XXXIV European Congress on Molecular Spectroscopy - **EUCMOS 2018**

E
U C
M O
S

Coimbra – Portugal

19 – 24 August 2018

ADDENDUM
TO THE
BOOK OF ABSTRACTS

Addendum to the
Book of Abstracts of the XXXIV European Congress on Molecular Spectroscopy
EUCMOS 2018
Coimbra, Portugal
August 19-24, 2018

Edited by:

Rui Fausto
Elisa M. Brás
Licínia L. G. Justino
Bernardo A. Nogueira

Department of Chemistry
University of Coimbra
R. Larga, s/n
P-3004-535 Coimbra (Portugal)

Printed and bound:

João Duarte, Unipessoal, Lda – OGAMI

Copies:

250

Legal Deposit:

443831/18

Note

Editing a **Book of Abstracts** is not an easy task. Last minute abstracts and last minute changes always appear. Sometimes, these are received after the book has been printed. In the case of EUCMOS 2018, fortunately, the number of last minute abstracts of requests for last minute changes was very small. Nevertheless, a few requests have arrived. Also, because the amount of information that we had to process was very large, and the editorial work was very complex and involving several people, there was the risk that something got lost or adulterated during the editorial processing. I am glad to say that, at least until this date, the number of such occurrences identified was extremely small. In any case, there is always the exception that confirms the rule, and we have to apologize the authors of *Poster 8.29* for having not included their abstract in the Abstracts Book.

This **Addendum** presents the last minute changes to the abstracts requested by the authors, and the missing abstract of *Poster 8.29*.

After the congress, the **final official version of the Abstracts Book** will be published, which will be available at the congress website for download. In that version, all abstracts appearing in the version distributed during the congress that correspond to communications that were not effectively presented will be removed, and the requested last minute changes and the missing abstract of *Poster 8.29* will be included. Any other mistake, missing data, etc. that meanwhile might be detected, will also be corrected.

Rui Fausto, Ph.D.

Chairman of EUCMOS XXXIV

P
8.29

Discrimination Analysis of Blood Plasma Associated with Schizophrenia Disease Using FTIR Spectroscopy

Gülce Ogruc Ildiz[a] and Sevgi Haman Bayari[b]
[a] *Department of Physics, Science and Letters Faculty, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Turkey*
[b]*Department of Physics Engineering, Hacettepe University, Beytepe, 06800, Ankara, Turkey*
g.ogruc@iku.edu.tr

Schizophrenia is a severe mental disorder in which people interpret reality abnormally. It will impact the individual's feelings and their ability to communicate, to focus, to complete tasks, to sleep, and to relate to others. The Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) spectroscopy is highly favored and sensitive analytical tool widely used to detect the changes in the functional groups and molecular conformations of biochemical composition, such as nucleic acids, proteins, and lipids of normal and disease states. In this study, ATR-FTIR spectroscopy coupled with hierarchical cluster analysis methods were used to determine the biochemical variations in the blood plasma of schizophrenic patients compared with those of healthy control group. The variations in the area under the spectral bands give information about concentration of the functional groups belonging to the relevant molecules. In order to investigate possible disease-induced variations, the ratio of the area of the bands assigned to lipids, proteins, and nucleic acids were calculated. The first, most striking difference occurs in the bands associated with lipids. The lipid to protein ratio was lower in schizophrenic patients than controls, suggesting a decrease in total lipid content, in accordance with other studies.[1] The band at around 1080 cm^{-1} is due to symmetric stretching vibrations of phosphodiester groups (PO_2^-) in nucleic acids. The area ratios of the 1080 to 1550 cm^{-1} (amide II; protein) bands could be used to probe nucleic acids. We also found a significant decrease in the phosphodiester content for the schizophrenic group compared to the control. The use of hierarchical clustering analysis (HC) enabled us to explore in an efficient way the spectra of healthy and diseases groups. The best results were achieved in the C-H (3100- 2800 cm^{-1}) and 1300-900 cm^{-1} spectral regions.

References

1. J. Matsumoto *et. al.*, *Scientific Reports*, 7 (2017) 45050.

Acknowledgements: This study has been funded by the Scientific and Technological Research Council of Turkey-TUBITAK 1001 Project (Project No.: 116Z294).

KL 1

Non Linear Optics at Interfaces: Sensitive Probing of Biomolecular Recognition by Sum Frequency Generation and the Quest of Super Resolution Infrared Microscopy of Biological Tissues

N. Hedaoui[a], C. Bouchened[b] and André Peremans[c]
[a] *Centre de Développement des Technologies Avancée (CDTA), Cité 20 août 1956 Baba Hassen, Alger.*
[b] *Université des Sciences et de la Technologie Houari Boumediene (USTHB), BP 32 El Alia, Bab Ezzouar 16111, Alger.*
[c] *Université de Namur (UNAMUR), PMR, 61 rue de Bruxelles, Namur, Belgique*
andre.peremans@unamur.be

Since the pioneering work of Guyot-Sionnest in 1987, vibrational spectroscopies exploiting the non-linear optical processes have opened new opportunities for the analysis of biological systems, as well as, for bypassing the spatial resolution limit imposed by diffraction in infrared microscopy.
Indeed, biological molecules are complex and their infrared spectroscopy signature barely modified upon the structural change resulting from bio-recognition interactions. However, the selection rules of sum-frequency generation (SFG) makes this technique particularly sensitive to these structural modifications, and adapted for the determination of the biological films configuration as we demonstrated for: avidin-biocytin, penicillin derivative molecule, and biomimetic lipid systems.
Chemical cartography of biological tissues is traditionally realized by anchoring fluorescent chromophores on specific chemical functions. In 1994, Hell demonstrated the possibility of bypassing the spatial resolution limit, due to diffraction, in fluorescent microscopy using the stimulated-emission-depletion (STED) process. We recently demonstrated that the intrinsic non-linear optical properties of vibrational transitions also enable to perform super-resolution infrared microscopy on semiconductor and polymer materials, opening the prospect of label-free super resolution vibrational microscopy.

P
4.2

Skin Permeabilization Tracking by Confocal Raman Spectroscopy

Rita Cardoso, Andreia M. Tabanez, Bernardo A. Nogueira and Rui Fausto
CQC, Department of Chemistry, University of Coimbra, 3004-535, Coimbra, Portugal
ritadascardoso@gmail.com

Confocal Raman Spectroscopy is a powerful non-invasive optical technique that allows one to obtain detailed information regarding the chemical composition of molecular compounds, with high specificity. This technique is based on the inelastic light scattering and detects the vibrational modes that are characteristic from each molecule, giving us the "fingerprint" of the studied molecule.

The skin is a special organ with the ability to protect the organism, which main goal is to guaranty the right homeostatic relationship between the body and the external environment. The main barrier that is involved in this function, the stratum corneum (SC), is also the barrier that needs to be overcome by a topically applied drug to get in the body.

The topic application of drugs has been gaining relevance, because strategies have been developed that allow to control the drug release. In this work, we have studied the skin permeability capacity of different compounds involved in the topical administration of a recently developed drug for photodynamic therapy of cancer. The investigations were performed in pig skin model samples, by collecting the Raman spectra of the different Z-points of the studied samples.

It was possible to follow the pattern of penetration of the studied components of the sampled formulation, and conclude that all of them are indeed able to overcome the SC. These results are in favor of the use of the studied formulation as vehicle for topical administration of the drug.

Acknowledgements: The Coimbra Chemistry Centre (CQC) is supported by FCT, through the project UI0313/QUI/2013, also co-funded by FEDER/COMPETE 2020-EU.

P
5.20

The Impact of Dextran Sulfate on the Radiolytic Synthesis of Magnetic Iron Oxide Nanoparticles

Tanja Jurkin[a], Ivan Marić[a], Goran Štefanić[b] and Marijan Gotić[b]
[a] *Radiation Chemistry and Dosimetry Laboratory, Ruđer Bošković Institute, Bijenička 54, 0000 Zagreb, Croatia*
[b] *Center of Excellence for Advanced Materials and Sensing Devices, Research Unit New Functional Materials, Bijenička 54, 10000 Zagreb, Croatia*
tjurkin@irb.hr

Recently, the new synthesis route to δ-FeOOH nanodiscs based on the γ-irradiation of a deoxygenated iron(III) chloride alkaline aqueous colloidal solution in the presence of diethylaminoethyl-dextran hydrochloride (DEAE-dextran) has been reported by Jurkin et al. [1]. In that work we supposed that γ-irradiation produced reducing conditions and that δ-FeOOH nanoparticles were formed through oxidation of obtained white suspension characteristic of $Fe(OH)_2$. In this work, we studied the impact of dextran sulfate polymer (DEX-sulfate) on the radiolytic synthesis of magnetic iron oxide nanoparticles. The syntheses started with γ-irradiation (130 kGy) of deoxygenated iron(III) chloride alkaline aqueous colloidal solution in the presence of 2-propanol and DEX-sulfate. The radiolytically synthesised samples were isolated by conventional process of sample isolation (centrifugation/washing with water or ethanol) or in the presence of glycerol. The XRD results showed that sample isolated in the presence of glycerol contained $Fe(OH)_2$, hydroxysulfate green rust II (GR SO_4^{2-}) and goethite (α-FeOOH). The Mössbauer results confirmed the presence of $Fe(OH)_2$ and hydroxysulfate green rust II (GR SO_4^{2-}) in this sample. The radiolytically synthesized samples that were isolated by centrifugation and washing with water or ethanol contained GR SO_4^{2-} and α-Fe_2O_3. Therefore, the DEX-sulfate favoured the formation of α-FeOOH and/or α-Fe_2O_3 through GR-II (SO_4^{2-}) intermediate product.

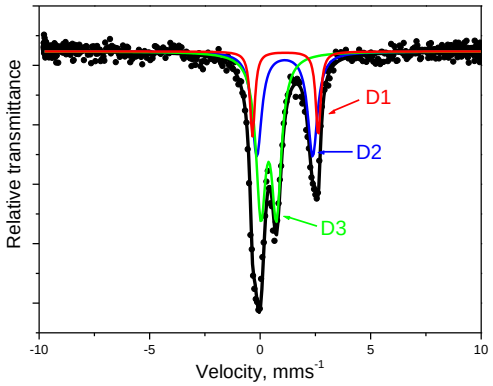


Figure 1 – Mössbauer spectrum of radiolytically synthesised sample that was isolated in the presence of glycerol. D1 and D2 doublets correspond to Fe(II) in $Fe(OH)_2$ and GR-II (SO_4^{2-}), respectively, whereas D3 corresponds to Fe(III).

References

1. T. Jurkin, G. Štefanić, G. Dražić and M. Gotić, *Mater. Lett.*, 173 (2016) 55.

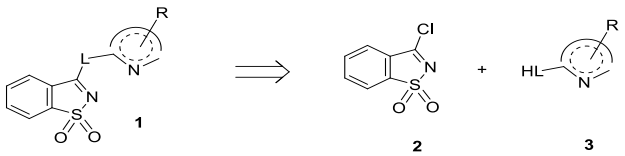
Acknowledgements: This work has been supported by Croatian Science Foundation under the project UIP-2017-05-7337 (POLRADNANOP).

OC 49

Saccharinate-based Ligands; Structure, Reactivity and Properties

Amin L. Ismael[a], Lília L. Cabral[a], Elisa Brás[b], Rui Fausto[b] and Maria L. S. Cristiano[a]
[a] *CCMAR and Dep. of Chemistry and Pharmacy, University of Algarve, 8005-139 Faro, Portugal*
[b] *CQC, Department of Chemistry, University of Coimbra, 3004-535, Coimbra, Portugal*
mcristi@ualg.pt

Saccharin (3-oxo-1,2-benzisothiazole 1,1-dioxide) and saccharinates have important applications in coordination chemistry, as ligands [1]. However, conjugates that combine the saccharyl system with other heterocycles have been scarcely explored hitherto, in spite of their expectable capabilities as bridging ligands. We have designed and prepared a representative library of saccharinate-based ligands **1** from tailored building blocks (**2**, **3**) [2], in view of exploring their potential as chelants. The monomeric structure and photochemistry of selected conjugates was investigated, using matrix isolation coupled to FTIR spectroscopy and molecular orbital calculations. Then their chelating properties towards divalent cations of transition metals were scrutinised, revealing properties that may support relevant applications of the ligands and corresponding complexes [3]. The journey from molecular design to the proposal of applications will be described, emphasizing the relevance of detailed structural studies for the optimisation of properties.



3 = unsaturated 5 membered rings:
Thiodiazole/Triazoles/Tetrazoles

R=H, alkyl, phenyl
L=-NH, S

References

1. D. W. Cho, S. W. Oh, D. U. Kim, H. J. Park, J. Y. Xue, U. C. Yoon, P. S. Mariano, *Bull. Korean Chem. Soc.*, 31 (2010) 2453.
2. L. Frija, R. Fausto, R. Loureiro, M. L. S. Cristiano, *J. Mol. Catal. A-Chemical*, 305 (2009) 142; A. Ismael, A. Borba, L. Duarte, B. M. Giuliano, A. Gómez-Zavaglia, M. L. S. Cristiano, *J. Mol. Struct.*, 1025 (2012) 105.
3. A. Ismael, A. Borba, M. S. C. Henriques, J. A. Paixão, R. Fausto, M. L. S. Cristiano, *J. Org. Chem.*, 80 (2015) 392; A. Ismael, M. S. C. Henriques, C. Marques, M. J. Rodrigues, L. Barreira, J. A. Paixão, R. Fausto, M. L. S. Cristiano, *RSC Adv.*, 6 (2016) 71628; L. Cabral, E. M. Brás, M. S. C. Henriques, C. Marques, L. Frija, L. Barreira, J. A. Paixão, R. Fausto, M. L. S. Cristiano, *Eur. J. Chem.*, 24 (2018) 3251.

Acknowledgements: We acknowledge Fundação para a Ciência e a Tecnologia (FCT)-Portugal and COMPETE (projects UID/Multi/04326/2013, UI0313/QUI/2013, PTDC/QEQ-QFI/3284/2014, PTDC/MAR-BIO/4132/2014). The Coimbra Chemistry Centre (CQC) is supported by FCT, through the project UI0313/QUI/2013, also co-funded by FEDER/COMPETE 2020-EU.


COMPETE
PROGRAMA OPERACIONAL FACTORES DE COMPETITIVIDADE


FCT
Fundação para a Ciência e a Tecnologia
MINISTÉRIO DA EDUCAÇÃO E CIÊNCIA


QUADRO
DE REFERÊNCIA
ESTRATÉGICO
NACIONAL
PORTUGAL 2007.2013