REGIONAL WORKSHOP ON ATOMIC AND MOLECULAR DATA

Belgrade, Serbia, 14-16 June 2012

BOOK OF ABSTRACTS

Edited by Milan S. Dimitrijević

Society of Astronomers of Serbia

Belgrade, 2013

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Regional Workshop on Atomic and Molecular Data

June 14 - 16, 2012, Belgrade, Serbia

Organized by:
Serbian Astronomical Society (http://www.das.org.rs/) and
Group for Astrophysical Spectroscopy, Astronomical Observatory, Belgrade

Co-organizer:
Faculty of Mechanical Engineering, University of Belgrade

The official conference website (http://poincare.matf.bg.ac.rs/~andjelka/VAMDC/)

SCIENTIFIC RATIONALE: Atomic and molecular data play an essential role in astrophysics, fusion, laboratory and industrial plasmas, lightning sciences and technologies, biomedicine and biophysics, combustion and environmental sciences as well underpinning many technologies, surface physics, optics and spectroscopy, optoelectronics, etc. In this meeting the need for (and applications of) such data in these fields will be reviewed, as well as discussion and presentation of some of the databases and data centres that collate and disseminate such data. The objective is both to show the state of the art in this field and provide information on the need for atomic and molecular data and the current status of atomic and molecular databases. It targets both at data producers and users and will be of interest to all scientists involved in fundamental research and/or technological applications.

A key part of the meeting will be the presentation of the Virtual Atomic and Molecular Data Center (VAMDC), an EU funded collaboration between groups involved in the generation, evaluation, and use of atomic and molecular data. VAMDC is building a reliable, open, flexible and interoperable e-science interface to existing atomic and molecular data. During the workshop there will be a VAMDC tutorial in order to explain and demonstrate to participants how to use services of VAMDC.

The meeting is particularly targeted at researchers based in the Balkans and south eastern Europe and some support for such researchers will be available.

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RADIATIVE PARAMETERS OF ATOMIC AND IONIC STATES

Kiril Blagoev

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In this report, a short survey of the experimental methods for determination of radiative parameters of excited atomic and ionic states will be given.

These are radiative lifetimes of the excited states, transition probabilities and oscillator strengths. The methods, which are used now days, will be discussed as well as their advantages and limitations. Some results as examples will be presented. Interesting application of Laser Induced Breakdown Spectroscopy will be presented, as well.

These investigations have been supported by contract D 02-274/2008 BNSF and Laser Lab in Europe.

DISSOCIATIVE ELECTRON ATTACHMENT IN MOLECULES - NEEDS AND CURRENT STATUS OF AVAILABLE DATA

Iztok Čadež

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A compact historical overview of the evolution of understanding of dissociative electron attachment (DEA) in molecules as well as on the increasing body of studied molecular species will be presented. Some experimental ambiguities which persist until modern time will be emphasised and discussed. Finally, current status of DEA studies and needs as well as perspective for the future development will be given.

Dissociative electron attachment in molecules is one of classical binary electron molecule collision processes which have been studied with variable intensity since late fifties. The fact that DEA is a resonant process on one side and a rearrangement process on another, make it an interesting case for the theory development and also an important process in various environments. New needs in advanced applications, more detailed modelling codes and also, the development of new experimental techniques enhanced the interest for DEA in recent years. The fields of research which are currently driving this interest for DEA are studies of free electrons in biological environment, astrochemistry (recent discovery of anions in space and planetary atmospheres), sensitive compound selective detection techniques, edge plasma in tokamaks and various technological plasmas.

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STARK BROADENING DATA – NEEDS AND APPLICATIONS

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Stark broadening data are of importance for a number of problems connected with the research and modelling of various astrophysical plasmas as well as for laboratory plasmas, inertial fusion plasma and technological plasmas investigations and for designing of laser equipment, For example in astrophysics, such data are needed for modelling and spectroscopic diagnostics of stellar atmospheres and envelopes. In fact stellar spectroscopy is a powerful tool for investigation of stellar plasma and by analyzing stellar spectral lines, we can determine for example the temperature in particular atmospheric layers, the chemical composition of stellar plasma, surface gravity, spectral type and effective temperature. For such purposes, Stark broadening data are often needed, since in a number of cases, the influence of collisions with charged particles on emitting/absorbing atoms and ions is important and its result is the broadening of spectral lines, so called Stark broadening.

We will review here the needs for Stark broadening data in various research topics and technology with the accent on significance of Virtual Atomic and Molecular Data Center for their search and for search of atomic data needed for determination of Stark broadening parameters.

ATOMIC AND MOLECULAR DATA - APPLICATION ON FORMATION OF MOLECULES IN DARK CLOUDS

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Our knowledge about composition and evolution of molecules in space is constantly changing through ground-based and space observations, as well as laboratory simulations and theoretical modeling. With observations we can obtain molecular abundances in a variety of environments. For example abundances of different molecules in dark clouds were measured by SWAS satellite. Here we present how input data can change resulting molecular abundances in dark clouds. We show this on H_2O and O_2 molecules. Resulting molecular abundances depend on many factors: physical parameters such as temperature, density or the amount of cosmic rays; initial abundances of different elements; chemical reaction and collision rates etc. In order to model chemistry of any environment many atomic and molecular data are needed. Virtual Atomic and Molecular Data Centre (VAMDC) can be used to search different databases in order to obtain needed data, for example collision rates that are used to model dark cloud chemistry.

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ELECTRON INTERACTIONS DATA BASE AS A STEP TOWARDS A DATA BASE FOR RADIATION DAMAGE IN BIOMOLECULAR SYSTEMS II

D. Janković[1], I. Maksimović[1], D. B. Marinković[1], S. Djordjević[2], M. Nešić[2], D. Radosavljević[2], S. Čonjagić[2] and B. P. Marinković[3]

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The formation of Belgrade electron cross section data base, IPBeMolDB, is foreseen as a part of a more comprehensive data base devoted to the research of radiation damage processes in biomolecular systems (RADAM DB). Belgrade data base should contain preferably those data that has been obtained in the measurements performed in the Laboratory for Atomic Collision Processes (LACP) at the Institute of Physics, University of Belgrade (IPB). Researchers in the LACP participate in the European network organization COST Action MP1002 entitled "Nano-scale insights in ion beam cancer therapy (Nano-IBCT)". Our focus of investigation is in obtaining the absolute differential cross sections for low and intermediate energy electron scattering by (bio)molecules. Electron interactions comprise elastic scattering, excitation, ionization and fragmentation of molecular targets. The IPBeMolDB will exploit the underlying infrastructure of VAMDC, Virtual Atomic Molecular Data Centre, with its applications capable of combining, extracting and processing data from all VAMDC member data bases. Data will be structured according VAMDC standard documentation and XSAMS reference guide. Our aim is to get better visibility and dissemination of experimental results obtained in LACP, and to make a platform for evaluation of different sets of data. In that sense, data from other sources will be included in the data base for those atomic species targets that have been studied in LACP.

Acknowledgement

This work has been partially supported by the Ministry of Education and Science of Republic of Serbia (Project 171020) and the bilateral project between Serbia and Germany (DAAD #54394840). It has been motivated by research within COST Action MP1002 Nano-IBCT and FP7 VAMDC project.

ATOMIC AND MOLECULAR DATA FOR STELLAR ATMOSPHERES MODELLING – EXAMPLE OF PHOENIX CODE

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For the investigation and modelling of stellar atmospheres atomic and molecular data for a huge number of neutral and ionized species are needed. In this contribution we will review such needs, on the example of PHOENIX, a general stellar atmosphere code, used from novae/supernovae to brown dwarfs/extrasolar planets - now even AGN's neutron stars etc. There are more than 500 papers concerning PHOENX, describing obtained results, and the used methods.

An illustration of the need for atomic and molecular data for stellar atmospheres modelling might be that PHOENIX has a list of ~42×10^6 atomic lines and ~10^9 molecular lines. We will review here the problems where AM data are needed for PHOENIX, highlights of results obtained with this code, ^{6}Li problem and Atmospheric models for evolutionary modelling and populations synthesis.

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ATOMIC AND MOLECULAR DATA FOR ACTIVE GALACTIC NUCLEI – Fe II LINES AND BALMER CONTINUUM

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Active Galactic Nuclei (AGNs) are the most luminous objects in the Universe. They produce a large amount of energy, resulting in a very complex spectrum that shows a number of strong emission lines. The properties of emission lines in AGN spectra are signature of the geometry, physical and kinematical properties of the emission gas.

The data basis with large and complete atomic data may help a lot in analysis of AGN spectra, and understanding of their nature. In this talk we demonstrate some examples of use of atomic databases in AGN investigation: the construction of the complex Fe II template, and calculation of Balmer continuum, which have practical use in AGN spectral analysis.

OVERVIEW ON THE VAMDC PROJECT

Friedrich Kupka and the VAMDC Collaboration (P.I. M.-L. Dubernet)

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In this presentation I will give an overview on the purpose, the functionality, and the current status of the Virtual Atomic and Molecular Data Centre (VAMDC, see M.L. Dubernet et al. 2010, JQSRT 111, 2151). VAMDC is an EU-FP7 e-infrastructure project which has been set up to build a common electronic infrastructure for the exchange and distribution of atomic and molecular data. Two dozen teams from six EU member states (Austria, France, Germany, Italy, Sweden, United Kingdom) as well as Russia, Serbia, and Venezuela have been working together since July 2009 and the three and a half year long project has now achieved many of its originals goals. Most importantly, it now offers a generic user interface, the VAMDC Portal, which allows access to currently 18 different atomic and molecular data bases in a unified way extending the original functionality of the individual data bases. In my presentation I will explain what is inside VAMDC and how it can be used, make a few user demonstrations, and also discuss some future perspectives.

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ELECTRON INTERACTIONS DATA BASE AS A STEP TOWARDS A DATA BASE FOR RADIATION DAMAGE IN BIOMOLECULAR SYSTEMS I

B. P. Marinković[1], D. Janković[2], I. Maksimović[2], D. B. Marinković[2], S. Djordjević[3], M. Nešić[3], D. Radosavljević[3], S. Čonjagić[3], A. V. Yakubovich[4], M. Hanauske[4] and A. V. Solov'yov[4]

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The study of radiation damage processes in biomolecular systems has been in focus of the European network organization COST (Co-operation in Science and Technology) since the adoption of COST Action P9 that started in 2003 and has been succeeded by COST Action MP1002 entitled "Nano-scale insights in ion beam cancer therapy (Nano-IBCT)". Recently it has been decided to create an comprehensive data base for radiation damage that would comprise both experimental and theoretical data relevant to the several topical areas of radiation damage processes. These include five areas: TA1 Ionic interactions, TA2 Electron/positron interactions, TA3 Photonic Interactions, TA4 Multiscale RADAM phenomena and TA5 Radiobiological scale effects. The planned data base, RADAM DB, will exploit the underlying infrastructure of VAMDC, Virtual Atomic Molecular Data Centre, with its applications capable of combining, extracting and processing data from all VAMDC member data bases. Data base for electron/positron interactions with biomolecules will collect data of cross sections (elastic, excitation, ionization, positronium formation, resonances), molecular fragmentation processes (dissociative electron attachment, relative fragmentation yields and mechanisms, DNA strand breaks) secondary particle production (yields of excited or ionized particle energy spectra, radicals productions, annihilation), energy transfer and doses (linear energy transfers, nanodosimetry, electron excitation exchanges, alignment and orientation parameters), swarm and transport processes (effective parameters, integral and momentum transfer cross sections, transport code results). Data will be structured according VAMDC standard documentation and XSAMS reference guide.

Acknowledgement

This work has been partially supported by the Ministry of Education and Science of Republic of Serbia (Project 171020) and the bilateral project between Serbia and Germany (DAAD #54394840). It has been motivated by research within COST Action MP1002 Nano-IBCT and FP7 VAMDC project.

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IMPORTANCE OF VERY LOW FREQUENCY RADIO SIGNAL DATA REGISTERED BY VLF-RECEIVER SYSTEM

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The ionosphere as a part of terrestrial atmosphere is very sensitive to numerous external factors. Variable influences coming from both the outer space and from different sources of Earth make the ionospheric plasma characteristics time dependent. The most significant perturber from the outer space originates in solar activity whose consequences can be either periodical (due to the solar cycle, and seasonal and diurnal variations) or transient (arising from solar flares and coronal mass ejections). Significant transient perturbations can also result from gamma ray bursts and gamma ray flares from various sources. In addition, there are some processes in the Earth lithosphere (such as volcanic eruptions, earthquakes) as well as in the atmosphere (such as lightnings) that cause non-periodic disturbances in the ionosphere.

The induced ionospheric disturbances may directly affect human activities on Earth related to, for example, radio communications, planned networks of mobile communications satellites, high precision applications of global navigation satellite systems, etc.

Investigation of physical processes under time varying conditions in the ionosphere is thus interesting not only for purely scientific reasons but it also has numerous important practical applications. The main way to study the low ionosphere (altitudes between 60 and 90 km) is based on properties of propagating VLF radio waves, i.e. on monitoring time variations of VLF radio signal amplitudes and phases and forming corresponding data bases. In the Institute of Physics in Belgrade this is done by two receiver systems incorporated in AWESOME and AbsPAL international networks.

DATA BASES FOR COLLISIONS AND TRANSPORT OF ELECTRONS AND POSITRONS IN IONIZED GASES

Z. Lj. Petrović, O. Šašić, J. Jovanović, S. Dujko, V. Stojanović, A. Banković, D. Marić, G. Malović

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Non-equilibrium plasmas are ofthen thought to be a man-made system aimed at favouring energy transfer ot electrons while ions and neutral particles remain at low, even room temperature. Those plasmas may be found in panetary atmospheres, interstellar coronas and gas clouds. Those plasmas however represent the basis for numerous down to earth application such as plasma processing for micro and nano electronics, plasma medical applications, plasmas in nanotechnologies and many more.

Any modeling of such plasmas is based on phenomenology, data and theoretical apparatus taken from the physics of swarms (i.e. physics of non interacting charged particles in unperturbed ionized gases). Even the techniques such as PIC or fully kinetic calculations that rely on the cross sections only need a swarm analysis to test whether the number, momentum and energy balances are fullfilled.

Data sets used in modeling of such plasmas have to be comprehensive. That means that they have to cover a wide range of energies from thermal to maximum avalable energy as often runaway phenomena occur. They have to include all processes and in different energy ranges different inelastic processes dominate the energy balance. Number changing collisions (attachment, ionization, etc.) affect the definition of transport coefficients and significant differences may occur between calculated and experimental data unless proper care of those processes is taken. The codes used in calculations all have to be tested against well known and well defined benchmarks.

Comparisons of trasport data calculated with the cross section set and those measured provide tests of whether overall balances are made but may lead to non-unique resulting cross sections, poor energy resolution and efefcts due to compensation of the processes below and above the energy range that is well covered by the swarm experiment. Thus the best strategy is to apply shapes of the cross sections from binary experiments and theories and use the swarm analysis to normalize them a to fill the missing processes.Typical error is in representing ionization, surely a critical parameter in any self sustained plasma.

In this talk we shall make a survey of the available data bases, how to use the binary collision data in plasma modeling and swarm analysis, different applications and finally we shall give some examples for data bases for positrons.

THE STARK-B DATABASE FOR SPECTRAL LINE BROADENING BY COLLISIONS WITH CHARGED PARTICLES

Sylvie Sahal-Bréchot

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Stark broadening theories and calculations have been extensively developed for about 50 years. Accurate spectroscopic diagnostics and modelling require the knowledge of numerous collisional line profiles.

Nowadays, the access to such data via an on line database becomes essential. The aim of STARK-B [1] is to reply to this need. It is a collaborative project between the Astronomical Observatory of Belgrade and the Observatory of Paris (LERMA). STARK-B is a database of widths and shifts of isolated lines of atoms and ions due to electron and ion collisions that we have calculated within the semiclassical impact perturbation theory and published in international refereed journals (more than 150 papers). It is devoted to modelling and spectroscopic diagnostics of stellar atmospheres and envelopes, laboratory plasmas, laser equipments and technological plasmas. Hence, the domain of temperatures and densities covered by the tables is wide and depends on the ionization degree of the considered ion. STARK-B has been fully opened since September 2008. Due to the considerable growing in the recent past years of spectral resolution, sensitivity, large ground-based telescopes and space-born missions, new data requests are increasing. So the database is very lively and we continue to feed it with new calculations.

STARK-B is a part of VAMDC (Virtual Atomic and Molecular Data Centre) [2] [3]. We will present STARK-B and its VAMDC context at the Workshop.

References

[1]STARK-B: http://stark-b.obspm.fr
[2]VAMDC: http://www.vamdc.eu
[3] Dubernet, M. L., Boudon, V., Culhane, J. L., et al.: 2010, *JQSRT*, **111**, 2151.

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ATOMIC DATA AND ELECTRON-IMPACT BROADENING OF SPECTRAL LINES OF RARE EARTHS

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Spectral lines of rare-earth elements are present in Solar as well as in stellar spectra, and they principally originate in layers of stellar atmospheres with higher electron density (photosphere or subphotosphere). Consequently, electron-impact broadening mechanism can be important, especially for hot (A and B) stars as well as for white dwarfs.

So, for modelling and spectroscopic diagnostics of stellar atmospheres and envelopes, it is important to have a set of electron-impact broadening data, also for the lines of ionized rare-earth elements.

For example, the reliability of the element abundance determinations in stellar atmospheres depends on a number of factors, where atomic data (transition probabilities, collisional widths, etc.) are among the most important. One of the needed set of atomic data for line synthesis are the electron-impact widths of spectral lines. They are needed in order to solve various problems in astrophysics and physics, for example, diagnostics and modeling of laboratory and stellar plasma, investigation of its physical properties and for abundance determination.

In this lecture, we review the needs for Stark broadening data of rare earth elements, and results of our investigation of influence of electron-impacts with rare earth atoms and ions on the broadening of stellar spectral lines.

VLF DATA ACQUISITION AND CENTRAL DATABASE STORING

Vladimir Srećković, Desanka Šulić, Aleksandra Nina, Anatolij Mihajlov, Ljubinko Ignjatović

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The ionosphere, having characteristics of plasma, is very sensitive to electromagnetic disturbances whose intensity and number mainly vary with solar activity. These disturbances cause numerous complicated physical, chemical and dynamical phenomena in the lower ionosphere and may directly affect human activities, especially in the telecommunications. Besides a pure scientific interest to study the influence of solar activity on the terrestrial atmosphere, the understanding and predicting the resulting turbulent regions of the ionosphere has important applications for radio communications, military operations in remote locations, planned networks of mobile communications satellites, high-precision applications of global navigation satellite systems, etc. The lower ionosphere such as the D region (60–90 km) where the altitude range is too low for satellites and too high for atmospheric balloons, requires measurements mostly based on radio wave propagation techniques. In the past few years, we study the influence of solar perturbations on electron concentration in the terrestrial ionospheric D-region by analyzing the amplitude and phase time variations of very low frequency (VLF) radio waves emitted by VLF transmitter all over the world and recorded by the AWESOME and ABSPAL receivers in Belgrade (Serbia) in real time. Naturally, there is a need to store these huge amount of collected data. Here, we will try to present a need of central database storing and exchange with other VLF stations and groups.

CHALLENGES OF HIGH RESOLUTION RADIATIVE TRANSFER IN DUST SUBLIMATION ZONES

Dejan Vinković

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Radiative transfer calculations are a key tool in reconstructing dust properties from observed spectra and images of circumstellar environments. What is traditionally required are dust optical properties and a model of dust distribution in space. But thanks to high resolution radiative transfer calculations, it has been recognized recently that this is an unsolvable problem for zones of dust sublimation on the surface of optically thick clouds. The inner region of protoplanetary disks, where we expect formation of terrestrial planets, is such an example. Solution might be reached by combining dust dynamics and gas properties with radiative transfer, but the set of input parameters and output possibilities is dramatically increased.

Program

14. June 2012, Thursday

9:30-10:00 Opening

Chairman: Milan S. Dimitrijević

10:00-10:45 Nigel Mason: ON THE APPLICATION OF ATOMIC AND MOLECULAR DATA

10:45-11:30 Iztok Čadež: DISSOCIATIVE ELECTRON ATTACHMENT IN MOLECULES – NEEDS AND CURRENT STATUS OF AVAILABLE DATA

11:30-12:00 **Coffee Break**

Chairman: Nigel Mason

12:00-12:45 Milan S. Dimitrijević: STARK BROADENING DATA – NEEDS AND APPLICATIONS

12:45-13:30 Darko Jevremović: ATOMIC AND MOLECULAR DATA FOR STELLAR ATMOSPHERES MODELLING – EXAMPLE OF PHOENIX CODE

13:30-15:00 **Lunch Break**

Chairman: Zoran Petrović

15:00-15:45 Dejan Vinković: CHALLENGES OF HIGH RESOLUTION RADIATIVE TRANSFER IN DUST SUBLIMATION ZONE

15:45-16:15 Jelena Kovačević: ATOMIC AND MOLECULAR DATA FOR ACTIVE GALACTIC NUCLEI – Fe II LINES

16:15-16:45 **Coffee Break**

Chairman: Friedrich Kupka

16:45-17:15 Kiril Blagoev: RADIATIVE PARAMETERS OF ATOMIC AND IONIC STATES

17:15-17:45 Zoran Simić, Milan S. Dimitrijević: ATOMIC DATA AND ELECTRON-IMPACT BROADENING OF SPECTRAL LINES OF RARE EARTHS

15. June 2012, Friday

Chairman: Bratislav Marinković

10:00-10:45 Sylvie Sahal-Bréchot: THE STARK-B DATABASE FOR SPECTRAL LINE BROADENING BY COLLISIONS WITH CHARGED PARTICLES

10:45-11:30 Alexander Yakubovich: DEVELOPMENT OF THE RADAM DATABASE

11:30-12:00 **Coffee Break**

Chair person: Sylvie Sahal-Bréchot

12:00-12:45 Zoran Petrović, O. Šašić, J. Jovanović, S. Dujko, V. Stojanović, A. Banković, D Marić, G. Malović: DATA BASES FOR COLLISIONS AND TRANSPORT OF ELECTRONS AND POSITRONS IN IONIZED GASES I

12:45-13:30 Zoran Petrović, O. Šašić, J. Jovanović, S. Dujko, V. Stojanović, A. Banković, D Marić, G. Malović: DATA BASES FOR COLLISIONS AND TRANSPORT OF ELECTRONS AND POSITRONS IN IONIZED GASES II

13:30-15:00 **Lunch Break**

Chairman: Alexander V. Yakubovich

15:00-15:45 Bratislav P. Marinković, D. Janković, I. Maksimović, D. B. Marinković, S. Djordjević, M. Nešić, D. Radosavljević, S. Čonjagić, A. V. Yakubovich, M. Hanauske, A. V. Solov'yov: ELECTRON INTERACTIONS DATA BASE AS A STEP TOWARDS A DATA BASE FOR RADIATION DAMAGE IN BIOMOLECULAR SYSTEMS I

15:45-16:30 D. Janković, I. Maksimović, D. B. Marinković, S. Djordjević, M. Nešić, D. Radosavljević, S. Čonjagić, Bratislav P. Marinković: ELECTRON INTERACTIONS DATA BASE AS A STEP TOWARDS A DATA BASE FOR RADIATION DAMAGE IN BIOMOLECULAR SYSTEMS II

16:30-17:00 **Coffee Break**

Chairman: Kiril Blagoev

17:00-17:30 Friedrich Kupka: VALD Database

17:30-17:45 Vladimir Srećković, Desanka Šulić, Aleksandra Nina, Anatolij A. Mihajlov, Ljubinko Ignjatović: VLF DATA ACQUISITION AND CENTRAL DATABASE STORING

17:45-18:00 Aleksandra Nina, Vladimir Čadež, Vladimir Srećković: IMPORTANCE OF VERY LOW FREQUENCY RADIO SIGNAL DATA REGISTERED BY VLF-RECEIVER SYSTEM

18:00-18:15 Aleksandra Dobardžić, Andjelka Kovačević: ATOMIC AND MOLECULAR DATA – APPLICATION ON FORMATION OF MOLECULES IN DARK CLOUDS CONTAINING DATA REGISTERED BY VLF RECEIVER SYSTEM

16. June 2012, Saturday

VAMDC INTRODUCTION

10:00-10:45 Friedrich Kupka: OVERVIEW ON THE VAMDC PROJECT

10:45-11:30 Nigel Mason: VIRTUAL ATOMIC AND MOLECULAR DATA CENTER - VAMDC I

11:30-12:00 **Coffee Break**

12:00-13:00 Nigel Mason: VIRTUAL ATOMIC AND MOLECULAR DATA CENTER - VAMDC II

13:00 **Closing**

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