CEQPAS

Centennial of Quantum Theory: Progress in Atomic and Molecular Structure

University of Belgrade | Institute of Physics Belgrade
National Institute of the Republic of Serbia

Institute of Chemistry, Technology & Metallurgy

University of Kent

3–5 November 2025 – Belgrade, Serbia

3–5. новембар 2025 – Београд, Србија

BOOK OF ABSTRACTS

Књига апстраката

CEQPAS 2025

International Year of Quantum Science and Technology

Science Fund of the Republic of Serbia

AtMolCol

MOLESs
MOLecular Excited State spectroscopy

https://www.moless-spectroscopy.org

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CEQPAS 2025

Book of Abstracts
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University of Belgrade - Institute of Chemistry, Technology and Metallurgy
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Conference Chairs:
Nigel J. Mason, University of Kent, UK
Bratislav P. Marinković, University of Belgrade, RS

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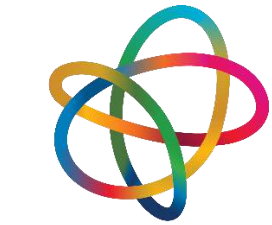

The organizers of CEQPAS 2025 acknowledge the support by the Science Fund of the Republic of Serbia, #6821, Atoms and (bio)molecules - dynamics and collisional processes on short time scale - ATMOLCOL.

A welcome to CEQPAS 2025

This year we celebrate a hundred years of the Nobel Prize in Physics awarded to James Franck and Gustav Hertz for their ingenious experimental finding that in collisions of electrons with atoms, the energy is absorbed in a quantized manner and proving the Niels Bohr model of the atom. It is also a year when we honour eighty years of Wolfgang Pauli's acceptance of the Nobel Prize for the discovery of the exclusion principle, named after him, the "Pauli principle", which underpins our understanding of the structure of matter. These two groundbreaking discoveries formed part of the emergence of quantum mechanics as the basis for unravelling the nature of the atomic and molecular world. Accordingly, 2025 was declared by the United Nations as the "International Year of Quantum Science and Technology (IYQ)", recognising 100 years since the initial development of quantum mechanics. Hence, we are organising the conference "Centennial of Quantum Theory: Progress in Atomic and Molecular Structure (CEQPAS)" to present the advancements of quantum physics in diverse fields such as:

- Atomic and molecular spectroscopy and its applications to atmospheric sciences and astronomy;
- Collisions and their applications in plasma physics;
- Studies in Chemical physics & physical chemistry;
- The application of quantum science to our wider understanding of phenomena, including radiation sciences;
- The use of Artificial Intelligence (AI) and Machine Learning (ML) for atomic and molecular data analysis and generation.

We are delighted to organise this conference in Belgrade, the capital of the Republic of Serbia, at two institutes of national importance: the Institute of Physics Belgrade and the Institute of Chemistry, Technology and Metallurgy. During the conference, more than 25 speakers will present the state of the art across the different topics represented in the conference; summaries of these talks are presented in this Book of Abstracts.
Immediately after the CEQPAS conference, we will hold the inaugural meeting of the MOLecular Excited State spectroscopy (MOLESs) Consortium. This consortium has been established to review the status of our knowledge of the electronic spectroscopy of molecules, revising and extending the classic series of Melvin Robin's three-volume books on "Higher Excited States of Polyatomic Molecules". A series of reviews of the electronic state spectroscopy of different molecular series in different phases —

gaseous, liquid and solid — will be presented together with reviews of different experimental and theoretical methods used to collect this data and a discussion of relevance to important applications.

We hope all participants enjoy the scientific content of the conference, allowing new collaborations to be formed. We also hope participants will take the opportunity to explore Belgrade.

Finally, we wish to thank all who have contributed to the success of the CEQPAS and MOLESs meeting and who will help to celebrate the IYQ.

On behalf of the Scientific Committee,

Nigel J. Mason & Bratislav P. Marinković

Content

ATOMIC AND MOLECULAR SPECTROSCOPY AND ITS APPLICATIONS TO ATMOSPHERIC SCIENCES AND ASTRONOMY

Ejected electron spectra from N_2O molecule obtained by OHRHA electron spectrometer

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Abstract: Electron spectrometer OHRHA (Jureta et al. 2025) is used to obtain ejected electron spectra from nitrous oxide (N_2O) molecule. The spectrum at 101.05 eV incident electron energy and in the range of kinetic energies from 5 eV to 9 eV is shown in Figure 1. The assignments of the peaks should be provided by TD-DFT calculations.

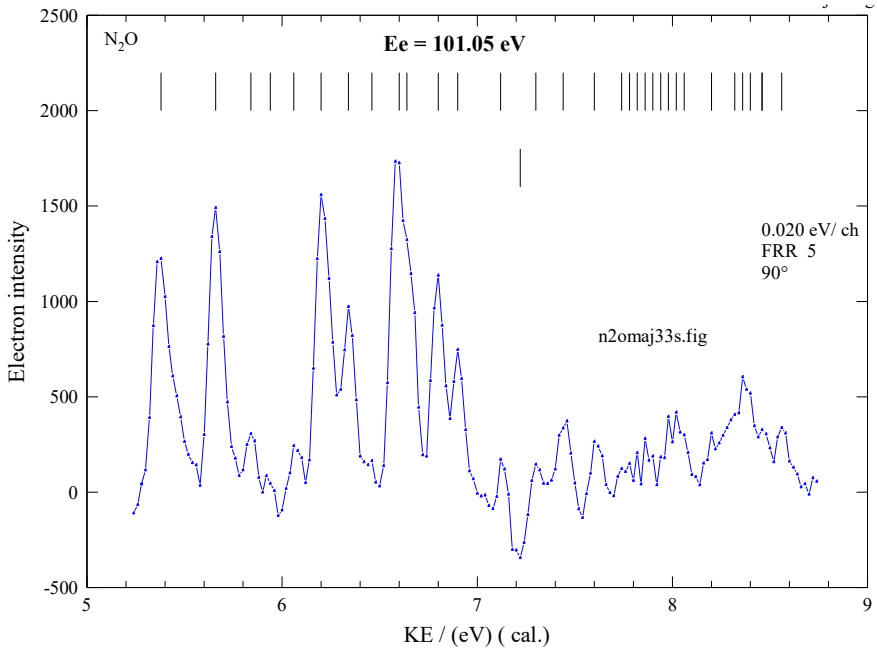

Figure 1 Ejected electron spectrum from N_2O molecule at 90° angle and101.05 eV impact electron energy. Kinetic energy range is from 5 eV to 9 eV. The most prominent peaks are at the KE=5.38; 5.66; 5.84; 5.94; 6.06; 6.20; 6.34; 6.60; 6.80; 6.90; 7.12; 7.22 (dip); 7.3; 7.44; 7.6 eV.

Keywords: Nitrous Oxide; Ejected Electron Spectra.

Acknowledgement
This research was supported by the Science Fund of the Republic of Serbia, Grant No. 6821, Project title – ATMOLCOL

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Study of Elastic Electron Scattering Cross Section for Desflurane at 200 eV in the Gaseous Phase

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Abstract: Motivated by the environmental impact of halogenated anesthetics, we investigated elastic electron scattering from desflurane ($C_3H_2F_6O$) at an incident energy of 200 eV using both experimental and theoretical approaches. The measurements were performed with a crossed-beam setup employing the relative-flow normalization method with argon as the reference gas. Theoretical differential cross sections were calculated within the IAM-SCAR+I (Independent Atom Model combined with the Screening Corrected Additivity Rule and interference effects) framework and compared with the experimental data, showing good overall agreement. Since desflurane, like other volatile anesthetics, is largely exhaled unchanged and contributes to greenhouse gas emissions, these results provide useful parameters for atmospheric modeling and assessing its environmental impact.

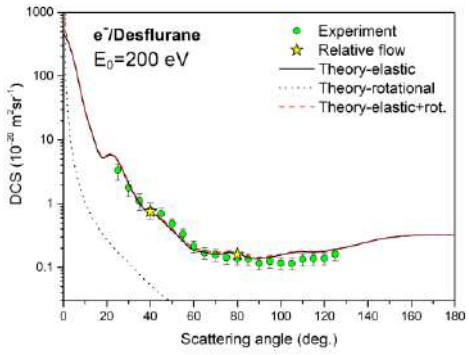

Figure 2. Differential cross section for elastic electron scattering from desflurane molecule.

Keywords: Electron Scattering; Desflurane; IAM-SCAR+I.

Acknowledgement
This research was supported by the Science Fund of the Republic of Serbia, Grant No. 6821, Project title – ATMOLCOL

COLLISIONS AND THEIR APPLICATIONS IN PLASMA PHYSICS

Collisions of electrons, photons and ions with atoms and (bio)molecule systems - ATMOLCOL project

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Abstract: The core of ATMOLCOL project is to study collisional processes involving atoms and (bio)molecules, especially focusing on very short time scales. Elastic scattering (Vukalović 2024) of electrons on atom/molecule, autoionization (Jureta 2024,), Ionization (Srećković 2025), photoionization (Delibašić 2024), electron autodetachment and dissociative electron attachment (Kopyra 2025) are accompanied processes that are examined. The planned experimental methodology is based on the cross-beam technique that provides conditions for the binary collision events (Vukalović 2024, Kopyra 2025), while the theoretical is based on first- and second-order theories (Delibašić et al). Both methodologies are supported with the numerical calculations and methods (IAM method, Gauss-Legendre and Gauss-Mehler quadratures). ATMOLCOL is bringing together experimental and theoretical knowledge which may lead to further technological developments and direct and indirect impacts on climate change, the environment science and human health.

Keywords: Electrons; Molecules; Collisions.

Acknowledgement: Acknowledge support of the Science Fund of the Republic of Serbia, Grant No. 6821, 'Atoms and (bio)molecules-dynamics and collisional processes on short time scale ATMOLCOL'.

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