage increases uniformly but scatters for virgin electrodes, while saturation occurs after approximately 30,000 breakdowns (Vb). The opposite behaviour was observed for single virgin electrodes where one of the electrodes was conditioned, and the other remained in a virgin state. In this case, the beginning of breakdown exhibits a linear steep increase.

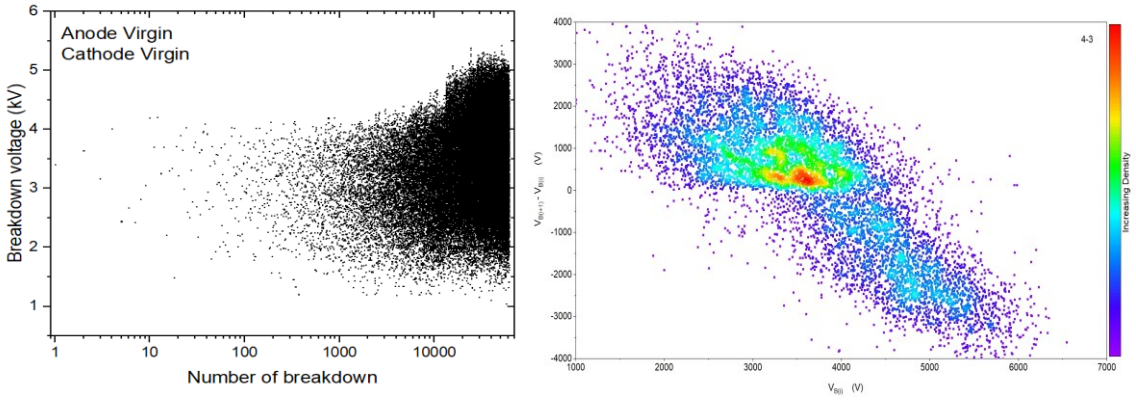

Figure 1: Evolution of the conditioning process of Virgin Cathode and Virgin Anode electrodes (left) and memory effect pattern for palladium microdischarges for 10μm (right).

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After saturation occurs, we conducted a statistical characterization of these seemingly stochastic breakdowns. Plotting the scatter density plot of Vb(i+1) − Vbi versus Vbi, we obtained a correlation pattern between breakdowns. This pattern clearly shows the evolution cycle of breakdowns. If the first breakdown occurs at a lower voltage under 4kV, the next voltage step increases until the breakdown voltage is higher than 4-5kV. After reaching values above this threshold, we observed a steep decrease in the breakdown. This indicates a memory dependency between each following breakdown—the memory effect. Figure 1

(right) illustrates the entire process repeating. This discovery confirms that the memory effect is also present in microdischarges.

Acknowledgement

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Characterization of 2-methyl-2-oxazoline and 2-ethyl-2-oxazoline by ion mobility spectrometry and mass-spectrometry

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Positive polarity atmospheric pressure chemical ionization of 2-Methyl-2-oxazoline and 2-Ethyl-2-oxazoline were studied using ion mobility spectrometry (IMS) and IMS combined with time-of-flight mass spectrometer (IMS-TOF MS) techniques, in the dry air at 373 K drift gas temperature. During measurements, the IMS was operated in the positive polarity mode at sub-atmospheric pressure (680 mbar) due to simple sampling of volatile organic compounds by the capillary inlet. As a drift gas, purified ambient air was used with a gas flow of 600 mL/min, while the sample flow was set to 50 mL/min. In the ionisation source, the reactant ions (RI) $H^+.(H_2O)_{3,4}$ and $NH_4^+.(H_2O)_{0,1}$ were generated, which were used for the chemical ionisation of studied compounds. The dominant ionization reaction was the direct proton transfer. The ionization resulted in the appearance of $M.H^+$ and $M.H^+(H_2O)$ ions for both substances. In the IMS spectrum of 2-Methyl-2-oxazoline, we have detected a monomer peak with the reduced ion mobility K_0 = 2.046 $cm^2.V^{-1}.s^{-1}$ and especially at lower concentrations a peak with the reduced ion mobility K_0 = 1.948 $cm^2.V^{-1}.s^{-1}$ corresponds to 2-propanol. The spectra of 2-Ethyl-2-oxazoline were measured under similar conditions to 2-Methyl-2-oxazoline. In the IMS spectrum, we have detected a monomer peak with the reduced ion mobility K_0 = 1.925 $cm^2.V^{-1}.s^{-1}$ and a small impurity with the reduced ion mobility K_0 = 2.044 $cm^2.V^{-1}.s^{-1}$ representing ethanol. We have calculated the limit of detection (LOD) for both investigated samples by calibration curves (51 ± 2ppb for 2-Methyl-2-oxazoline, and 84 ± 3ppb for 2-Ethyl-2-oxazoline).

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Detection of explosives from various surfaces using laser desorption technique and ion mobility spectrometry

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The present study showcases the successful integration of ion mobility spectrometry (IMS) with laser desorption (LD) for the effective detection of explosives on diverse surfaces, including aluminium, stainless steel, ceramic, PVC, glass, drywall, paper, wood, cotton, and denim. In this study, IMS with corona discharge (CD) as the ion source, and C_2Cl_6 as a dopant, was employed for detection. The LD sampling technique emerged as a robust method for desorbing low-volatile compounds, particularly explosives, facilitating subsequent analysis by IMS. However, the study revealed that the performance of LD-IMS is influenced by the composition of the surface material. While explosives were successfully detected on nearly all surfaces, challenges arose with materials such as paper, wood, and textiles due to the occurrence of burning after laser focusing. Favorable responses were observed on PVC and drywall surfaces, while ceramic and metal materials presented challenges due to laser reflection. Successful desorption was achieved through additional darkening of the sample application site. Reduced ion mobility values were assigned to individual explosives, including TNT (1.44 $cm^2.V^{-1}.s^{-2}$), 2,4-DNT (1.55 $cm^2.V^{-1}.s^{-2}$), 3,4-DNT (1.52 $cm^2.V^{-1}.s^{-2}$), 2,6-DNT (1.46 $cm^2.V^{-1}.s^{-2}$), RDX and C-4 (1.39 $cm^2.V^{-1}.s^{-2}$), and PETN and Semtex (1.16 $cm^2.V^{-1}.s^{-2}$). Limits of detection (LOD) were determined for each explosive during laser desorption from various surfaces, with values of 7 ng/mm^2 for TNT, 15 ng/mm2 for RDX, C-4, PETN, and Semtex, and approximately 50 ng/mm^2 for DNTs. Slightly diminished sensitivity was observed for all explosive samples on drywall material.

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Influence of water vapor on electrical discharge initiated processes in prebiotic atmospheres

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The aim of the presented work is study of chemical process in extraterrestrial atmosphere and the synthesis of organic compounds formed in electrical discharged in gaseous mixtures. This study focuses on the influence of water molecules on chemical processes initiated by electrical discharges in probiotic atmospheres. This work is focused on the simulation of nitrogen atmosphere and carbon dioxide atmosphere. These gases were chosen because they represent the main components of some known atmospheres. The atmosphere of Titan, second largest moon of solar system. The most common composition of the gaseous mixture was methane (2-4 sccm) in 200 sccm of nitrogen. The second study atmosphere was atmosphere of Mars. The most common composition of the gaseous mixture was nitrogen (2-4 sccm) in 200 sccm of carbon dioxide. A glow discharge generated in a special reactor at atmospheric pressure and a flow of pure N_2 or CO_2 was used for the simulation. Part of the measurement took place only in pure gas, into which water vapor with a flow rate of 0, 5, 10, 15 and 20 sccm was gradually introduced.

In the second part of the measurement, the influence of admixtures was studied. In the case of a nitrogenous gaseous mixture, methane flow rates of 2 and 4 sccm were used. In the case of a gaseous mixture with CO_2, the nitrogen flow is 2 and 4 sccm. Again, the analysis of the effect of water was carried out for all created atmospheres.

The products formed were analysed using proton ionization mass spectrometry and a time-of-flight analyser. Simple aliphatic hydrocarbons, alcohols, aldehydes, and ketones were detected. As the number of additives increased, more complex aromatic substances were also formed. In case of nitrogenous gaseous mixture, the most important gas detected was ammonia, followed by propane-2-ol, ethanol and most likely diethylamine. In case of carbon dioxide gaseous mixture, the most important gas detected was hydrogen cyanide, methenamine or acetonitrile. At the same time, plasma diagnostics was carried out using optical emission spectroscopy.

The substances detected in this work are in good agreement with the available literature and with substances detected in Mars and Titan's atmosphere by the Cassini interplanetary probe with the Huygens module.

Study of low temperature plasma direct application on mixed and individual cultures

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This work focuses on the study of the interaction of low-temperature microwave plasma with yeast Candida glabrata and bacteria Staphylococcus epidermidis and Escherichia coli. Co-cultivations of these microorganisms were also treated.

Each microorganism was treated individually on selected solid nutrient media and also in suspension (PBS and selected nutrient media). Co-cultivation of the mentioned microorganisms were treated only on selected solid nutrient media.

The surface wave microwave discharge was used, with argon as a working gas. For the experiment on solid nutrient media, a constant gas flow rate of 5 Slm was maintained. Power fluctuated between 8-10 W throughout the experiment. The microorganisms treated on solid nutrient media were inhibited and also uncultivable after plasma treatment.

For the experiment in suspension, a constant gas flow rate of 2 Slm and power 13 W were maintained throughout the experiment. We found that individual cells were killed when microorganisms were treated in suspension. However, the efficiency of this treatment wasn't sufficient. This was probably caused by the setup of experiment. Plasma was only being formed in argon because the capillary of the plasma torch was submerged in the treated suspension, which led to a low generation of reactive species.