

21st CEUM

21st Central European NMR Symposium & Bruker Users Meeting



BOOK OF ABSTRACTS

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Preface

The 21st Central European NMR Symposium & Bruker users meeting (CEUM) is an important scientific and professional event for all NMR users in Central Europe.

It has already a long history and has travelled along many counties in Europe.

It has always been an important occasion to share experience and know-how inside the community and meet scientists working mainly in the close countries (but not only!) in order to built up a stronger NMR community and have also a vision on new applications of NMR and new developments in the Magnetic Resonance Technology.

We are sincerely grateful to the lectures and guests coming from Greece, Bulgaria, Romania, Moldovia, Croatia, Slovenia, Bosnia and Herzegovina, Hungary, the Netherlands, US and from different cities from Serbia to have jointed this meeting.

He sincerely hope that all our effort will be lead also this year in this very nice city to a interesting and successful conference.

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IN SITU IRRADIATION NMR SPECTROSCOPY IN THE DESIGN OF NEW FUNCTIONAL MATERIALS

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In situ irradiation NMR spectroscopy includes illumination of the samples inside the NMR spectrometer [1]. The setup, which includes LEDs as light sources, allows application of whole variety of NMR methods to photochemical reactions. In addition to the standard NMR spectroscopic approaches feasible for reactions in the dark, a special hyperpolarization technique applicable exclusively to photoreactions, the Photo-CIDNP spectroscopy provides a molecular fingerprint of reactive intermediates at a nanosecond time scale.

The setup includes control unit connected directly to the NMR spectrometer through three BNC connections. The first connection can switch between CW and Pulse mode, the second one can setup the optical power of used LED source and third one can switch on and off the illumination. The setup has three LEDs (365-470 nm, 440-460 nm and 650-670 nm), which are coupled to optical fiber. The other end of the optical fiber is inserted in a coaxial insert and can illuminate the NMR sample.

The equipment was successfully tested on photoisomerization of azobenzene [2] by *in situ* UV irradiation using LED source at 365 nm. The Photo-CIDNP spectroscopy was demonstrated on photo-induces reaction between benzophenone triplet and hydroquinone [3]. The possibilities of novel methodology for thiol-ene modification of (co)polymers accomplished under LED UV-irradiation without any photoinitiator were tested [4].

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REFERENCES

[1] P. Nitschke, N. Lokesh, R. Gschwind, Prog. Nucl. Magn. Reson. Spectrosc. 2019, 114–115, 86.

[2] H. M. D. Bandarab, S. C. Burdette, Chem. Soc. Rev. 2012, 41, 1809.

[3] R. Amorati, I. valgimigli, C. Viglianisi, M. Schmallegger, D. Neshchadin, G. Gescheidt, *Chem. Eur. J.* **2017**, 23, 5299.

[4] N. Toncheva-Moncheva, M. Dangalov, N. G. Vassilev, C. P. Novakov, PHOTOINITIATED THIOL-ENE COUPLING REACTION USING LED NMR SPECTROSCOPY (poster).