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Inelastic interactions of electrons with molecules and clusters examined using crossed-beam methods

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Abstrakt

V rámci tejto dizertačnej práce boli skúmané tri druhy nepružných zrážok elektrónov s molekulami a klastrami na dvoch aparátúrach. Elektrónmi indukovaná fluorescencia bola skúmaná na aparátúre EIFA (skratka z angl. Electron Induced Fluorescence Apparatus) pre molekuly vodíka a deutéria, ako i nitrometánu a pentakarbonýlu železa v oddelených štúdiách. Emisné spektrá v ultrafialovej (UV, z angl. ultra violet) a viditeľnej (VIS, z angl. visible) časti elektromagnetického spektra boli zaznamenávané a analyzované, ako i účinné prierezy pri rôznych energiách elektrónov. Žiarenie kontinua vodíka a deutéria boli prvýkrát skúmané experimentálne vo viditeľnej oblasti. Účinné prierezy pre Balmersové čiary a vetvy Fulcher α pásu boli pre niektoré čiary zmerané prvýkrát, a iné boli overené a spresnené. Výsledky tohoto výskumu majú využitie v diagnostike a modelovaní vodíkovej plazmy. Emisné spektrum nitrometánu bolo namerané pri lepšom optickom rozlíšení ako je dostupné v literatúre, vibračná štruktúra neutrálnych fragmentov bola pozorovaná na EIFA. Výskum najjednoduchšej nitro-zlúčeniny môže mať využitie v astrochémii. Relatívne účinné prierezy pre emisiu železo pentakarbonýlu po interakcii s elektrónmi pri energiách 5 až 100eV boli skúmané prvýkrát v rámci tejto dizertačnej práce, ako i vysokorozlíšené spektrá v UV/VIS. Bola pozorovaná úplná fragmentácia molekuly na atóm železa a CO skupiny, a je veľmi podstatným výsledkom nášho štúdia. Má dôležité implikácie pre fabrikáciu nano štruktúr obsahujúcich atómy železa. Druhá časť nášho výskumu v rámci doktorandského štúdia bola uskutočnená na aparátúre HEM (hemisférický elektrónový monochromátor). Disociatívny elektrónový záchyt imidazolu a 2-nitroimidazolu boli pozorované v plynnom skupenstve pri náraze pomalých elektrónov (0 až 15eV). Niekoľko fragmentov imidazolu bolo zaznamenaných pri energiách 7eV a 11eV, a nakoniec aj úplná abstrakcia vodíkových atómov, kým najsilnejší signál bol pozorovaný pre stratu jedného vodíka pri energiách nižších ako 3eV. Potenciálny radiosensitizer, 2 nitroimidazol, bol experimentálne študovaný a výsledky boli porovnané so štúdiom jeho izomerických foriem, 4 a 5-nitroimidazolu. Rozsiahla teoretická analýza bola spojená s experimentálnymi výsledkami a viedla k záveru, že 2-nitroimidazol môže byť lepším kandidátom pre rádioterapiu. HEM aparátúra bolo použitá aj na tretiu časť výskumu, kde boli skúmané neónové klastre v oblasti prahových energií. Aj formovanie kladných a záporných iónov dopovaných neónových klastrov s CO₂ boli študované na HEM. Ionizácia cez Rydbergové stavy je navrhnutá ako možný mechanizmus produkcie kladných iónov neónu pri náraze elektrónov na čisté neónové klastre. Zmiešané klastre CO₂ a neónu podliehajú Penningovej ionizácii cez metastabilné excitované stavy neónu. Výsledné pozorovanie kladných CO₂ klastrov podporuje navrhnutý mechanizmus ionizácie zmiešaných klastrov neónu a CO₂. Konečne, disociatívny elektrónový záchyt na zmiešaných klastroch CO₂ a neónu sa vyznačuje tromi rezonanciami: pri 1eV, 2eV a 3eV, ktoré boli pozorované pri formovaní záporného iónu tetraméru CO₂. Predbežné vysvetlenie komplexného mechanizmu fragmentácie tohto klastra a posunu pozície rezonancie, ktorý je závislý na začiatočnej veľkosti klastra, je dostupné v tejto práci.

Kľúčové slová: elektrónmi indukovaná fluorescencia, disociatívny elektrónový záchyt, ionizácia.

Abstract

Inelastic electron interaction with molecules and clusters were investigated within the framework of this thesis. Two experimental setups were used for probing three different interaction. First, Electron Induced Fluorescence apparatus (EIFA) was used for the investigation of the electron interaction with hydrogen, deuterium, nitromethane and iron pentacarbonyl in separated studies. The emission spectra in ultra violet (UV) and visible (VIS) region were investigated, and photon efficiency curves (PEC) were measured. Hydrogen and deuterium continuum was investigated in VIS region for the first time. New and or improved cross section data for hydrogen Balmer series as well as the Fulcher alpha band are reported here with strong impact on diagnostics and modeling of hydrogen plasmas. Nitromethane emission spectrum was obtained with optical resolution better than found in literature so that the vibrational structures of neutral fragments were observable. The astrochemical context of this simplest nitro-compound is emphasized. Iron pentacarbonyl PECs were investigated for the first time in region 5-100 eV, and high resolution emission spectra in UV - VIS were recorded. Complete fragmentation into iron and CO was observed with strong implications for the nanofabrication of iron structures. The second part of the investigation was conducted on a Hemispherical electron monochromator (HEM) setup. Gas phase measurements were performed on imidazole and 2-nitroimidazole. Dissociative electron attachment (DEA) was investigated upon interaction of slow electrons (0-15 eV) with both molecules. Imidazole dissociates into variety of fragments at around 7 eV and 11 eV impact energy, leading up to all four hydrogen loss, while the loss of one hydrogen atom at energies lower than 3 eV is the strongest observed DEA channel. A potential radiosensitizer, 2-nitroimidazole, has been studied and analyzed in comparison to its isomeric variants, 4 and 5-nitroimidazole. Extensive theoretical work was coupled with this experimental investigation and led to the conclusion that 2-nitroimidazole might be a better candidate for the radiation treatment. The third study was also conducted on the HEM setup, where clusters of neon were investigated at the threshold of positive ion formation. Also doped neon clusters with CO₂ were investigated, both positive and negative ions. Ionization via Rydberg states was proposed as a possible mechanism for positive cluster ion formation from bare neon clusters. Penning ionization via metastable excited states of neon was observed upon the formation of CO₂ clusters from mixed CO₂/Ne clusters. Finally, three dominant resonance peaks were observed upon DEA to CO₂/Ne clusters, around 1 eV, 2 eV and 3 eV, resulting in negative tetramer ion of CO₂. A potential explanation of the complex mechanism of the size dependent resonance shifts is presented in this thesis.

Key words: electron induced fluorescence, dissociative electron attachment, ionization.

1 Introduction

The reason why we are still interested in examining the effects of electron molecule interactions after more than hundred years from the discovery of electrons by Sir J. J. Thomson [1], is the great impact these interactions have on the world around us [2], on top of how intriguing and simply exciting new findings about this subject can be. In this thesis a brief overview on the most recent improvements of the existing data sets on inelastic cross sections, relative or absolute in scale is presented. There are many more unanswered questions about “simple” electron molecule interaction worth of giving our attention to, and the aim of the thesis is to give a contribution in form of new data and the improvement of the knowledge in this field.

The impact of the free electrons on molecules depends on the kinetic energy of electrons and the structural characteristics of the involved molecules [3]. We are interested in low energy electrons, energies ranging from about zero up hundred electron volts. These so called “low energy electrons”¹ are able to excite, ionize and/or dissociate molecules by interacting with electrons of the valence shells of molecules. A subsequent change of the energy distribution in the electron – target system occurs, as well as in the geometry of the resulting species, and either or both can lead to further interaction of the products with the surrounding environment.

For astrochemistry [4], an emerging field of space science, it is of great importance to observe small hydrocarbons and nitro compounds interacting with electrons under laboratory conditions where the environment of outer space is simulated [5]. These interactions may lead to production of the simplest amino acids, which could give an answer to the question of the origin of life. Within the work conducted during my PhD studies, the simplest nitro-compound was examined. Nitromethane doesn't necessarily have to be the key species in formation of amino acids, but there is proof of its existence in interstellar medium and it is thus an astrochemically relevant molecule.

It has been long known that low energy electrons can cause damage on DNA [6]. This can be beneficial if the damage is oriented towards malignant tissues – tumors. Although there is still no step-by-step explanation of the mechanisms, it may become an established routine to use radiosensitizers in radiotherapy to enhance the efficiency of the treatment. We investigated potential radiosensitizer, 2-nitroimidazole, compared its reactivity upon electron interaction by means of mass spectrometry with other nitroimidazole isomers in order to better understand the electron induced chemistry on the molecular level. Experiments with imidazole, which is the building block of nitroimidazolic compounds and another biologically relevant molecules, are also covered in this thesis [7].

Aside from cancer related issues, the modern world is fighting the upcoming energy crisis. The development of tokamaks, thermonuclear fusion reactors, may be a solution of this problem in sense of efficiency, sustainability and environmental impact [8]. These reactors will use plasmas based on hydrogen isotopes as the source of the electrical power. The materials planned to be used for inner walls of the reactor are still under investigation in order to optimize the parameters of the reactor. Absolute cross sections upon the interaction of electrons with hydrogen and deuterium have to be as accurate as modern science allows. In the electron induced fluorescence laboratory in Bratislava, small hydrocarbons which can be formed upon interaction of electrons, atoms and molecules in the region close to the wall of the vessel, were investigated in the past [9]. In continuation to this work, hydrogen and deuterium have been re-examined and the results are reported in this thesis.

Interaction of electrons with matter close to the surface is not only an issue in thermonuclear fusion research. In industry, mainly in microelectronics, the necessity for production of pure atomic monolayers in order to deliver smaller devices, led to an increased interest in elementary processes, such as electron – atom and electron – molecule interactions. One of the main goals of the ongoing COST action, CELINA (Chemistry of ELectron Induced NANolayers) [10] is the better understanding of low energy electron interactions with the precursor molecules used for the atomic layer growth in

¹ the definition of “low energy” differs in literature

focused electron beam techniques. This thesis provides insight into electron induced fluorescence of iron pentacarbonyl, which is a widely used precursor in focused beam techniques.

Inelastic electron – molecule interactions are particularly important in plasmas, where excited particles, both neutrals and ions, represent reactive species that are able to change the properties of the object they interact with [11-17]. The list of scientific fields and research areas which are tightly related to the aforementioned interactions, is immense.

To bridge the gap between single electron – molecule interactions and electron interaction with solids or liquids, the field of cluster physics embarked in twentieth century giving the opportunity to get an insight on how properties of the matter change when going from isolated molecule to the bulk. [18] Given the multitude of different media where clusters are present and applications in which they can be used, as well as many variations in their composition, clusters and cluster physics have a lot to offer [19].

The first chapter of this thesis will give an introduction about the beginnings of the experimental research using crossed-beam methods and show the connection of optical spectroscopy and mass spectroscopy with the presented studies. With the emphasis on the theoretical background of the investigated field, the second chapter will give the basis for the understanding of the studied processes between electrons and molecules, as well as clusters. Two experimental setups were used for the investigation of molecules and clusters within this thesis, and both will be described in the Experimental setup chapter. Results obtained during this study will be presented in chapter four to six. Electron induced fluorescence, investigated in Bratislava, will be presented in the fourth chapter containing the results and the discussion on hydrogen and deuterium investigation, as well as nitromethane and ironpentacarbonyl studies. In the Appendix A and B two published papers can be found, on hydrogen and ironpentacarbonyl, respectively. Gas phase measurements performed on the HEM setup in Innsbruck will be introduced in the following chapter, while the respective submitted paper draft on nitroimidazoles and published paper on imidazole can be found in the Appendix C and D of this thesis. The last chapter of the thesis contains results on neon cluster investigations. Positive ion studies on bare clusters, as well as on CO₂/Ne mixed clusters will be shown. Preliminary results of dissociative electron attachment to CO₂/Ne mixed clusters will be given at the end of the last chapter.

2 Experimental setups

Two crossed – beam setups were used for the research during my PhD studies. Common feature of the setups is the principle of the operation: monoenergetic beam of electrons produced in an electron monochromator collides with a beam of molecules (atoms or clusters) and the products of various electron induced reactions are observed. On the other hand, crucial difference is the detection system of the two: Electron Induced Fluorescence Apparatus (EIFA) is used for the observation of the radiative transitions upon electron interaction, whereas the Hemispherical Electron Monochromator setup (HEM setup) is used for the detection of ions.

2.1.1 General overview on EIFA

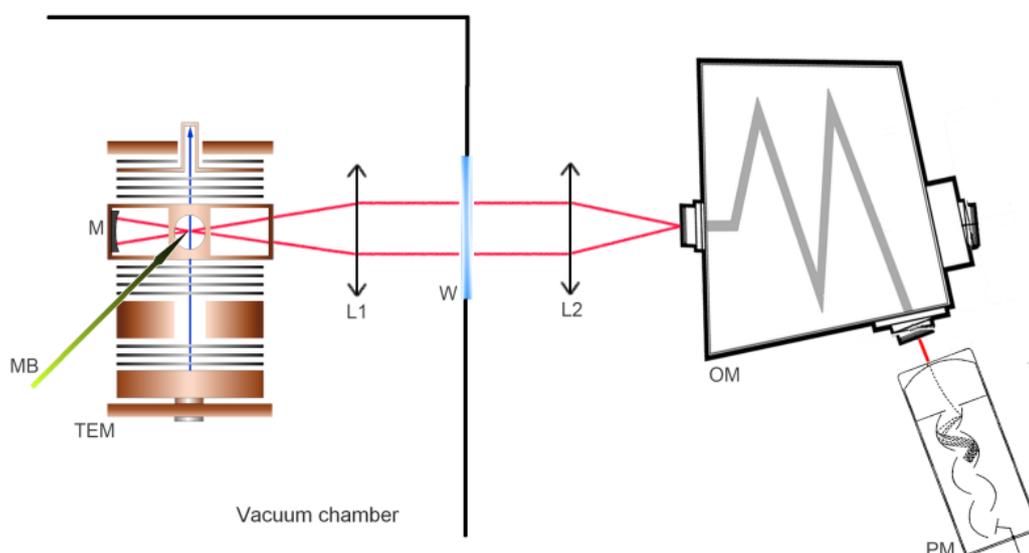


Figure 2.1. The scheme of the EIFA. MB-molecular beam, TEM-trochoidal electron monochromator, M-mirror, L1-lens, W-window, L2-lens, OM-Czerny-Turner optical monochromator, PM-photomultiplier. Adjusted from [20].

EIFA consists of the ultra – high vacuum chamber, 6-way cross made of stainless steel sealed with CF (Con – Flat) flanges with copper gaskets (Fig.2.1). The chamber is pumped out by two stage vacuum system consisting of the three-stage membrane pump, *Pfeiffer Vacuum MVP 055-3*, for generation of pre-vacuum and the *Pfeiffer Vacuum TNU 261*, the turbo pump for the final background pressures typically 10^{-8} mbar after the baking of the chamber with resistive wire. Pressure measurement inside the vacuum chamber is done by Penning gauge, *Pfeiffer Vacuum IKR 251*, operating in range 1×10^{-2} – 2×10^{-9} mbar. Measurement of the pre-vacuum, between the turbo and the membrane pumps is done by Pirani gauge, *Pfeiffer Vacuum TRP 281*, operating in range between 1×10^3 – 5×10^{-4} mbar. The gas inlet system consists of standard Swagelok VCR tubes with outer and inner diameter of 6 mm and 4 mm, respectively. Tubes are made of steel and connected with copper gaskets forming the double cross with six ends. Two of the ends are used for the pumping and pressure monitoring: the inlet system is pumped by the rotary pump, and the pressure is monitored by piezo-electric vacuum gauge, *Pfeiffer Vacuum APR 260*, with operating range 1.1×10^3 – 1×10^{-1} mbar. Inlet system has three free ends for the sample supply connection, either for the gas cylinders or liquid sample holder. The sixth end connects the inlet system with the vacuum chamber through the effusive capillary, with 5 mm length and 0.5 mm inner diameter. The pressure in the capillary is measured by *Pfeiffer Vacuum CMR 364*, absolute capacitance gauge, operating in range of 1.1 – 1×10^{-4} mbar, and regulated by fine

needle valve, *Pfeiffer Vacuum UDV 046*. In the vacuum chamber, effusive molecular beam meets monoenergetic beam of electrons in the reaction chamber of the trochoidal electron monochromator (TEM), or the electron gun (EG). The monochromator has been designed and manufactured in our group [16]. It consists of 18 electrodes with adjustable potentials so the kinetic energy of electrons can be varied in range between around 0 eV to 100 eV (changing the voltage source we could perform measurements at higher energies). Electrons are thermally emitted for a commercial tungsten hairpin filament, *Agar Scientific A054*, due to the heating of the filament to temperatures of about 2000K with current flowing through the filament (2 – 2.25 A). Except electrons, filament emits photons as well, so the cavity of the first and the second electrodes is covered with the colloidal graphite. Interaction of monochromatized beam of electrons and effusive molecular beam occurs in the interaction region of the TEM. Working pressure inside the chamber is 10^{-4} mbar ensuring the single collision event. Electrons that do not interact with molecules are passing through next three electrodes until they reach the fourth electrode having the role of the electron collector – Faraday cup, connected with picoammeter *Keithley 6485*. Electron current is typically 10^1 - 10^2 nA, in case of TEM, while with monochromator we can achieve higher currents μ A, but in contrast to energy resolution of TEM of about 300 meV at 10^2 nA, energy resolution of EG has not been better than 0.5 eV. Collection of the optical signal from the EIF, DE or DIE is done by optical elements (mirror, lenses, window, and optical monochromator) and photomultiplier. Currently we are using the *Oriel Cornerstone™ 260 Czerny – Turner* optical monochromator with operating range 180 – 1400 nm given by two different grids: 180 – 650 nm holographical grid and 200 – 1400 nm standard grid. Optical resolution of the monochromator is determined by the width of the entrance and exit slits. At 200 μ m opening, the resolution on the Ar 294.3 line is about 0.7 nm whilst at 100 μ m 0.4 nm resolution is achieved. The working range in UV – VIS demands usage of optical elements made of UV suitable materials: the lenses are made of UV fused silica, mirror is coated with UV enhanced aluminum and window separating the vacuum and non-vacuum region is made of MgF_2 . Detection of the photon signal which passes through the optical monochromator is done by the photomultiplier, *Hamamatsu R4220P*. The photomultiplier working range is 185 – 710 nm and it is thermoelectrically cooled to -15° C to assure very low noise intensity (less than 2counts/s) and high quantum efficiency.

2.1.2 General overview on the HEM setup

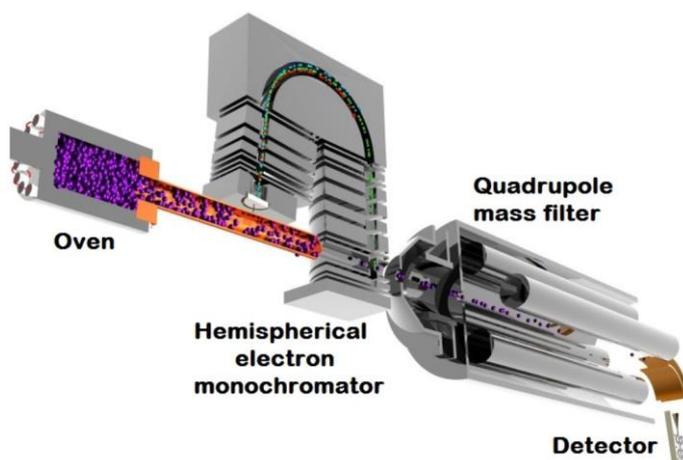


Figure 2.2. The scheme of the HEM. [21]

Similarly as EIFA, the HEM setup comprises of 6-way cross stainless steel ultra – high vacuum chamber sealed with CF flanges and copper gaskets or rubber sealing rings (Fig.2.2). On the bottom side, a *Pfeiffer Vacuum TMU 521 P* turbomolecular pump is attached to the chamber. For generation

of pre-vacuum (~ 1 mbar) a three stage *Vacuubrand MD 4C NT* diaphragm pump is used. With this vacuum system, the HEM chamber can be pumped down to pressures of 10^{-8} mbar. Pre-vacuum pressure measurement is performed with a *Varian ConvecTorr P-Type gauge*, which is a thermal conductivity gauge with operation range starting at atmospheric pressure and going down to 10^{-4} mbar, whereas at high vacuum the pressure is measured with a hot cathode Bayard-Alpert ionization gauge, *UHV-24 Nude of Varian Agilent*, covering the range 10^{-3} - 10^{-10} mbar. In order to prevent the hemispherical electron monochromator (HEM) from getting severely covered with layers of molecules and molecular residues of samples measured in HEM setup, the chamber is heated with halogen lightbulbs which are placed inside the chamber in close proximity of the HEM. By heating the chamber up to approximately 90°C and pumping down for couple of days base pressures in range of 5×10^{-9} mbar can be achieved. The HEM is placed in the chamber from the upper side of the 6-way cross with all electrical connections on the same flange as the monochromator, which makes the installation of the HEM into the chamber more practical on this setup in contrast to the EIFA where the electrical connections and the TEM are placed on the separate flanges. The HEM will be discussed in more detail in the next section. For the mass selection of ionic fragments formed in the interaction region of the HEM, a quadrupole mass selector is used. It is attached to the chamber 90° in respect to the HEM. The quadrupole used in this study is commercially available *QMG 700 HiQUAD* from *Pfeiffer Vacuum*. Several high frequency heads for examination of ions belonging to different mass regions are available: *QMH 400-5* (up to 512 u), *QMH 410-1* (up to 1024 u) and *QMH 410-2* (up to 2048 u). Between the monochromator and the quadrupole, the ion optics is placed in such way that the ions produced in the interaction region are extracted towards the quadrupole. The first lens of this system is a conically shaped lens, *Optik aussen (O_a)*, positioned in close proximity to the interaction region (< 0.05 mm). O_a should be kept on voltage values in the range 30-70 V to avoid the extraction of electrons into the quadrupole. As a part of the Einzellens system, *Optik innen (O_i)* is placed after the O_a . The quadrupole DC component (field-axis, *FA*) is manually tunable, and it is used for the focusing of the ions into the quadrupole. The second function of *FA* is the adjustment of kinetic energy of the ions in combination with *Ionenergie*, where latter is the floating potential of all of the lenses of the HEM in respect to ground. Adjusting the *Ionenergie* and *FA* is used for optimizing the ion signal on the detector. Maximizing the signal of the specific fragment deteriorates the mass resolution. At the exit of the quadrupole region, two deflectors of parabolic shape, *Def i* and *Def a*, are placed. This configuration provides homogenous electric field which guides the ions from the quadrupole to the detector. The drawback to this design is contribution of the metastables to the ion signal. Since the directed beam of neutrals can pass through the quadrupole metastables with lifetimes in range of microseconds and larger can reach the *Def a* and produce secondary electron species that are further accelerated towards the detector and result in false ion signal. Finally, for the detection of the ions, a secondary electron multiplier detector, a Channel Electron Multiplier (CEM) from *Dr. Sjuts Optotechnik GmbH*, model *KBL 510*, is used. A gas inlet system for introduction of calibration gases into the chamber is connected via Swagelok VCR tubes. Simultaneous or separate introduction of CCl_4 and SF_6 in the gas phase is possible via series of precession valves and separate gas inlet lines connected to a common gas inlet pre-vacuum pump. An important part of the WIPPI setup is the vacuum security. The vacuum security serves to prevent unwanted events that are leading to an increase of the pressure (higher than 9×10^{-6} mbar) in the chamber to damage filament of the HEM, quadrupole and the detector by switching the aforementioned devices off in case of such an event. Three pairs of coaxial coils (Helmholtz coils) are used to produce magnetic field that reduces Earth's magnetic field and stray magnetic fields in the HEM region and thus allows to achieve high resolution electron energy beam. Since low energy electron trajectories are strongly influenced by the magnetic field, proper settings of the Helmholtz coils are crucial for the performance of the HEM setup.

3 Fluorescence measurements on EIFA

3.1 Hydrogen and deuterium

The extensive study on hydrogen molecule by means of electron induced fluorescence has been performed using EIFA. In thesis of Marian Danko the ongoing research on Balmer lines and Fulcher series was summarized [22]. After the additional measurements and analysis the results regarding Balmer series and Fulcher alpha band were published in Plasma Sources Science and Technology [23]. Also, the continuum radiation of hydrogen molecule was examined and the detailed study is planned to be published together with theoretical calculations concerning this system. Further, we have examined the deuterium molecule in order to compare the emission spectra and photon efficiency curves for particular transitions with corresponding analogues of hydrogen molecule.

We have studied PECs of $H_2(a^3\Sigma_g^+ \rightarrow b^3\Sigma_u^+)$ continuum at several different wavelengths in the region between 5 – 100 eV electron impact energy. [22] As a benchmark for the analysis of the PECs the excitation cross section $H_2(a^3\Sigma_g^+ \leftarrow X^1\Sigma_g^+)$ from Ajello and Shemansky was used [24]. PECs obtained at 230 nm and 650 nm on EIFA were compared to the excitation cross section and showed strong correlation in shape: both yields show the threshold around 12 eV and the peak maximum around 15 eV which is followed by the rapid falloff with the electron impact energy (Figure 4.5 a). However, in the region higher than 40 eV possible contribution of cascades can play role in the photon yield measured with EIFA and result in difference between the excitation cross section from previous authors and our data. We would like to point out that the shapes of PECs measured at 230 nm and 650 nm are very similar which implies that both originate from the transition $H_2(a^3\Sigma_g^+ \rightarrow b^3\Sigma_u^+)$ which is proven for the first time [22]. No other hydrogen molecular bands nor hydrogen atom lines are predicted to appear at 650 nm, thus it can be concluded that the PEC obtained at 650 nm on EIFA is the result of purely continuum radiation. In deuterium, measurements of the PECs at 230 nm, 360nm, and 650 nm were performed and the threshold energies were determined. For the measurement at 650 nm, filter for low wavelength cut off (400 nm) was used and the obtained curve is shown in Figure 3.1.

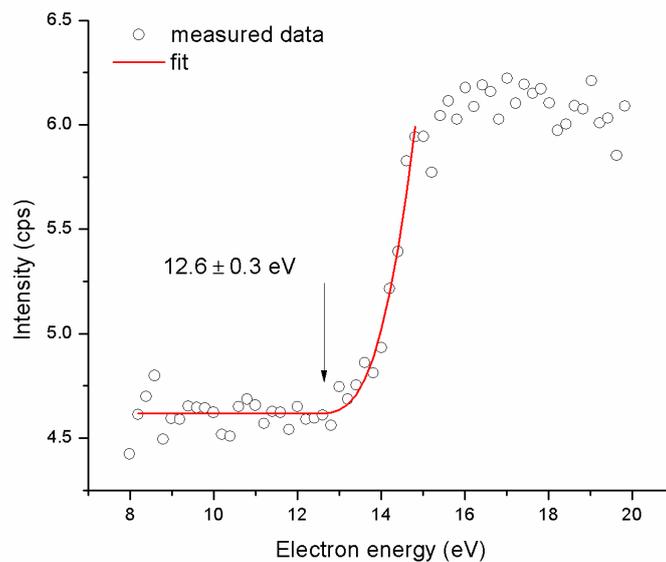


Figure 3.1. PECs recorded at 650 nm in deuterium corresponding to $D_2(a^3\Sigma_g^+ \rightarrow b^3\Sigma_u^+)$ continuum radiation.

3.2 Nitromethane

The electron induced emission spectrum of nitromethane in the range between 200 – 670 nm was recorded and the most intense lines and bands were identified, hydrogen Balmer lines, CH bands and CN violet bands. Although very low in intensity, photon yield in UV region proves the OH radical formation at low energy electron impact to nitromethane. High threshold of overlapping bands, CN ($B^2\Sigma^+ \rightarrow X^2\Pi$) and CH ($B^2\Sigma^- \rightarrow X^2\Pi$) around 388 nm, observed in PEC indicates efficient energy transfer to internal degrees of freedom to fragmented nitromethane in electron impact dissociation process. Presence of CN tail bands in emission spectrum obtained at 50 eV supports this assumption.

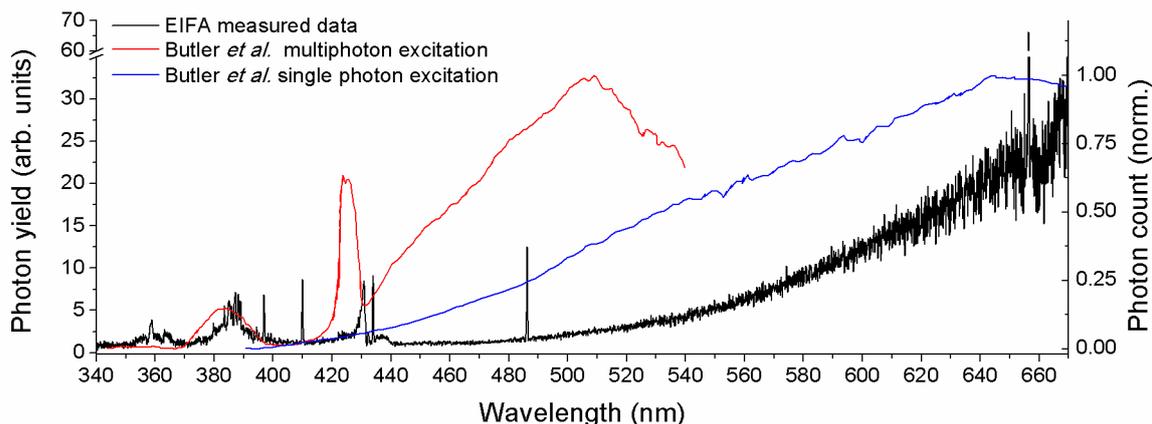


Figure 4.11. NO_2 continuum radiation in comparison to previous studies. [25].

Strong oxidation of the tungsten filament used on EIFA in presence of nitromethane caused frequent interruptions of the measurements and prevented from more detailed investigation of the molecule. The problem can be solved by using a filament made of chemically resistant material in presence of nitromethane, which would inquire major reconstruction of the current setup, thus at this point it is inconvenient to proceed with the investigation.

3.3 Ironpentacarbonyl

Ironpentacarbonyl was investigated on EIFA within the framework of CELINA [10]. One of the goals of this COST action is to gain a better understanding of the elementary processes occurring within focused electron-beam induced deposition (FEBID) [10]. Elementary processes of ironpentacarbonyl of electrons and photons have been investigated in the past, as well as the electronic structure and of the molecule, experimentally and theoretically [26-35]. Recently, also the aggregates of this molecule were probed [36]. Fluorescence of this molecule has been studied in the past by Hale [35], and much improved data set was obtained now on EIFA. Dissociative excitation study of ironpentacarbonyl molecule on EIFA was enclosed with a paper, which is published in European Physics Journal D and it is available in the Appendix B. The paper is a result of a joint effort of all coauthors. The experimental investigation was mainly performed by myself, with the assistance of Marian Danko and Juraj Orszagh, as well as Filipe Ferreira da Silva, who visited the lab with a Short Term Scientific Mission. Full analysis of the data as well as the preparation of the manuscript was done by myself, with the input from all of the authors. The whole study was led by prof. Matejčík.

4 Gas phase measurements on the HEM setup

4.1 2-Nitroimidazole

Researchers have found compounds that specifically target cancer cells, make them more sensitive to ionizing radiation and thus enhance the radiation damage to the target tissue. These compounds are referred to as *radiosensitizers* [37], and the effect which they have on the tumor tissue development differs from one type of the radiosensitizer to another. It is crucial to gain a better understanding of processes in the radiated cell on molecular scale. It has long been known that nitroimidazoles increase DNA damage caused by ionizing radiation in hypoxic cells. In general, it is considered that the ionizing radiation is responsible for free radical formation and subsequent damage to DNA. Nevertheless, we still don't have a clear understanding of elementary processes on electron-molecular scale in hypoxic tumor cells in presence of nitroimidazoles [38]. However, recently the interaction of nitroimidazolic compounds with LEEs was investigated by means of mass spectroscopy for the first time [39, 40]. Simple bond cleavages resulting in NO_2 , NO_2^- formation or H loss were observed at electron attachment energies below 8 eV for 4-nitroimidazole (4NI) and its methylated derivatives, 1-methyl-4-nitroimidazole (Me4NI) and 1-methyl-5-imidazole (Me5NI) [39]. More complex reactions, such as loss of NO, HNO_2 , or CN^- formation also take place at low electron energies. More importantly, high ion yield for the loss of OH^* from 4NI has been detected at energies below 2eV with maximum very close to 0 eV [40]. Investigation of the methylated derivatives of 4NI showed complete quenching of DEA channels close to 0 eV, thus lowering the reactivity of the compound. Going back to radiosensitive properties of nitroimidazoles, this finding of effective generation of radicals from 4NI at very low energies, might be the key to understanding of its radiosensitizing property.

Another isomeric form of nitroimidazole, 2-nitroimidazole (2NI), was investigated within my studies. The investigation was performed on the HEM setup, at similar conditions as for the previous study with 4-nitroimidazole. The manuscript submitted to Chemistry – A Eur. J. is accompanied with the extensive supporting material, mainly containing the details on calculations. Also, additional graphs and the table with the experimental results are included in the supporting material, also included in the thesis.

4.2 Imidazole

Imidazole is a simple heterocyclic nitrogen containing molecule, which is a structural constituent of many biologically relevant molecules, e.g. histidine (amino acid), or purine derivatives, such as adenine and guanine, the DNA purine nucleobases. The pyrimidine nucleobases, cytosine, thymine and uracil, are chemically related to benzimidazole, which also contains imidazole in its structure. Thus, the motivation to study and gain a better understanding on imidazole reactivity in presence of slow electrons ($\sim 0\text{-}10^2$ eV) is great, not only due to the questions related to electron induced astrochemistry, but also to understand the interactions of slow electrons with imidazolic compounds in biological tissues [7]. Imidazole is a building block of many antifungal drugs and antibiotics. As it has been pointed out in previous sub chapter on the potential radiosensitizers, 2NI and 4NI, are imidazolic compounds proposed as potential radiosensitizers [41].

In the course of my PhD thesis the formation of negative ions upon DEA to imidazole was studied. The results were published in PCCP [42] and showed surprising loss of all four hydrogens in DEA at energies above the ionization energy of imidazole.

5 Clusters measurements on the HEM setup

The examination of meteorites proved that neon, as well as other rare gases, such as argon or helium, have a role in mineral formation in outer space [43]. It is, possible that the formation of more complex systems is mediated by neon in atomic form, or even more likely upon interaction with aggregates of neon. Astrochemically relevant complexes, such as fullerenes, are examined in cold matrices under laboratory controlled conditions to get information that could be later directly compared with the outer space observations. Considerable work has been done using solid neon, e.g. deposited on rhodium-coated sapphire plate at temperatures as low as 6K and observing the behavior of the system altered upon laser ablation and absorption spectroscopy [44].

However, these examples prove that the neon cluster is a peculiar system where both classical and quantum approaches have to be employed to understand the behavior of the system upon its growth. Also it is apparent that the doping of neon clusters at carefully regulated experimental conditions using specific experimental techniques can lead to valuable information about the structure and the dynamics of the system. With the setup such as HEM we have an opportunity to improve the existing knowledge on neon clusters behavior upon the interaction with low energy electrons, and to investigate electron attachment, a technique which has never so far been used for neon clusters. Based on the charge state of the products observed, this research is divided into positive ion and negative ion studies. Both, pristine neon clusters and the neon clusters doped with CO₂ using the pickup technique were studied. Thus, this section is divided into two sub-sections where the results of the studies will be presented: appearance energy determination (positive ions) and the electron attachment study (negative ions). The first sub-section contains the results and the discussion on the pristine clusters and doped clusters. The attachment study was performed with CO₂ doped neon clusters and the results and the discussion will follow the appearance energy sub-section.

5.1 Bare neon clusters

In the present study of bare neon clusters a 20 μm pinhole nozzle was used. The nozzle was cooled down to temperatures as low as 60 K at neon pressures from 2 bar up to ~5 bar. The focus was placed on the examination of the appearance energies of neon clusters and two data sets at approximately the same conditions were obtained. The formation of all probed cluster ion sizes (2-7 in this study) requires less energy than the ionization energy of neon atom. We propose here for the first time that neon clusters, similarly as argon clusters, are formed via autoionizing Rydberg states.

Table 5.1. The AEs and exponents (exp.) from the fits are presented for neon clusters of sizes N=2-7 obtained in two independent measurements in the present study marked as data set 1 and data set 2; the average of two data sets is presented further, as well as the results of Fiegele and Trevor [45, 46].

ion	present results (eV)					Fiegele (eV)	Trevor (eV)
	data set 1	exp.	data set 2	exp.	average		
Ne ⁺	21.565 ± 0.01	1.265	21.565 ± 0.02	1.38		21.567	21.567
Ne ₂ ⁺	20.89 ± 0.18	1.70	21.12 ± 0.08	1.36	21.00 ± 0.09	21.004*	20.33±0.08
Ne ₃ ⁺	21.15 ± 0.05	1.30	21.29 ± 0.03	1.31	21.22 ± 0.03	21.028	
Ne ₄ ⁺	20.96 ± 0.06	1.54	21.06 ± 0.04	1.46	21.01 ± 0.04	21.048	
Ne ₅ ⁺	21.13 ± 0.04	1.28	21.27 ± 0.05	1.30	21.20 ± 0.03	21.048	
Ne ₆ ⁺	20.81 ± 0.39	1.72	21.10 ± 0.21	1.38	20.95 ± 0.21	21.039	
Ne ₇ ⁺	20.97 ± 0.54	1.54	21.16 ± 0.42	1.37	21.06 ± 0.34	21.066	

*the value is probably obtained at 70K in contrast to N=3-7 obtained at 80K

The difference between the results obtained in this study and previous studies might be explained by the initial neutral cluster size distribution. The ionization mechanisms employed in the formation of positive ion of specific size from smaller clusters could lead via higher excited Rydberg states which results in higher AE. In order to better interpret the experimentally obtained values of the appearance energies, further computational input is necessary.

5.2 Positive ion investigation of CO₂ doped Ne clusters

The beam of neon clusters doped with CO₂ was crossed with the beam of electrons and examined by means of mass spectrometry on the HEM setup. Positive ion formation from neutral mixed CO₂/Ne clusters was observed for the first time in the region of electron impact energies near threshold for ionization. Also, positive ion formation was examined at energies around 70 eV.

Investigation of positive ions formed from the electron impact of CO₂ doped neon clusters showed the dominance of ions of $[(\text{CO}_2)]_k^+$ type in the examined m/z region at 70 eV electron energy. Further, analysis of the obtained ion efficiency curves revealed four major ionization mechanisms: ionization via CO₂ ionization, neon atom excitation into the metastable excited states, neon ionization and possible neon cluster ionization prior to fragmentation and formation of $[\text{CO}_2]_k^+$ type ions. Further development of the threshold fitting technique would improve the analysis of this high-resolution electron impact study. Theoretical calculations could support suggested ionization pathways, thus the further investigation of this system is preferable prior to conclusion on the behavior of small neon clusters doped with CO₂.

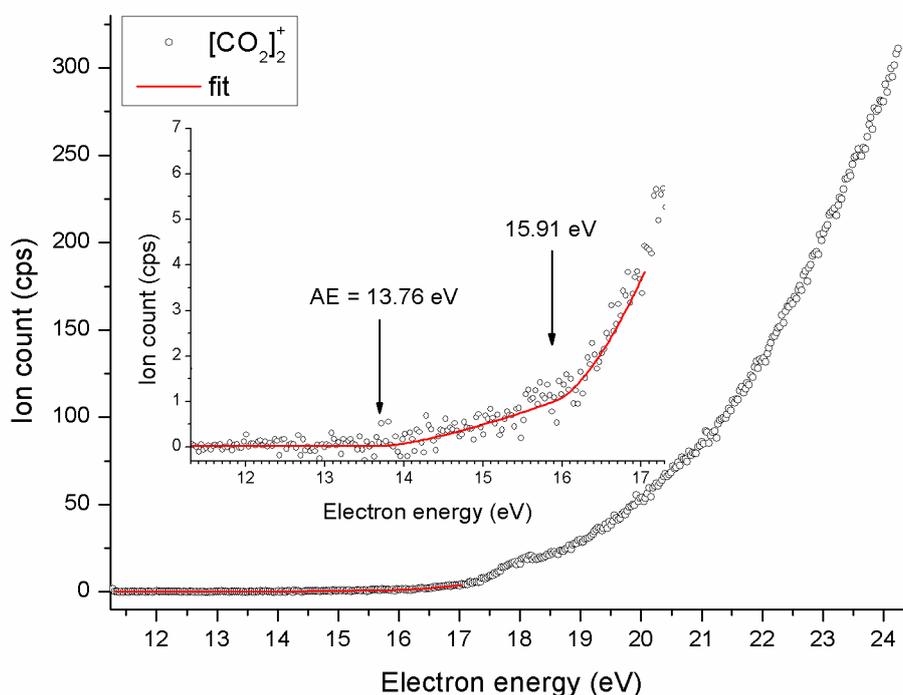


Figure 5.1. Ion efficiency curve corresponding to $[\text{CO}_2]_2^+$ measured at 4.8 bar neon stagnation pressure before the 20 μm pinhole nozzle cooled down to the temperature of 50 K after the background subtraction. Inserted panel is a close-up of the threshold region.

5.3 DEA to CO₂ doped neon clusters

The study on DEA to CO₂ doped neon clusters brought interesting, but rather complex results for the interpretation. In summary three main points of the investigation can be drawn:

- 1) The nature of the clusters work against each other here: CO₂ clusters with the increase of the size shift the features such as resonance positions to lower energies due to polarization effect (red-shift) while neon clusters provide finite barrier (blue shift) for the incoming electron, which is also size dependent property.
- 2) The initial neutral neon cluster size distribution is possible to calculate, while the size of CO₂ clusters formed on such neon clusters is quantitatively unavailable parameter, although qualitatively with the increase of the mean cluster size of neon also CO₂ cluster size should increase.
- 3) The postulate that the simplest answer is usually the right one has failed here: all three observed resonances seem to come from different neutral precursor size.

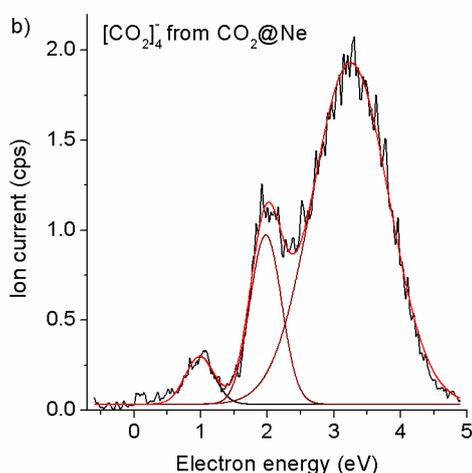


Figure 5.2. Electron energy scan of $[CO_2]_4^-$ from the electron impact study of CO₂ doped Ne clusters.

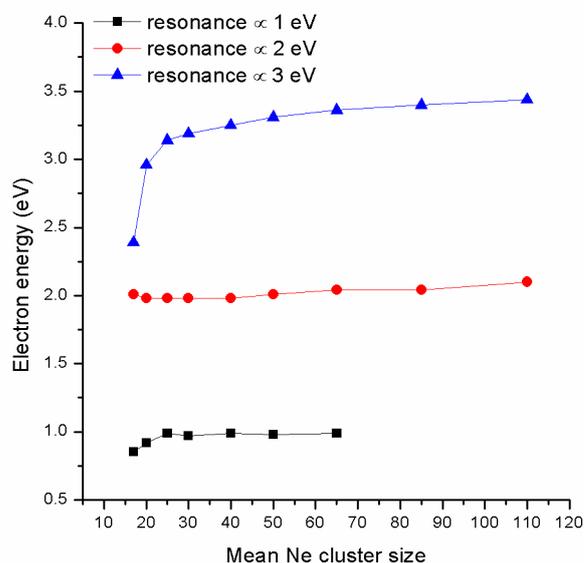


Figure 5.3. Change of the resonance position with the mean size of neon clusters

The lowest resonance is situated at around 1 eV, and in range of probed neon cluster sizes, $\langle N \rangle_{Ne} = 17 - 110$, its position shows minor dependence on the cluster size. The position is the lowest when the smallest neon clusters are formed, 0.85 eV, and the highest, 0.99 eV, for the largest investigated neon matrix. This resonance is attributed to VFRs observed in pristine clusters, which are here shifted due to the neon matrix. The second resonance, appearing in range 2.01 – 2.10 eV depending on the cluster size, shows greater cluster size dependence. It is, however, attributed to the resonant scattering feature observed in both gas phase scattering experiments as well as in DEA to pristine clusters. The position of the resonance is shifted towards lower energies in this study in respect to the pristine cluster investigation probably due to the larger CO₂ cluster size which are formed by pickup on neon matrix in this study. At this resonance, the effect from both cluster species is recognizable: the blue shift is present when going to larger neon matrix clusters, but it superimposes to the red shift due to the larger CO₂ clusters in respect to pristine cluster study. The third resonance, observed around 3 eV, is associated with the ${}^2\Pi_u$ shape resonance. It has similar behavior as the resonance at around 2 eV with more prominent blue shift due to the increase of the neon matrix. It must be noted that the shifts within one measurement are not the same for the two

higher resonances, indicating that the neutral precursor for the resulting negative ion cluster is not the same. The ratio of the intensities of the resonances around 3 eV and the one around 2 eV becomes larger with the increased size of the cluster, which is in line with observations in pristine clusters.

Summary and outlook

Seemingly broad subject introduced already in the title was divided into three main experimentally investigated themes: fluorescence induced by electrons, gas phase molecular interactions with electrons probed by means of mass spectroscopy, and investigation of clusters of atoms and molecules. Studies were conducted on two experimental setups, EIFA for the fluorescence measurements and the HEM setup for mass spectrometric research.

In the electron induced fluorescence study hydrogen, deuterium, nitromethane and ironpentacarbonyl were investigated. First three are astrochemically relevant molecules. Hydrogen is the most abundant specie in space and it plays a significant role in interactions with other species, but its emission is also an important diagnostic parameter. The improvement of the knowledge on the absolute cross sections, here more specifically emission cross sections induced by electrons of energies in range 5 – 100 eV, is crucial not only for the astro-community, but also for plasma diagnostics. The results presented in this thesis were published in *Plasma Sources Science and Technology* titled Electron induced fluorescence of the H₂ molecule-Balmer lines and Fulcher alpha system. In the study, absolute cross sections for some of the transitions within the Balmer series were presented for the first time, as well as the rovibronic lines of Fulcher alpha system, both being important diagnostic parameters in plasmas. Nowadays, subject of energy sources that will provide us with healthier environment and reduce the emission of greenhouse gases is more important than ever. Tokamaks, reactors that will be using energy from the fusion of hydrogen isotopes to produce electrical energy, are hope for a better tomorrow. Hand in hand with this challenge, deuterium molecule was further studied by means of electron induced fluorescence and found to emit observable continuum radiation in visible region of electromagnetic spectrum, which has never been observed by optical spectroscopy before. The results are presented here and compared with recently discovered hydrogen emission in same region by our group. Nitromethane molecule investigation was a challenging task which resulted in the observation of the emission spectrum with resolved vibrational structures of several molecular bands, features that were observed for the first time in this quality. Production of vibrationally excited fragments from nitromethane could have implications for the chemistry of interstellar medium, where small nitro compounds are proven to be present, but have to date insufficiently well understood role in possible formation of more complex molecules. The last molecule presented in this thesis within the experimental study of electron induced fluorescence is ironpentacarbonyl. Fruitful cooperation within CELINA community led to the publication in *EPJD* available in this thesis on Dissociative excitation study of ironpentacarbonyl. This molecule is widely used in deposition techniques, such as FEBID, and in this study it was confirmed that the products of electron (0 – 100 eV) interaction with this molecule are mostly excited species of iron and carbonyl group. The emission spectrum, as well as photo efficiency curves were measured in region 200 – 470 nm and showed the dominance of iron lines and to some extent carbonyl bands.

Moving from the technological advances towards the human tissue, two nitro compounds were investigated in terms of mass spectrometry, 2-nitroimidazole and imidazole, by detecting negative ions from the dissociative electron attachment reactions. This resonant process is known to have very large cross sections, for some molecules even higher than the ionization cross section. For the two investigated molecules, dissociation by electron attachment in the electron range between

~0 – 15 eV has never been investigated in the gas phase before, to the best of my knowledge. This energy range is very significant due to the high abundance of such electrons in biological tissue upon radiation treatment. As imidazolic compound, 2-nitroimidazole is a potential radiosensitizer, molecule which can enhance the eradication of tumorous cells upon radiation treatment. In this thesis, the paper draft was included with the comparison of the reactivity of nitroimidazole isomers. It was shown that 2-nitroimidazole has more dissociative channels than 4(5)-nitroimidazole observable upon DEA. This, from our perspective, puts it in front of the 4(5)-nitroimidazole when it comes to the role of a radiosensitizer. Additionally, investigation of imidazole, the constituent of both investigated nitroimidazoles, but also purine basis, histamine, other drugs, etc., showed astonishing multiple bond breakage upon interaction with electrons with energies lower than 15 eV. Most of the resonances were observed around 7 eV and 11 eV, while the formation of dehydrogenated anion was triggered at energies lower than 2 eV. The paper was published in Physical Chemistry and Chemical Physics and it was included in this thesis.

The most complex investigation conducted within this study was certainly the investigation of pure neon clusters, and neon clusters doped with CO₂. Appearance energies for small neon clusters were observed in the range below the ionization energy of neon, implicating that Rydberg states are involved in this ionization pathway. Autoionization via Rydberg states is offered as an ionization mechanism responsible for the formation of neon clusters starting with the dimer. To investigate the influence of neon matrix on interaction of electrons with doped species, neon clusters were doped with CO₂ and positive ions of CO₂ cluster were studied at the threshold of their formation. Three distinct pathways of ion formation of CO₂ clusters were found, namely direct ionization of the CO₂ cluster, Penning ionization via electronically excited states of neon, and ionization via initial ionization of a neon atom. The interpretation of data obtained in dissociative electron attachment study of the doped neon clusters with CO₂ was challenging and is still preliminary. The distribution of both neon clusters and CO₂ clusters is statistic parameter which strongly differs for the two due to the mechanism of their formation. The size of target complex is known only to the limited extent and that is the mean neon cluster size prior to doping. Mixed clusters showed affinity towards electrons in such manner that dissociative electron attachment was observable via formation of negative ions of carbondioxide clusters. The most abundant cluster anion [CO₂]₄⁻ was investigated in this study at different conditions, meaning cluster sizes. Other negatively charged CO₂ clusters were observed in negative ion mass spectra, but more detailed investigation was out of the scope of the current research. Three resonances resulting in [CO₂]₄⁻ formation were observed, each originating probably from a different parent cluster. The opposite influence of the neon solvent, which tend to form a barrier for the incoming electron, and CO₂ clusters, which on the other hand have a positive electron affinity, made this investigation even more complex. The dependence of the resonance position on the parent cluster size, as well as the change of ratio of their intensities due to the neutral cluster size was observed for the two higher resonances, having the peak around 2 eV and 3 eV. Surprisingly, VFRs observed in pristine clusters around 0 eV were not observed in this energy region even at the smallest neon clusters size, which was 17 in this investigation.

Hydrogen and deuterium have been extensively studied throughout the history, but technical improvements of the experimental setups will lead to more reliable cross sections, which would refine the modeling results and lead to better understanding of elementary processes. Thus, for example, further investigation of continuum radiation from both hydrogen and deuterium is necessary. Investigation of the photon efficiency curves of nitromethane, especially in the threshold region, would contribute to the knowledge on neutral species formation in the interstellar medium. Extending the research conducted on imidazole and 2-nitroimidazole to fluorescence study is technically challenging but possibly beneficial step towards better understanding of neutral fragment

formation from these molecules. Neutral radicals, such as OH, CH or H have rich emission spectra in UV-VIS region, and thus can be observed on EIFA. However, compounds with low vapor pressure which are solids at normal conditions have never been investigated on this setup before. Many other potential radiosensitizers or radiosensitizers that have already been used, such as nimorazole, could be investigated by both, DEA and fluorescence study. In addition, the neon cluster source used in this study, offers wide variety of possibilities for future studies. Probing larger clusters, doping neon with biologically relevant molecules to mimic cold environment of outer-space ices where potentially life could have been formed, investigating the bulk properties by controlled size change of the target complexes are just handful of vast possibilities that this system offers.

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Zoznam publikácií

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Registrované v: wos, scopus
Ohlasy (4):
[o1] 2016 De Teresa, J. M. - Fernandez-Pacheco, A. - Cordoba, R. - Serrano-Ramon, L. - Sangiao, S. - Ibarra, M. R.: Review of magnetic nanostructures grown by focused electron beam induced deposition (FEBID). In: Journal of Physics D-AppliedPhysics, Vol. 49, No. 24, 2016, Art. No. 243003 - SCI ; SCOPUS
[o1] 2016 Lengyel, J. - Fedor, J. - Farnik, M.: Ligand Stabilization and Charge Transfer in Dissociative Ionization of Fe(CO)(5) Aggregates. In: Journal of Physical Chemistry C, Vol. 120, No. 31, 2016, s. 17810-17816 - SCI ; SCOPUS
[o1] 2016 Lengyel, J. - Kocisek, J. - Farnik, M. - Fedor, J.: Self-Scavenging of Electrons in Fe(CO)(5) Aggregates Deposited on Argon Nanoparticles. In: Journal of Physical Chemistry C, Vol. 120, No. 13, 2016, s. 7397-7402 - SCI ; SCOPUS
[o1] 2017 Skoviera, J. - Neogrady, P. - Louis, F. - Pitonak, M. - Cernusak, I.: Caesium hydride: MS-CASPT2 potential energy curves and A(1)Sigma(+)-> X-1 Sigma(+) absorption/emission spectroscopy. In: Journal of Chemical Physics, Vol. 146, No.10, 2017, Art. No. 104304 - SCI ; SCOPUS
- ADC03 Al Maalouf, Elias Jabbour (50%) - Reitsammer, Julia (5%) - Ribar, Anita [UKOMFKEFd] (20%) - Scheier, Paul (10%) - Denifl, Stephan (15%): Helium anion formation inside helium droplets
Lit. 39 záz. n., 3 obr., 2 tab.
In: European Physical Journal D. - Vol. 70, No. 7 (2016), Art. No. 148, s. 1-5
Registrované v: wos, scopus
Ohlasy (1):
[o1] 2016 Lengyel, J. - Fedor, J. - Farnik, M.: Ligand Stabilization and Charge Transfer in Dissociative Ionization of Fe(CO)(5) Aggregates. In: Journal of Physical Chemistry C, Vol. 120, No. 31, 2016, s. 17810-17816 - SCI ; SCOPUS
- ADC04 Danko, Marián [UKOMFKEFs] (30%) - Ribar, Anita [UKOMFKEFd] (30%) - Országh, Juraj [UKOMFKEF] (10%) - Matejčík, Štefan [UKOMFKEF] (10%) - Ďurian, Michal [UKOMFKEFd] (20%): Electron induced fluorescence of the H-2 molecule-Balmer lines and Fulcheralpha system
Lit. 34 záz. n.
In: Plasma Sources Science & Technology. - Vol. 25, No. 6 (2016), Art. No. 65007, s. 1-8
Registrované v: wos

ADC05 Ribar, Anita [UKOMFKEFd] (70%) - Fink, Katharina (5%) - Li, Z. (5%) - Ptasińska, Sylwia (5%) - Carmichael, I. (5%) - Feketeová, L. (5%) - Denifl, Stephan (5%): Stripping off hydrogens in imidazole triggered by the attachment of a single electron
Lit. 65 záz., 8 obr., 1 tab.
In: Physical Chemistry Chemical Physics. - Vol. 19, No. 9 (2017), s. 6406-6415
Registrované v: wos

AFC Publikované príspevky na zahraničných vedeckých konferenciách

AFC01 Danko, Marián [UKOMFKEFs] (40%) - Országh, Juraj [UKOMFKEF] (25%) - Ribar, Anita [UKOMFKEFd] (25%) - Matejčík, Štefan [UKOMFKEF] (8%) - Denifl, Stephan (2%): Population of excited states of hydrogen leading to balmer series emission and their threshold energies studied by electron induced fluorescence in methane molecule
Recenzované
Lit. 12 záz., 4 obr.
In: WDS 2012: Proceedings of Contributed Papers: Part II Physics of Plasmas and Ionized Media. - Prague : MATFYZPRESS, 2012. - S. 111-117. - ISBN 978-80-7378-225-2
[WDS 2012 : Week of Doctoral Students : Annual Conference of Doctoral Students. 21st, Prague, 29.5.-1.6.2012]

AFC02 Danko, Marián [UKOMFKEFs] (25%) - Országh, Juraj [UKOMFKEF] (25%) - Ribar, Anita [UKOMFKEFd] (25%) - Matejčík, Štefan [UKOMFKEF] (25%): Electron induced emission of methane
Lit. 3 záz.
In: 21st Europhysics Conference on Atomic and Molecular Physics of Ionised Gases: Proceedings [elektronický zdroj]. - Lisbon : European Physical Society, 2012. - s. 1-2 [CD ROM]. - ISBN 2-914771-74-6
[ESCAMPIG 2012 : Europhysics Conference on Atomic and Molecular Physics of Ionised Gases. 21st, Viana do Castelo, 10.-14.7.2012]

AFC03 Országh, Juraj [UKOMFKEF] (25%) - Danko, Marián [UKOMFKEFs] (25%) - Matejčík, Štefan [UKOMFKEF] (25%) - Ribar, Anita [UKOMFKEFd] (25%): Fluorescence of methane induced by electron impact
Lit. 8 záz., 2 obr.
In: HAKONE XIII. - Lublin : Lublin University of Technology, 2012. - S. 225-227. - ISBN 978-83-62596-99-7
[HAKONE 2012 : International Symposium on High Pressure Low Temperature Plasma Chemistry. 13th, Kazimierz Dolny, 9.-14.9.2012]

AFC04 Ribar, Anita [UKOMFKEFd] (50%) - Danko, Marián [UKOMFKEFs] (20%) - Országh, Juraj [UKOMFKEF] (20%) - Matejčík, Štefan [UKOMFKEF] (10%): Study of dissociative excitation processes of Fe(CO)₅
Lit. 6 záz., 5 obr.
In: WDS 2014 : Part-Physics. - Praha : MATFYZPRESS, 2014. - S. 296-301. - ISBN 978-80-7378-276-4
[WDS 2014 : Week of Doctoral Students : Annual Conference of Doctoral Students. 23rd, Prague, 3.-5.6.2014]

AFC05 Ribar, Anita [UKOMFKEFd] (40%) - Szymańska-Skolimowska, Ewelina (10%) - Danko, Marián [UKOMFKEFs] (20%) - Matejčík, Štefan [UKOMFKEF] (20%) - Mason, Nigel J. (10%): Low energy electron interactions with nitromethane
Popis urobený 20.1.2015
Lit. 10 záz., 2 obr. 1 tab.
In: 27th Summer School and International Symposium on the Physics of Ionized Gases : Contributed Paper [elektronický zdroj]. - Belgrade : Institute of Physics, 2014. - S. 86-89 [online]. - ISBN 978-86-7762-600-6
[SPIG 2014 : Summer School and International Symposium on the Physics of Ionized Gases. 27th, Belgrade, 26.-29.8.2014]
URL: <http://www.spig2014.ipb.ac.rs/doc/SPIG2014-book-online.pdf>

AFD Publikované príspevky na domácich vedeckých konferenciách

- AFD01 Danko, Marián [UKOMFKEFs] (20%) - Országh, Juraj [UKOMFKEF] (20%) - Ribar, Anita [UKOMFKEFd] - Kočišek, Jaroslav [UKOMFKEFd] (20%) - Matejčík, Štefan [UKOMFKEF] (20%): Electron impact excitation of the second positive system of N₂
 Recenzované
 Lit. 5 záz., 4 obr., 1 tab.
 In: HAKONE XII. - Bratislava : FMFI UK, 2010. - S. 103-107. - ISBN 978-80-89186-72-3
 [HAKONE 2010 : International Symposium on High Pressure Low Temperature Plasma Chemistry. 12th, Trenčianske Teplice, 12.-17.9.2010]
- AFD02 Danko, Marián [UKOMFKEFs] (25%) - Országh, Juraj [UKOMFKEF] (25%) - Ribar, Anita [UKOMFKEFd] (50%): Electron impact induced fluorescence of second positive system of N₂ molecule
 Recenzované
 Lit. 6 záz., 5 obr., 1 tab.
 In: 18th Symposium on Application of Plasma Processes [elektronický zdroj]. - Bratislava : Knižničné a edičné centrum FMFI UK, 2011. - S. 316-320 [CD ROM]. - ISBN 978-80-89186-77-8
 [SAPP 2011 : Symposium on Application of Plasma Processes. 18th, Vrátna, 15.-20.1.2011]
 [Workshop on Plasmas as a Planetary Atmosphere Mimics. Vrátna, 15.-20.1.2011]
- AFD03 Ribar, Anita [UKOMFKEFd] (100%) : Electron induced fluorescence of hydrogen
 Lit. 14 záz., 6 obr., 1 tab.
 In: Študentská vedecká konferencia FMFI UK, Bratislava 2013 : Zborník príspevkov. - Bratislava : Fakulta matematiky, fyziky a informatiky UK, 2013. - S. 127-131. - ISBN 978-80-8147-009-7
 [Študentská vedecká konferencia FMFI UK 2013. Bratislava, 23.4.2013]
- AFD04 Danko, Marián [UKOMFKEFs] (40%) - Ribar, Anita [UKOMFKEFd] (30%) - Országh, Juraj [UKOMFKEF] (10%) - Matejčík, Štefan [UKOMFKEF] (20%): Comparison of results from electron induced fluorescence study of deuterium and hydrogen molecule
 Popis urobený 18.3.2015
 Lit. 16 záz., 5 obr.
 In: 20th Symposium on Application of Plasma Processes SAPP ; COST TD1208 Workshop on Application of Gaseous Plasma with Liquids [elektronický zdroj]. - Bratislava : Department of Experimental Physics FMFI UK, 2015. - S. 179-183 [online]. - ISBN978-80-8147-027-1
 [SAPP 2015 : Symposium on Application of Plasma Processes. 20th, Tatranská Lomnica, 17.-22.1.2015]
 [COST TD1208 : Workshop on Application of Gaseous Plasma with Liquids. Tatranská Lomnica, 17.-22.1.2015]
 URL: http://neon.dpp.fmph.uniba.sk/sapp/base.php?stranka=Book of Contributed Papers&http://neon.dpp.fmph.uniba.sk/sapp/download/SAPP_XX_2015.pdf
- AFD05 Ribar, Anita [UKOMFKEFd] (50%) - Danko, Marián [UKOMFKEFs] (30%) - Országh, Juraj [UKOMFKEF] (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Differences between fluorescence spectra of various hydrocarbons with emphasis on nitromethane
 Popis urobený 18.3.2015
 Lit. 15 záz., 5 obr., 2 tab.
 In: 20th Symposium on Application of Plasma Processes SAPP ; COST TD1208 Workshop on Application of Gaseous Plasma with Liquids [elektronický zdroj]. - Bratislava : Department of Experimental Physics FMFI UK, 2015. - S. 217-221 [online]. - ISBN978-80-8147-027-1
 [SAPP 2015 : Symposium on Application of Plasma Processes. 20th, Tatranská Lomnica, 17.-22.1.2015]
 [COST TD1208 : Workshop on Application of Gaseous Plasma with Liquids. Tatranská Lomnica, 17.-22.1.2015]
 URL: http://neon.dpp.fmph.uniba.sk/sapp/base.php?stranka=Book of Contributed Papers&http://neon.dpp.fmph.uniba.sk/sapp/download/SAPP_XX_2015.pdf
- AFD06 Danko, Marián [UKOMFKEFs] (40%) - Ribar, Anita [UKOMFKEFd] (20%) - Ďurian, Michal [UKOMFKEFd] (20%) - Országh, Juraj [UKOMFKEF] (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Electron induced emission of Balmer lines and Fulcher Alpha bands of H₂
 Lit. 8 záz.
 In: ESCAMPIG XXIII : Europhysics Conference [elektronický zdroj]. - [Mulhouse] : European Physical Society, 2016. - S. 390-391 [USB kľúč]. - ISBN 979-10-96389-02-5
 [ESCAMPIG 2016 : Europhysics Conference on Atomic and Molecular Physics of Ionised Gases. 23rd, Bratislava, 12.-16.7.2016]

AFD07 Országh, Juraj [UKOMFKEF] (50%) - Danko, Marián [UKOMFKEFs] (20%) - Ďurian, Michal [UKOMFKEFd] (10%) - Ribar, Anita [UKOMFKEFd] (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Electron impact excitation of nitrous oxide
Lit. 7 záz.
In: ESCAMPIG XXIII : Europhysics Conference [elektronický zdroj]. - [Mulhouse] : European Physical Society, 2016. - S. 56-57 [USB kľúč]. - ISBN 979-10-96389-02-5
[ESCAMPIG 2016 : Europhysics Conference on Atomic and Molecular Physics of Ionised Gases. 23rd, Bratislava, 12.-16.7.2016]

AFD08 Ribar, Anita [UKOMFKEFd] (80%) - Holzer, Georg Alexander (5%) - Matejčík, Štefan [UKOMFKEF] (5%) - Denifl, Stephan (10%): Electron attachment to doped Neon clusters
Lit. 4 záz.
In: ESCAMPIG XXIII : Europhysics Conference [elektronický zdroj]. - [Mulhouse] : European Physical Society, 2016. - S. 60-61 [USB kľúč]. - ISBN 979-10-96389-02-5
[ESCAMPIG 2016 : Europhysics Conference on Atomic and Molecular Physics of Ionised Gases. 23rd, Bratislava, 12.-16.7.2016]

AFE Abstrakty pozvaných príspevkov zo zahraničných konferencií

AFE01 Országh, Juraj [UKOMFKEF] (25%) - Danko, Marián [UKOMFKEFs] (25%) - Ribar, Anita [UKOMFKEFd] (25%) - Matejčík, Štefan [UKOMFKEF] (25%): Excitation reactions studied by electron induced fluorescence method
Lit. 2 záz., 1 obr.
In: CEPAS 2011 & CEAMPP 2011. - Belgrade : Institute of Physics, 2011. - S. 18. - ISBN 978-86-82441-32-8
[CEPAS 2011 : Conference on Elementary Processes in Atomic Systems. 5th, Belgrade, 21.-25.6.2011]

AFG Abstrakty príspevkov zo zahraničných vedeckých konferencií

AFG01 Ribar, Anita [UKOMFKEFd] (100%) : Electron induced fluorescence of methane
Popis urobený 26.3.2014
Lit. 8 záz., 1 obr., 2 tab.
In: 3. Česko-slovenská studentská konferencie ve fyzice [elektronický zdroj]. - Praha : Univerzita Karlova, 2012. - nestr. [4 s.] [online]
[Česko-slovenská studentská vědecká konference ve fyzice. 3., Praha, 17.-18.5.2012]
URL: http://neon.dpp.fmph.uniba.sk/svk13/download/zbornik_2012.pdf

AFG02 Ribar, Anita [UKOMFKEFd] (25%) - Danko, Marián [UKOMFKEFs] (25%) - Országh, Juraj [UKOMFKEF] (25%) - Matejčík, Štefan [UKOMFKEF] (25%): Dissociative excitation of Fe(CO)₅ studied using electron induced fluorescence apparatus
Lit. 2 záz.
In: The first meeting of COST Action CM1301. - [Erlangen] : [University of Erlangen], 2014. - S. 54
[CELINA 2014 : COST Action CM1301 : Kick-off Meeting. 1st, Erlangen, 19.-22.3.2014]

AFG03 Danko, Marián [UKOMFKEFs] (40%) - Ribar, Anita [UKOMFKEFd] (30%) - Országh, Juraj [UKOMFKEF] (20%) - Matejčík, Štefan [UKOMFKEF] (10%): Fulcher alpha radiation after electron impact excitation of hydrogen molecule
Popis urobený 14.10.2015
Lit. 3 záz., 1 obr.
In: POSMOL 2015 [elektronický zdroj]. - [Lisboa] : [Universidade Nova], 2015. - S. 29 [online]. - ISBN 978-989-20-5845-0
[EMS 2015 : Electron-Molecule Collisions and Swarms : International Symposium. Lisboa, 17.-20.7.2015]
Registrované v: URL zdrojového dokumentu

AFG04 Országh, Juraj [UKOMFKEF] (40%) - Danko, Marián [UKOMFKEFs] (30%) - Ribar, Anita [UKOMFKEFd] (20%) - Matejčík, Štefan [UKOMFKEF] (10%): Dissociative excitation of iron pentacarbonyl by impact of slow electrons
Popis urobený 14.10.2015
1 obr.

In: POSMOL 2015 [elektronický zdroj]. - [Lisboa] : [Universidade Nova], 2015. - S. 60 [online]. - ISBN 978-989-20-5845-0
[EMS 2015 : Electron-Molecule Collisions and Swarms : International Symposium. Lisboa, 17.-20.7.2015]
Registované v: URL zdrojového dokumentu

AFG05 Ribar, Anita [UKOMFKEFd] (80%) - Holzer, Georg Alexander (5%) - Matejčík, Štefan [UKOMFKEF] (5%) - Denifl, Stephan (10%): Electron interactions with doped neon clusters
Popis urobený 28.9.2016
Lit. 4 záz. n.
In: 28th Summer School and International Symposium on the Physics of Ionized Gases : Contributed Paper [elektronický zdroj]. - Belgrade : University of Belgrade, Faculty of Physics, 2016. - S. 10 [online]. - ISBN 978-86-84539-14-6
[SPIG 2016 : Summer School and International Symposium on the Physics of Ionized Gases. 28th, Belgrade, 29.8.-2.9.2016]
URL: <http://www.spig2016.ipb.ac.rs/spig2016-book-online.pdf>

AFG06 Ribar, Anita [UKOMFKEFd] (75%) - Neustetter, M. (5%) - Jabbour Al Maalouf, E. (5%) - Mauracher, Andreas (5%) - Lim?o-Vieira, P. (5%) - Denifl, Stephan (5%): Low-energy electron interaction with tungsten hexacarbonyl clusters
Lit. 3 záz. n.
In: The 3rd CELINA Meeting. - [Siedlce] : [Siedlce University], 2016. - S. 21
[CELINA 2016 : COST Action CM1301 : Chemistry for ELection-Induced NAnofabrication. 3rd, Kraków, 18.-20.5.2016]

AFG07 Ribar, Anita [UKOMFKEFd] (70%) - Tanzer, Karin (5%) - Fink, Katharina (5%) - Matejčík, Štefan [UKOMFKEF] (5%) - Denifl, Stephan (15%): Secondary electron interaction with radiosensitizers
Popis urobený 28.9.2016
Lit. 4 záz. n.
In: 6th CMBI Meeting [elektronický zdroj]. - Innsbruck : CMBI, 2016. - Art. No. P38, S. 40 [online]
[CMBI Annual Meeting 2016. 6th, Gnadental, 3.-4.3.2016]
URL: https://www.uibk.ac.at/cmbi/downloads/meeting/abstract-band_cmbi-meeting.pdf

BEF Odborné práce v domácich zborníkoch (konferenčných aj nekonferenčných)

BEF01 Országh, Juraj [UKOMFKEF] (25%) - Matejčík, Štefan [UKOMFKEF] (25%) - Danko, Marián [UKOMFKEFs] (25%) - Ribar, Anita [UKOMFKEFd] (25%): Fluorescence induced by monoenergetic electrons
Lit. 15 záz. n.
In: 19th Symposium on Application of Plasma Processes and Workshop on Ion Mobility Spectrometry [elektronický zdroj]. - Bratislava : Department of Experimental Physics FMFI UK, 2013. - S. 105-109 [CD-ROM]. - ISBN 978-80-8147-004-2
[SAPP 2013 : Symposium on Application of Plasma Processes. 19th, Vrátna, 26.-31.1.2013]
[Workshop on Ion Mobility Spectrometry 2013. Vrátna, 26.-31.1.2013]

BEF02 Ribar, Anita [UKOMFKEFd] (40%) - Danko, Marián [UKOMFKEFs] (20%) - Országh, Juraj [UKOMFKEF] (20%) - Matejčík, Štefan [UKOMFKEF] (20%): Dissociative excitation of Fe(CO)₅ studied using electron induced fluorescence apparatus
Popis urobený 20.1.2015
Lit. 11 záz. n., 3 obr.
In: Contributed Papers of the 6th Conference on Elementary Processes in Atomic Systems [elektronický zdroj]. - Bratislava : Comenius University Faculty of Mathematics Physics and Informatics, 2014. - S. 87-90 [online]. - ISBN 978-80-8147-021-9
[CEPAS 2014 : Conference on Elementary Processes in Atomic Systems. 6th, Bratislava, 9.-12.7.2014]
URL: http://neon.dpp.fmph.uniba.sk/cepas2014/downloads/CEPAS_2014_Book_of_Contributions.pdf

BEF03 Ribar, Anita [UKOMFKEFd] (50%) - Szymańska-Skolimowska, Ewelina (10%) - Mason, Nigel J. (10%) - Matejčík, Štefan [UKOMFKEF] (30%): Dissociative electron attachment to nitromethane studied by velocity slice imaging
Popis urobený 20.1.2015
Lit. 10 záz. n., 4 obr., 1 tab.

In: Contributed Papers of the 6th Conference on Elementary Processes in Atomic Systems [elektronický zdroj]. - Bratislava : Comenius University Faculty of Mathematics Physics and Informatics, 2014. - S. 91-94 [online]. - ISBN 978-80-8147-021-9
[CEPAS 2014 : Conference on Elementary Processes in Atomic Systems. 6th, Bratislava, 9.-12.7.2014]
URL: http://neon.dpp.fmph.uniba.sk/cepas2014/downloads/CEPAS_2014_Book_of_Contributions.pdf

BFA Abstrakty odborných prác zo zahraničných podujatí (konferencie, ...)

- BFA01 Országh, Juraj [UKOMFKEF] (30%) - Ribar, Anita [UKOMFKEFd] (30%) - Danko, Marián [UKOMFKEFs] (30%) - Matejčík, Štefan [UKOMFKEF] (10%): Excitation of hydrogen by impact of monoenergetic electrons
Popis urobený 21.6.2013
Lit. 7 zázň., 1 obr.
In: 10th Frontiers in Low Temperature Plasma Diagnostics [elektronický zdroj]. - Eindhoven : Technische Universiteit, 2013. - S. P2-3 [online]
[FLTPD 2013 : Frontiers in Low Temperature Plasma Diagnostics. 10th, Kerkrade, 28.4.-2.5.2013]
Registrované v: URL zdrojového dokumentu
- BFA02 Danko, Marián [UKOMFKEFs] (40%) - Ribar, Anita [UKOMFKEFd] (40%) - Országh, Juraj [UKOMFKEF] (10%) - Matejčík, Štefan [UKOMFKEF] (10%): Electron induced emission of acetone
Popis urobený 27.10.2014
Lit. 2 zázň., 1 obr.
In: HAKONE XIV : Book of Abstracts [elektronický zdroj]. - Greifswald : Institute of Physics at the University of Greifswald and the Leibniz Institute for Plasma Science and Technology, 2014. - S. 29 [online]
[HAKONE 2014 : International Symposium on High Pressure Low Temperature Plasma Chemistry. 14th, Zinnowitz, 21.-26.9.2014]
URL: http://www.hakone2014.org/downloads/book_of_abstracts.pdf
- BFA03 Országh, Juraj [UKOMFKEF] (30%) - Ribar, Anita [UKOMFKEFd] (20%) - Danko, Marián [UKOMFKEFs] (20%) - Utke, Ivo (10%) - Matejčík, Štefan [UKOMFKEF] (20%): Dissociative excitation of iron pentacarbonyl by electron impact
Lit. 5 zázň.
In: 5th Workshop on Focused Electron Beam Induced Processing. - Frankfurt am Main : [Goethe University], 2014. - S. 202-203
[FEBIP 2014 : Focused Electron Beam Induced Processing : Workshop. 5th, Frankfurt am Main, 21.-24.7.2014]
URL: http://febip2014.physik.uni-frankfurt.de/FEBIP_2014/Program_files/abstract_book_final_with_update_remark.pdf
- BFA04 Országh, Juraj [UKOMFKEF] (40%) - Danko, Marián [UKOMFKEFs] (30%) - Ribar, Anita [UKOMFKEFd] (20%) - Matejčík, Štefan [UKOMFKEF] (10%): Electron induced dissociative excitation of C₂H₂
Popis urobený 11.11.2015
Lit. 3 zázň., 1 obr.
In: ICPEAC 2015 : Conference Program [elektronický zdroj]. - Barcelona : Grupo Pacifico, 2015. - Art. No. FR-105 [1 s.] [online]
[ICPEAC 2015 : International Conference on Photonic, Electronic and Atomic Collisions. 29th, Toledo, 22.-28.7.2015]
URL: <https://intranet.pacifico-meetings.com/amsysweb/publicacionOnline.jsf?id=236>
- BFA05 Ribar, Anita [UKOMFKEFd] (30%) - Danko, Marián [UKOMFKEFs] (30%) - Országh, Juraj [UKOMFKEF] (30%) - Matejčík, Štefan [UKOMFKEF] (10%): Hydrogen and Deuterium Continuum Radiation (α_3 Sigma g^+ ? β_3 Sigma u^+) Induced by Electron Impact
Popis urobený 11.11.2015
Lit. 2 zázň., 2 obr.
In: ICPEAC 2015 : Conference Program [elektronický zdroj]. - Barcelona : Grupo Pacifico, 2015. - Art. No. FR-103 [1 s.] [online]
[ICPEAC 2015 : International Conference on Photonic, Electronic and Atomic Collisions. 29th, Toledo, 22.-28.7.2015]

BFB Abstrakty odborných prác z domácich podujatí (konferencie, ...)

BFB01 Lacko, Michal [UKOMFKEFd] (30%) - Papp, Peter [UKOMFKEF] (20%) - Danko, Marián [UKOMFKEFs] (10%) - Ribar, Anita [UKOMFKEFd] (10%) - Országh, Juraj [UKOMFKEF] (10%) - Matejčík, Štefan [UKOMFKEF] (20%): Electron induced dissociation of FEBIDprecursors
Lit. 7 záz.

In: 2nd Annual Meeting of the COST Action CM1301, CELINA : Book of Abstracts. - [Bratislava] : [Comenius University], 2015. - S. 8
[CELINA 2015 : COST Action CM1301 : Chemistry for Electron-Induced NAnofabrication. 2nd, Bratislava, 6.-9.5.2015]

BFB02 Országh, Juraj [UKOMFKEF] (30%) - Danko, Marián [UKOMFKEFs] (30%) - Ribar, Anita [UKOMFKEFd] (30%) - Matejčík, Štefan [UKOMFKEF] (10%): Electron induced fluorescence as a tool for studying precursor dissociation

Lit. 3 záz., 1 obr.

In: 2nd Annual Meeting of the COST Action CM1301, CELINA : Book of Abstracts. - [Bratislava] : [Comenius University], 2015. - S. 46
[CELINA 2015 : COST Action CM1301 : Chemistry for Electron-Induced NAnofabrication. 2nd, Bratislava, 6.-9.5.2015]

BFB03 Ribar, Anita [UKOMFKEFd] (50%) - Danko, Marián [UKOMFKEFs] (15%) - Országh, Juraj [UKOMFKEF] (15%) - Silva, Filipe Ferreira da (5%) - Utke, Ivo (5%) - Matejčík, Štefan [UKOMFKEF] (10%): Electron induced fluorescence study of iron pentacarbonyl:Carbonyl bands

1 obr.

In: 2nd Annual Meeting of the COST Action CM1301, CELINA : Book of Abstracts. - [Bratislava] : [Comenius University], 2015. - S. 50
[CELINA 2015 : COST Action CM1301 : Chemistry for Electron-Induced NAnofabrication. 2nd, Bratislava, 6.-9.5.2015]

BFB04 Ribar, Anita [UKOMFKEFd] (50%) - Danko, Marián [UKOMFKEFs] (15%) - Országh, Juraj [UKOMFKEF] (15%) - Silva, Filipe Ferreira da (5%) - Utke, Ivo (5%) - Matejčík, Štefan [UKOMFKEF] (10%): Electron induced fluorescence study of iron pentacarbonyl:Iron atom lines

1 obr.

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[SAPP 2015 : Symposium on Application of Plasma Processes. 20th, Tatranská Lomnica, 17.-22.1.2015]

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excitation of H2 and D2 leading to continuum radiation

Popis urobený 13.10.2015

Lit. 8 záz., 3 obr.

In: ICPIG 2015 [elektronický zdroj]. - [Iasi] : [Alexandru Ioan Cruza University], 2015. - Art. No. P2.06 [2 s.] [online]

[ICPIG 2015 : International Conference of Phenomena in Ionized Gases. 32nd, Iasi, 26.-31.7.2015]

URL: <http://www.icpig2015.net/ShowPage/?PageName=PosterInformation>

Štatistika kategórií (Záznamov spolu: 40):

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