EuCMOS

European Congress on Molecular Spectroscopy

Book of Abstracts

24.08.2025 - 29.08.2025

Wrocław, Poland

EuCMOS

European Congress on Molecular Spectroscopy

EUCMOS
European Congress on Molecular Spectroscopy

Book of Abstracts

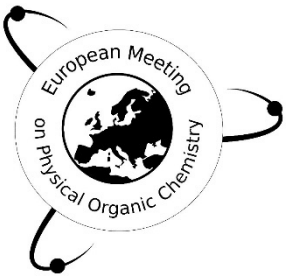
EUCMOS 2025 & EMPOC 2025

XXXVI. European Congress on Molecular Spectroscopy

XLIV. European Meeting on Physical Organic Chemistry

24 – 29 August 2025

Wrocław, Poland



ISBN 978-83-60043-45-5
Editor Justyna Krupa

Organizers:

Faculty of Chemistry, University of Wrocław

Faculty of Chemistry, Wrocław University of Science and Technology

Institute of Low Temperature and Structure Research, Polish Academy of Sciences

Honorary Patronage:

Rector of the University of Wrocław

Rector of the Wrocław University of Science and Technology

President of the Polish Academy of Sciences

Polish Chemical Society

Lower Silesian Governor

Marshal of the Lower Silesian Voivodeship

Mayor of Wrocław

Patronages:

EUCMOS International Committee

R. Fausto (Coimbra, Portugal) - President
S. Turrell (Villeneuve D'ascq, France) -Vice-President
M. Schmitt (Düsseldorf, Germany) - Vice-President
L. Bañares (Madrid, Spain)
M. Barańska (Cracow, Poland)
S. Bayari (Ankara, Turkey)
W. V. Buma (Amsterdam, Netherlands)
A. Császár (Budapest, Hungary)
C. Castiglioni (Milan, Italy)
M. Czarnecki (Wroclaw, Poland)
V. Deckert (Jena, Germany)
G. Dovbeshko (Kiev, Ukraine)
H. M. Heise (Iserlohn, Germany)
P. Herdewyn (Leuven, Belgium)
S. Kazarian (London, UK)
H. Kjaergeard (Copenhagen, Denmark)
J. Kneipp (Berlin, Germany)
B. Lendl (Vienna, Austria)
R. López-Ramírez (Malaga, Spain)
J. Lundell (Helsinki, Finland)
T. Mamose (Vancouver, Canada)
S. Melandri (Bologna, Italy)
A. Mezzetti (Paris, France)
I. Nemec (Prague, Czech Republic)
G.O. Ildiz (Istanbul, Turkey)
K. Orzechowski (Wrocław, Poland)
S. Riedel (Berlin, Germany)
R. Romano (La Plata, Argentina)
M. Schnell (Hamburg, Germany)
E. Ventura do Monte (João Pessoa, Brazil)
W. Yang (Durham, USA)

EUCMOS Honorary Members

J. Bellanato (Madrid, Spain)
T. A. Ford (Durban, South Africa)
H. Hamaguchi (Hsinchu, Taiwan)
J. Laane (College Station, Tx, USA)
H. Ratajczak (Wrocław, Poland)
G. Zerbi (Milan, Italy)

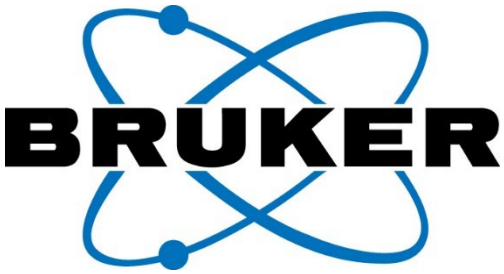
Local Organizing Committee

Kazimierz Orzechowski - Chair
Mirosław Czarnecki - Vice-chair
Maria Wierzejewska - Vice-chair
Justyna Krupa-Secretary and Book of Abstract Editor
Dariusz Bieńko (PWr)
Katarzyna Cieślik-Boczula (UWr)
Marta Gordel-Wójcik (UWr)
Karol Kułacz (UWr)
Magdalena Malik (PWr)
Tomasz Mazur (PWr)
Karolina Mucha (UWr)
Maciej Ptak (INTiBS PAN)

Sponsors

spectroscopy journal
an Open Access Journal by MDPI

Uniwersytet Wrocławski



BRUKER

RENISHAW®

OXFORD INSTRUMENTS

ChemLand®

Programme

Sunday, August 24th

Faculty of Chemistry (Fryderyka Joliot-Curie 14 - entry near the University Library)

14:00 - 21:00 **Registration** - Student's entrance

15:00 - 17:00 **Bruker Workshop**
OPUS Unlocked: Getting the Most Out of Your FT-IR Spectrometer, Room 145

19:00 - 21:00 **Get-together party** - drinks, snacks, and music, Main Hall

Monday, August 25th

University Library (Fryderyka Joliot-Curie 12)

08:30 **Registration** - Main Hall

Lecture hall III

9:00 - 9:30 **Opening Ceremony**

CHAIR: **prof. Kazimierz Orzechowski**

9:30 - 10:00 **PL-1** **Rui Fausto** (Coimbra, Portugal)
Tunnelling-Driven Chemistry: From Conformational Changes to Optically-Controlled Tunnelling-Based Molecular Switches

10:00 - 10:30 **PL-2** **Maria Luisa Saladino** (Palermo, Italy)
Non Invasive Spectroscopy for Cultural Heritage

10:30 - 11:00 **Coffee break**

CHAIR: **prof. Rui Fausto**

11:00 - 11:30 **PL-3** **Małgorzata Barańska** (Kraków, Poland)
Raman Probes for Multiplex Bioimaging

11:30 - 12:00 **PL-4** **Klaus Gerwert** (Bochum, Germany)
Protein-Misfolding as Fluid Biomarker in Morbus Alzheimer and Parkinson Measured with the iRS (immuno-Infrared Sensor)

12:00 - 12:10 **OC-1** **Maria Rosa Lopez-Ramirez** (Málaga, Spain)
Highly Effective Core@shell AuAg Nanoparticles as Potential SERS Pubstrates

12:10 - 12:30 **OC-2** **Anna Pieczara** (Kraków, Poland)
Raman-Based Biochemical Profiling of Adrenaline's Action on Lipid Metabolism in Endothelial Cells

12:30 - 12:50 **OC-3** **Halina Abramczyk** (Łódź, Poland)
A New Modality for Cancer Tracking-Raman Imaging, NanoIR Imaging, Fluorescence and AFM Studies Combined with AI Analysis

12:50 - 13:00 **OC-4** **Adriana Adamczyk** (Kraków, Poland)
A Spectroscopic Evaluation of the Erythroid Differentiation Process Induced by Drugs of Different Mechanisms of Action

13:00 - 15:00 **Lunch**

CHAIR: **prof. Herbert Michael Heise**

15:00 - 15:20 **OC-5** **Beata Brożek-Płuska** (Łódź, Poland)
Exploring The Therapeutic Molecules Effects in Colon Cells Using Integrated Raman Imaging-AFM-Femtosecond Laser Spectroscopy

15:20 - 15:40 **OC-6** **Rares-Ionut Stiufiuc** (Cluj-Napoca, Romania)
The Role of Spectroscopic Liquid Biopsy in Early Disease Detection

15:40 - 16:00 **OC-7** **Andreas Barth** (Stockholm, Sweden)
The Structure of Amyloid-β Oligomers Studied by Experimental and Computational Isotope-Edited Infrared Spectroscopy

16:00 - 16:20 **OC-8** **Sylwester Mazurek** (Wrocław, Poland)
Carotenoid Profile of Bee Pollen Fractions Based on Raman Spectra

16:20 - 16:40 **OC-9** **Katarzyna Cieślik-Boczula** (Wrocław, Poland)
FTIR Studies of the Structure of Lipid Membrane Models for Protein/Peptide-Lipid Matrix Interaction and for Carriers in the Transport of Biologically Active Substances

16:40 - 16:50 **OC-10** **Ewa Szczęsny-Małysiak** (Kraków, Poland)
Monitoring of Cytochrome C Oxidation State in Live Cells with Resonance Raman Imaging

16:50 - 17:00 **OC-11** **Patrycja Dawiec** (Kraków, Poland)
Spectroscopic Profiling of Pharmacologically Induced Metabolic Shifts in Sensitive and Resistant Blood Cancer Cells

17:00 - 17:30 **Coffee break**

19:00 - 21:00 **Barbecue at the Botanical Garden** (Henryka Sienkiewicza 23)

Tuesday, August 26th

University Library (Fryderyka Joliot-Curie 12)

08:30 **Registration** - Main Hall

Lecture hall III

CHAIR: **prof. Sylvia Turrell**

9:00 - 9:30 **PL-5** **Peter Gardner** (Manchester, UK)
Infrared Imaging of Prostate Tissue: From Diagnosis to Prognosis

9:30 - 10:00 **PL-6** **Herbert Michael Heise** (Iserlohn, Germany)
Infrared Biospectroscopy with ATR Measurement Technology for the Investigation of Insulin-Dependent Intracellular Processes in the Monocytic Cell Line

10:00 - 10:30 **PL-7** **Maxim S. Pshenichnikov** (Groningen, Netherlands)
Self-Assembly of Artificial Light-Harvesting Complexes: A Molecular Spectroscopist's Perspective

10:30 - 11:00 **Coffee break**

CHAIR: prof. Klaus Gerwert

11:00 - 11:30 **PL-8** **Michael Schmitt** (Düsseldorf, Germany)
The Concept of the Dipole Moment: Why is it still relevant for Chemistry?

11:30 - 11:40 **OC-12** **Barbara Gieroba** (Lublin, Poland)
Application of Fourier Transform Infrared Spectroscopy (FT-IR) in the Evaluation of Drug Release from Polysaccharide Matrices

11:40 - 11:50 **OC-13** **Marta Gordel-Wójcik** (Wrocław, Poland)
Tailoring Diverse Light–Matter Interactions by Combining Plasmonic, Dielectric, and Quantum-Confined Nanostructures in Hybrid Nanosystems

11:50 - 12:00 **OC-14** **Wiktoria Korona** (Kraków, Poland)
A New Approach to Spectral Analysis of Lipid Pathways in Cancer Cells Using Labeled Raman and O-PTIR Technique

12:00 - 12:10 **OC-15** **Jakub Dybaś** (Kraków, Poland)
Spectroscopic Analysis of Biochemical Composition of Red Blood Cells in Polycythemia Vera Patients

12:10 - 12:20 **OC-16** **Anna Kołodziej** (Kraków, Poland)
Spectroscopic Study of Magnetic Composites Modified with Hydroxyapatite for Regenerative Medicine Applications

12:20 - 12:30 **OC-17** **Vlada Pashynska** (Kharkiv, Ukraine)
Molecular Interactions Between Anticancer Drugs and Ascorbic Acid: Insights into Drug Activity Modulation

12:30 - 12:50 **OC-18** **Ahmad Salman** (Beer-Sheva, Israel)
Rapid Infection Diagnosis Using Infrared Microscopy, Peripheral Blood Tests, and an Expert System in Febrile Pediatric Oncology

12:50 - 13:00 **Conference Photo**

13:00 - 15:00 **Lunch**

CHAIR: prof. Małgorzata Barańska

15:00 - 15:20 **OC-19** **Ivan Němec** (Prague, Czech Republic)
Combined Spectroscopic and Structural Study of Promising NLO Crystals Based on 2D Molecular Building Units

15:20 - 15:30 **OC-20** **Thomas Golin Almeida** (Copenhagen, Denmark)
Atmospheric Oxidation Reaction Kinetics of Ethanolamines Employed in Carbon-Capture

15:30 - 15:40 **OC-21** **Ružica Marković** (Copenhagen, Denmark)
Vibrational Spectroscopy of Monohydrated Radical Cation Complexes

15:40 - 15:50 **OC-22** **Piotr Najgebauer** (Opole, Poland)
Molecular Modeling of Non-Covalent Interactions Between Orellanine and Graphene Oxide Models

15:50 - 16:00 **OC-23** **Nanna Falk Christensen** (Copenhagen, Denmark)
Calculated Absorption Cross Sections and Photolysis Rates of Ketohydroperoxides

CHAIR: **prof. Mirosław Czarnecki**

16:00 - 17:00 **Poster - Flash presentations**

17:00 - 19:00 **Poster session with coffee**

Wednesday, August 27th

University Library (Fryderyka Joliot-Curie 12)

08:30 **Registration** - Main Hall

Lecture hall III

CHAIR: **prof. Michael Schmitt**

9:00 - 9:30 **PL-9** **Jan Lundell** (Helsinki, Finland)
Light-Induced Chemistry in Low Temperature Matrices

9:30 - 10:00 **PL-10** **Marcus Meuwly** (Basel, Switzerland)
Computational Vibrational Spectroscopy in the Era of Machine Learning

10:00 - 10:30 **PL-11** **Małgorzata Biczysko** (Wrocław, Poland)
Simulation of Vibrational Signatures from the Mid Infrared (MIR) to the Vacuum Ultraviolet (VUV)

10:30 - 11:00 **Coffee break**

CHAIR: **prof. Maxim Pshenichnikov**

11:00 - 11:30 **PL-12** **Søren Balling Engelsen** (Copenhagen, Denmark)
Near Infrared Spectroscopy in Food Science and Industry

11:30 - 11:50 **OC-24** **Marek Drozd** (Wrocław, Poland)
About Metamaterials and Other Second Harmonic Generators

11:50 - 12:10 **OC-25** **Václav Profant** (Prague, Czech Republic)
Terahertz Raman Optical Activity as a New Window into Supramolecular Chirality

12:10 - 12:30 **OC-26** **Natalia Piergies** (Kraków, Poland)
Stability of Drug–Metal Nanoparticle Conjugates as a Key Determinant of Their In Vitro Efficacy

12:30 - 12:40 **OC-27** **Przemysław Dopieralski** (Wrocław, Poland)
Impact of Water on the Nanomechanical Degradation of Functionalized Gold Surface

12:40 - 13:00 **OC-28** **Karolina A. Haupa** (Ettlingen, Germany) **BRUKER**
Spectroscopy for Sustainability: The Role of FTIR in Green Technologies

13:00 - 15:00 **Lunch**

13:55 - 14:55 **Bruker Workshop - Lecture hall IV**
Getting up to speed with Infrared laser imaging

SESSION 1 - Lecture hall III

CHAIR: prof. Jacek Waluk

15:00 - 15:20 **OC-29** **Casper Vindahl Jensen** (Copenhagen, Denmark)
Resonance Tuning of the Water-Trimethylamine Complex in Three Different Experimental Media

15:20 - 15:40 **OC-30** **Aleksandra Wesełucha-Birczyńska** (Krakow, Poland)
Raman and Nanomechanical Studies of Polymer Mats with Carbon Nano-additives

15:40 - 16:00 **OC-31** **Vili-Taneli Salo** (Copenhagen, Denmark)
Kinetics of Atmospheric Oxidation of Ammonia

16:00 - 16:20 **OC-32** **Dhritabrata Pal** (Copenhagen, Denmark)
Dimethyl Ether-Water Hydrogen Bond Complex: Room Temperature Gas-Phase Detection and Determination of Formation Gibbs Energy

16:20 - 16:40 **OC-33** **Andrzej Teisseyre** (Wrocław, Poland)
The Inhibitory Effects of Genistein and Resveratrol on Voltage-Gated Potassium Channels in Cancer Cells – Putative Role in Anti-Cancer Activity

16:40 - 16:50 **OC-34** **Sándor Góbi** (Budapest, Hungary)
Hydrogen-Atom-Assisted Thione–Thiol Tautomerization of Thiourea Derivatives in para-H_2 Matrix

SESSION 2 - Lecture hall IV

CHAIR: prof. Richard Buchner

15:00 - 15:20 **OC-35** **Tomasz Pawel Czaja** (Copenhagen, Denmark)
Using ASCA to Study Sampling in Spectroscopy

15:20 - 15:40 **OC-36** **Eva Kočišová** (Prague, Czech)
Metal Oxides and Metal Oxides/Metal Nanostructures for Surface-Enhanced Raman Scattering (SERS) Spectroscopy

15:40 - 15:50 **OC-37** **Ali Muhieddine** (Orsay, France)
Photodetachment of Cooled Deprotonated Chlorophyll Pigments in the Gas Phase

15:50 - 16:00 **OC-38** **Szymon Smółka** (Wrocław, Poland)
Physicochemical Properties and Phase Transition Mechanisms of Lead Halides Comprising Small Organic Cations in the Structure: Novel Perovskites with Tunable Optoelectronic Properties

16:00 - 16:10 **OC-39** **Vera Staun Hansen** (Copenhagen, Denmark)
Absorption Cross-Section of Gas-Phase Isoprene in the Entire JWST Region

16:10 - 16:20 **OC-40** **Andras Sun Poulsen** (Copenhagen, Denmark)
Generation and Consideration of Trioxyl Radical

16:20 - 16:30 **OC-41** **Natalia Dutkiewicz** (Warsaw, Poland)
Porphyrin-acene Dyads for Controlled Singlet Oxygen Generation and Depletion

16:30 - 16:50 **OC-42** **Kazimierz Orzechowski** (Wrocław, Poland)
Dielectric Spectroscopy in Breast Cancer Imaging

17:00 - 17:30 **Coffee break**

19:30 - 20:30 **Classical music concert at the Oratorium Marianum**
In the concert hall of the main building of the University of Wrocław (Plac Uniwersytecki 1)

Thursday, August 28th

University Library (Fryderyka Joliot-Curie 12)

Lecture hall III

CHAIR: **prof. Poul Erik Hansen**

9:00 - 9:30 **PL-13** **Richard Buchner** (Regensburg, Germany)
Dielectric Spectroscopy in Solution Chemistry - Advantages and Pitfalls

9:30 - 10:00 **PL-14** **Henrik G. Kjaergaard** (Copenhagen, Denmark)
The Effect of Temperature on OH-stretching Bands of Hydrogen Bound Complexes

10:00 - 10:30 **PL-15** **Bernhard Lendl** (Wien, Austria)
Enhancing Mid-IR Sensing Through Laser Technology and Integrated Photonics

10:30 - 11:00 **Coffee break**

CHAIR: **prof. Jan Lundell**

11:00 - 11:20 **OC-43** **Jacek Waluk** (Warsaw, Poland)
Photostability: Proper Determination and Control

11:20 - 11:40 **OC-44** **Maciej Ptak** (Wrocław, Poland)
Mechanism of Phase Transition in Layered 2-Fluoroethylammonium Cadmium Chlorobromide

11:40 - 12:00 **OC-45** **Iwona Płowaś-Korus** (Poznań, Poland)
Molecular Dynamics and Interactions in Aqueous Solutions of Skin Care Ingredients

12:00 - 12:10 **OC-46** **Eaindra Lwin** (Göttingen, Germany)
The Universal Vibrational Dynamics of Water Bound to Tertiary Amines: More Than Just Fermi Resonance

12:10 - 12:20 **OC-47** **Ivan Kopal** (Prague, Czech Republic)
Underrated Surface Phenomena Influencing Surface-Enhanced Raman Scattering at Plasmonic Interfaces

12:20 - 12:30 **OC-48** **Valerie Smeliková** (Prague, Czech Republic)
Treatment of MoS2 Monolayers by Atomic Deuterium

12:30 - 12:40 **OC-49** **Karol Kułacz** (Wrocław, Poland)
Complexity and Various Dynamic States of Interlayer Water in Nontronite: Insights from Dielectric Spectroscopy and TG–DSC Analysis

12:40 - 13:00 **OC-50** **Agnieszka Sozańska** (Warsaw, Poland) **RENISHAW**
Remote and in situ Sampling with the Virsa™ Raman Analyser

13:00 - 15:00 **Lunch**

13:55 - 14:55 **Bruker Workshop - Lecture hall IV**
Unleash the real speed of Raman imaging on any sample

SESSION 1 - Lecture hall III

CHAIR: **prof. Marcus Meuwly**

15:00 - 15:20 **OC-51** **Marek Procházka** (Prague, Czech Republic)
Surface-Enhanced Raman Scattering (SERS) Spectroscopy on Conductive Polymers and Hybrid Metal/Conductive Polymers Materials

15:20 - 15:40 **OC-52** **Justyna Grabska** (Innsbruck, Austria)
Integration of NIR Spectroscopy and Anharmonic Chemical Calculations for Applied Analysis

15:40 - 15:50 **OC-53** **Aleksandra Szymańska** (Warsaw, Poland)
Seeing Red and Orange: Tailored Nanostructured SERS Substrates for Azo Dye Detection

15:50 - 16:00 **OC-54** **Veranika Kuzmina** (Warsaw, Poland)
Insights into the Photochemical Behavior of Coumarin Derivatives via UV-Vis and NMR: From Reversible Rotation to Irreversible Photodegradation

16:00 - 16:20 **OC-55** **Barbara Golec** (Warsaw, Poland)
Photostability of Azaaromatic Compounds

16:20 - 16:40 **OC-56** **Alicja Dabrowska** (Vienna, Austria)
Towards on-Chip Mach-Zehnder Interferometer for Complex Refractive Index Sensing of Liquids in the Mid-Infrared

16:40 - 16:50 **OC-57** **Shiva Ghasemi** (Hamedan, Iran)
Chemometric Deconvolution of Raman Spectra in Multi-Doped Carbon Nanomaterials

SESSION 2 - Lecture hall IV

CHAIR: **prof. Małgorzata Biczysko**

15:00 - 15:20 **OC-58** **Jože Grdadolnik** (Ljubljana, Slovenia)
The Physical Origin of Hydrophobicity

15:20 - 15:40 **OC-59** **Rafał Szabla** (Wrocław, Poland)
Stacking and Chalcogen Bonding Enhance Photoinduced Electron Transfer in Nucleic Acids

15:40 - 15:50 **OC-60** **Roel van de Ven** (Nijmegen, Netherlands)
Finding a Needle in a Needle Stack: Leveraging Vibrational Spectra and Machine Learning to Guide Conformational Search

15:50 - 16:00 **OC-61** **Anjali Sangwan** (Delhi, India)
Formation of Ethanolamine-Mediated Surfactant-Free Microemulsions Using Hydrophobic Deep Eutectic Solvents

16:00 - 16:10 **OC-62** **Kamil Wojtkowiak** (Wrocław, Poland)
Theoretical Study of Selected Halogen-Bonded Complexes: Case of Methionine and Its Derivatives

16:10 - 16:20 **OC-63** **Štěpán Jílek** (Prague, Czech Republic)
Investigation of the Structural Plasticity of Lithium Stabilized Mononucleotide G-Quadruplexes via Raman Optical Activity

16:20 - 16:40 **OC-64** **Galyna Dovbeshko** (Kyiv, Ukraine)
Vibrational Markers of Model Metastatic Circulating Tumor Cells: FTIR, Raman, CARS Spectroscopy and Microscopy

17:00 - 17:30 **Coffee break**

19:30 - 22:00 **Conference banquet**
Hotel HP Park Plaza Wrocław (Bolesława Drobnera 11-13)

Friday, August 29th

University Library (Fryderyka Joliot-Curie 12)

Lecture hall III

CHAIR: **prof. Søren Balling Engelsen**

9:00 - 9:30 **PL-16** **Piotr Piecuch** (Michigan, USA)
Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation

9:30 - 10:00 **PL-17** **Poul Erik Hansen** (Roskilde, Denmark)
A Kalejdoscopic View of Intramolecular Hydrogen Bonds

10:00 - 10:30 **PL-18** **Sylvia Turrell** (Lille, France)
From Alzheimer's Disease to Functional Nanomaterials: 100 Years of Advances in Vibrational Spectroscopy

10:30 - 11:00 **Closing Ceremony**

11:00 - 11:30 **Coffee break & snacks**

Plenary Lectures

PL-1: Rui Fausto

PL-2: Maria Luisa Saladino

PL-3: Małgorzata Barańska

PL-4: Klaus Gerwert

PL-5: Peter Gardner

PL-6: Herbert Michael Heise

PL-7: Maxim S. Pshenichnikov

PL-8: Michael Schmitt

PL-9: Jan Lundell

PL-10: Marcus Meuwly

PL-11: Małgorzata Biczysko

PL-12: Søren Balling Engelsen

PL-13: Richard Buchner

PL-14: Henrik G. Kjaergaard

PL-15: Bernhard Lendl

PL-16: Piotr Piecuch

PL-17: Poul Erik Hansen

PL-18: Sylvia Turrell

Tunnelling-Driven Chemistry: From Conformational Changes to Optically-Controlled Tunnelling-Based Molecular Switches

Rui Fausto
IMS-CQC, Department of Chemistry, University of Coimbra, P-3004-535 Coimbra, Portugal
ERA-Chair Spectroscopy@IKU, Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Ataköy Campus, Bakirköy, Istanbul, Türkiye
rfausto@ci.uc.pt

In this lecture, we will explore chemical processes occurring in cryogenic matrix media via the quantum mechanical tunnelling (QMT) mechanism. These processes range from simple conformational changes to more complex bond-breaking and bond-forming reactions. Strategies for generating appropriate reactant species in conformations favourable for tunnelling will be discussed. A wide array of QMT-driven processes will be presented, including competitive heavy-atom tunnelling (Figure 1), optically controlled QMT-based molecular switches, and solvent-coupled hydrogen transfer reactions exhibiting small isotopic kinetic isotope effects.

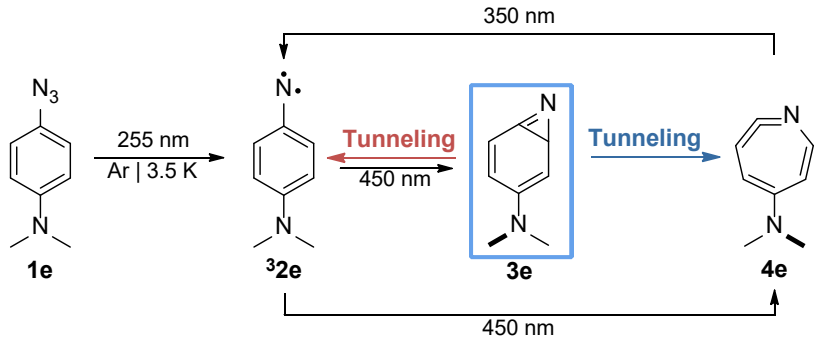


Figure 1 – Summary of the observed QMT-driven reactivity involving 4-dimethylamino-2*H*-benzazirine (**3e**) generated in an Ar matrix at 3.5 K from an azide precursor (**1e**)

References
1. R. Fausto, G. O. Ildiz, C. M. Nunes, *Chem. Soc. Rev.*, 51 (2022) 2853.

Acknowledgements: The author thanks the Horizon-Widera-2023-Talents-01 ERA-Chair 1011848998 Spectroscopy@IKU "Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals", which is Funded by the European Union. The IMS-CQC is funded by the Portuguese Science Foundation, projects UIDB/00313/2025 (https://doi.org/10.54499/UIDB/00313/2025), UIDP/00313/2025 (https://doi.org/10.54499/UIDP/00313/2025) and IMS-LA/P/0056/2020 (https://doi.org/10.54499/LA/P/0056/2020).

Non Invasive Spectroscopy for Cultural Heritage

Maria Luisa Saladino
Dipartimento di Scienze e Tecnologie Biologiche Chimiche e Farmaceutiche (STEBICEF) and INSTM-Palermo, Università degli studi di Palermo, Viale delle Scienze, Ed.17, I-90128 Palermo, Italy
IPCF-CNR, Istituto per i Processi Chimico Fisici, V.le F. S. d'Alcontres 37, I- 98158 Messina, Italy
marialuisa.saladino@unipa.it

The preservation and knowledge of cultural heritage artifacts necessitate physical chemical methods that are both informative and non-destructive. Non-invasive spectroscopic techniques have emerged as invaluable tools in this domain, enabling in-situ analysis without compromising the integrity of the objects. A sustainable, non-invasive approach is implemented through the use of portable instruments. XRF, IR, Raman and FORS spectroscopy offers molecular-level insights, facilitating the identification of pigments and/or corrosion products in artworks and archaeological items. By using the micro-XRF or micro-IR variants, a precise elemental or molecular analysis and mapping of surface compositions can also be obtained. Luminescence-based techniques provide complementary information on organic materials, varnishes, and certain mineral phases. These methods are particularly useful in the detection of aged varnishes, binders, and certain alteration compounds that exhibit characteristic emission behavior under specific excitation wavelengths.
The integration of these spectroscopic methods, often complemented by chemometric and multivariate analysis, as well as the machine learning approaches, provides a comprehensive and multi-faceted approach to the characterization, conservation, and authentication of cultural heritage materials, especially for collections constituted by thousands of objects [1,2].
Predictive and classification models using machine learning algorithms are useful to analyze archaeological and physico-chemical data, presenting itself as an innovative solution for sustainable diagnostics of cultural heritage. Here, some case studies, mainly paintings and metals, will be introduced in order to show the application, strengths, and drawbacks of different spectroscopic techniques, combined with chemiometric and machine learning approaches.

References

1. F. Armetta, M. Baublytė, M. Lucia, R.C. Ponterio, D. Giuffrida, M. L. Saladino, S. Orecchio, *J. Am. Chem. Soc.* 146 (2024) 35321.
2. S. Wang, Z. Wu, S. Dai, D. Jiang, *Angew. Chem. Int. Ed.*, 60(22) (2021) 12289.

Acknowledgements: The authors thank the Project MML-ARCH - "Metodologie di machine learning applicate all'archeometria: una nuova frontiera per l'interpretazione materica dei Beni Culturali", Programma "CHANGES Cultural Heritage Active iNnovation for Sustainable Society" CUP B53C22003890006 - Codice Identificativo PE_00000020, finanziato dall'Unione Europea – Next Generation EU sui fondi PNRR MUR – M4C2 – Investimento 1.3 "Partenariati estesi a Università, centri di ricerca, imprese e finanziamento progetti di ricerca" Avviso pubblico per la presentazione di Proposte di intervento per la creazione di "Partenariati estesi alle università, ai centri di ricerca, alle aziende per il finanziamento di progetti di ricerca di base".

Raman Probes for Multiplex Bioimaging

Anna Pieczara[a], Wiktoria Korona[a,b], Anna Nowakowska[a], Krzysztof Brzozowski[a], Barbara Orzechowska[a], Malgorzata Baranska[a]

[a]*Jagiellonian University in Krakow, Faculty of Chemistry, 2 Gronostajowa Str., Krakow, Poland*
[b]*Jagiellonian University in Kraków, Doctoral School of Exact and Natural Sciences, 11 Lojasiewicza St., Krakow, Poland*
m.baranska@uj.edu.pl

The main goal of this study is to overcome methodological and technical limits of Raman imaging in detecting small organelles and specific molecules within cells by harnessing physics, chemistry, medicine, pharmacology, biology, engineering, and data analysis, to use these advanced technologies in life sciences. The combination of specificity and sensitivity of the Raman probes with information obtained from spontaneous Raman spectroscopy and SRS/CARS on living cells gives diagnostic potential to these methods. They can support classic approaches in tracking cellular processes, studying chemoresistance, and characterizing drug-cell interactions.

The use of molecular probes in Raman imaging is a relatively new technique in subcellular research, however, very fast and dynamically developing. Compared to the label-free method, it allows for a more sensitive and selective visualization of organelles within a single cell. Directly visualizing biological structures and activities at the cellular and subcellular levels remains by far one of the most intuitive and powerful ways to study biological problems.

For hyperspectral detection and imaging of living cells, it is very desirable to use probes with strong and unique Raman vibrations in the biological silent region (1800 – 2800 cm-1). Here it is shown a biorthogonal chemical imaging of cells to track biochemical changes associated with mitochondrial function at the cellular level in an in vitro model. Both commercially available and newly synthesized highly sensitive Raman probes for selective imaging of mitochondria in live cells is presented. In addition to spontaneous Raman microscopy, nonlinear techniques were used for rapid cell imaging.

Acknowledgements: This research was funded in whole or in part by the National Science Center Poland (NCN), Maestro 2022/46/A/ST4/00054 to Malgorzata Baranska.

Protein-Misfolding as Fluid Biomarker in Morbus Alzheimer and Parkinson Measured with the iRS (immuno-Infrared Sensor)

Klaus Gerwert
Ruhr-Universität Bochum, Germany
klaus.gerwert@ruhr-uni-bochum.de

Early-stage blood-based biomarkers for Alzheimer´s disease (AD) are coming into focus. Especially, those that indicate the risk for dementia at a symptom-free stage, before irreversible brain-damage damage occurs, might provide the best therapy response. Blood-based biomarkers will allow, in contrast to current expensive PET scans and invasive CSF measurements, pre-screening of the elderly population. Complementary to the established concentration-based Aβ and p-tau biomarkers in body fluids for the symptomatic clinical stage, we have examined Aβ misfolding as structure based biomarkers for preclinical stages. With the innovative infrared-immuno-sensor (iRS), we measure the secondary structure distribution of all Aβ isoforms in body-fluids as misfolding biomarker [1]. The new iRS platform technology uses quantum cascade lasers as light source, ATR crystals to measure fluids in thin films and surface-bound antibodies to concentrate the biomarkers in the evanescent wave. A blocking layer prevents unspecific binding. The iRS overcomes the challenges of traditional infrared spectroscopy and allows targeted measurements of targets in aqueous solutions.

Initial misfolding of Aβ is followed by β-sheet oligomerization and aggregation to much larger nanoscale fibrils. After several years, these fibrils were deposited in macroscopic large amyloid plaques, which can be visualized by in PET scanning at the macroscopic scale. We have shown in a discovery study that the misfolding biomarker indicates probable AD in a prospective cohort [1]. We extended this to earlier mild cognitive impaired [2]. We also investigated the performance of Aβ misfolding as a prescreening plasma biomarker for the development of AD in a symptom-free population-based cohort up to 17 years before clinical diagnosis [3].

Recently, we extended this approach to Parkinson´s disease using alpha-synuclein misfolding as biomarker. This provides a sensitivity of 94% and specificity of 96% [4].

This highlights the potential of the misfolding biomarker as a blood-based- biomarker and as a screening method for the aging population to determine the risk of future clinical AD and PD. Thus, early intervention of Alzheimer's can be achieved by the new FDA-approved drugs.

References

1. A. Nabers, *et al.*, *J.Biophotonics.*, 9(3) (2016) 224.
2. A. Nabers, *et al.*, *EMBO.Mol.Med.*, 10(5) (2018).
3. L. Beyer, *et al.*, *Alzheimer's Dement.,* 19 (2023) 1020.
4. M. Schuler, *et al.*, *EMBO.Mol.Med.*, 17 (2025) 1203.

Infrared Imaging of Prostate Tissue: From Diagnosis to Prognosis

Dougal Ferguson, Claire A. Hart, Mick Brown, Diego F. Sanchez, Pedro Olivera, Noel Clark, Ashwin Sachdeva, Peter Gardner

[a]*Photon Science Institute, University of Manchester, Oxford Road, Manchester, M13 9PL,UK;*
[b]*Department of Chemical Engineering, School of Engineering, University of Manchester, Oxford Road, Manchester, M13 9PL.*
[c]*Division of Cancer Sciences, University of Manchester, UK*
[d]*Cancer Research UK Manchester Institute, Wilmslow Road, Manchester UK, M20 4GJ*
[e]*Department of Pathology, The Christie Hospital NHS Foundation Trust, UK*
[f]*Department of Surgery, The Christie Hospital NHS Foundation Trust, UK*
[g]*Department of Urology, Salford Royal Hospital, UK*
peter.gardner@manchester.ac.uk

It has long been established that infrared spectroscopic imaging of biopsy tissue can be used to separate cell types, identify cancerous tissue from non-cancerous tissue and also identify Gleason grades. This can potentially reduce current intra-observer variability and thus feed into the diagnostic pathway. However, it does not provide any additional prognostic information and is therefore of limited clinical utility. In this study we demonstrate that linking data with patient outcome rather than pathology can lead to new information that is potentially much more useful to clinicians. The identification of high-risk non-metastatic prostate cancers is extremely challenging. This means that most of these patients are put into the low risk group and the most common treatment option is to go onto active surveillance. This involves the clinicians keeping a watch on your condition (say every 6 months) without any aggressive intervention. However, it is well known that a small number of men in this situation suddenly develop aggressive prostate cancer (tigers) and have a survival rate similar to those men who present with metastatic disease. The identification of these cases is beyond current standard pathology practice. In this study, we have measured ~1400 archived FFPE tissue cores from 183 patents using infrared spectroscopic imaging (both conventional FTIR and QCL). From this data, we use various machine learning approaches to identify the key tissue components and then, using outcome data we have been able to stratify the tissue. Importantly, in the low risk non-metastatic group we have identified a high-risk sub-population who go on to develop aggressive disease. These results have important implications for clinical practice since this could alter current treatment options for these patients.

References

1. M.J. Baker, E. Gazi, M.D. Brown, J.H. Shanks, P. Gardner, N.W. Clarke, *British Journal of Cancer*, 99 (2008) 1859.
2. M.J. Baker, E. Gazi, M.D. Brown, J.H. Shanks, N.W. Clarke, P. Gardner, *J. Biophotonics*, 2 (2009) 104.
3. D. Ferguson, N. Kroeger-Lui, D. Dreisbach, C. Hart, D. Sanchez, P. Oliveira, M. Brown, N. Clarke, A. Sachdeva, P. Gardner, *Analyst*, 150 (2025) 1741.

Acknowledgements: The authors thank Niels Kroeger-Lui, Domenic Dreisbach from Bruker Optics for access to the Bruker LUMOS II ILIM microscope.

Infrared Biospectroscopy with ATR Measurement Technology for the Investigation of Insulin-Dependent Intracellular Processes in the Monocytic Cell Line

S. Paramasivam, W. Widdowson, S. Stoppelkamp, H.M. Heise
Interdisciplinary Center for Life Sciences, South-Westphalia University of Applied Sciences, Frauenstuhlweg 31, D-58644 Iserlohn, Germany
heise.h@fh-swf.de

FTIR-spectroscopy has been applied to various fields of biospectroscopy with the advantages of being non-destructive and label free. [1] Our interest was in monocytes as part of white blood cells, which play essential roles in inflammation and adaptive immunity. Glucose is a major energy source for activated monocytes while its uptake is facilitated by glucose transporters. We hypothesized that insulin dependent monocytes could be used as tools to study insulin action at the cellular level and facilitate the investigation of insulin activity. [2] Cells from the human monocytic cell line MONO-MAC-6 [3] were cultivated in a very-low endotoxin RPMI cell medium, enriched with amino acids and fetal bovine serum. Previously, such cells had been studied under different insulin concentrations in the culture medium for monitoring the glucose metabolization within the exponential growth stage. [4]
ATR-spectroscopy has been utilized to monitor transient states of the cells under treatment or activation. Spectra were recorded from dry-film samples at the interface as the evanescent wave exponentially decays within a few micrometers. The hydration level was monitored to support our spectral interpretations. For sample preparation, the isolated cells were re-suspended in physiological NaCl solution. Washed cell pellets were placed on an ATR-diamond or Germanium cone element with a following monitoring of the drying process. The spectral interpretation in the fingerprint region is complicated, but main interest was in the protein amide I and II bands. Cells were monitored over five days of cultivation with insulin addition at the first day. Further experiments were carried out for investigating the dynamic cellular response within two hours after under different insulin concentrations. After stimulation, spectral features not apparent in resting MM6 cells became obvious. Alternative biochemical methods such as FACS (fluorescence-activated cell sorting) and ICC (immune-cytochemistry) staining for proving the translocation of the GLUT4 proteins to the cellular membrane were also tested.

References

1. M.J. Baker, J. Trevisan, P. Bassan, et al., *Nat. Protoc.,* 9 (2014) 1771.
2. Y. Mavros, D. Simar, M.A. Fiatarone Singh, *Diabetes Research and Clinical Practice,* 84 (2009) 123.
3. H.W.L. Ziegler-Heitbrock, E. Thiel, A. Fütterer, et al., *Int. J. Cancer*, 41 (1988) 456.
4. A. Krolinski, S. Delbeck, Y. Dederich, et al., *Proc. SPIE* 11236 (2020) 112360O.

Self-Assembly of Artificial Light-Harvesting Complexes: A Molecular Spectroscopist's Perspective

Maxim S. Pshenichnikov
Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 3, 9747 AG Groningen, The Netherlands
m.s.pchenitchnikov@rug.nl

Molecular self-assembly, the spontaneous organization of molecules into supramolecular structures, is a powerful bottom-up strategy for fabricating nanostructures, with examples including liquid crystals, light-harvesting complexes, and protein-based materials. Understanding the mechanisms that govern these processes is key to unlocking nature's efficient design principles. However, this challenge is compounded by substantial molecular disorder and a wide range of timescales, necessitating a combination of structural and functional analytical techniques.

Here we demonstrate how two-dimensional correlation spectroscopy can unravel the pathways of supramolecular double-wall nanotube self-assembly, which closely mimic the natural light-harvesting antennae of green sulfur bacteria. By employing a microfluidic setup, we translate the temporal progression of self-assembly into a spatial coordinate, enabling us to reveal structure–property relationships under realistic dynamic conditions. More broadly, this work establishes a novel platform for real-time investigation of out-of-equilibrium self-assembly processes at both molecular and structural levels.

The Concept of the Dipole Moment: Why is it still relevant for Chemistry?

Michael Schmitt, Marie-Luise Hebestreit
Heinrich-Heine-University Düsseldorf, Germany
mschmitt@uni-duesseldorf.de

Dipole moments are among the most important physical parameters of molecules. They relate with the state of aggregation of substances and strongly affect solubilities and reactivities. Whereas the dipole moment of the molecular ground state is easily accessible through measurement of the permittivity, the determination of the dipole of short-lived species, like molecules in their excited states, or photochemical transients is far more challenging. The abstraction of charge distribution in molecules as electric dipole moment, is one of the basic concepts in chemistry, since it was originally introduced by Max Reinganum in 1903[1] and later, independently by Peter Debye in 1905[2]. An appealing aspect of this concept, is the idea of bond dipoles, which can be added up in a vectoral manner in order to result in a microscopically interpretable picture of the origin of molecular dipole moments. For electronically excited states, however, neither magnitude nor direction of the dipole moment can be deduced from simple vector addition of bond dipole moments. We will present a resume of current methods for determining dipole moments and their relevance for answering basic chemical questions.

References
1. M. Reinganum, *Ann. Phys. (Leipzig)*, 315 (1903) 334.
2. P. Debye, *Phys. Z.*, 13 (1912) 97.

Light-Induced Chemistry in Low Temperature Matrices

Jan Lundell
Department of Chemistry, University of Helsinki, P.O.Box 55 (A.I.Virtasen aukio 1), 00014 University of Helsinki, Finland
jan.lundell@helsinki.fi

In chemistry, the interaction between light and matter holds promises for identification, modification, and tailoring applications of substances. One of the great challenges of basic chemistry research is the selective modification of the molecular structures of matter and thereby resulting chemical reactivity. Use of selective light sources opens wide opportunities for production of chemical structures for various needs, from medicine through materials and environmental sciences to the energy economy. A broad understanding of the interaction between light and matter, benefiting from the insights and expertise in chemistry and its methodologies, provides scientific capital as a basis for the development of fundamental understanding of natural phenomena and applications.

Light have been widely used to study chemical properties and reactivity in combination of low temperature solid environments. Matrix isolation technique provides a convenient (i.e. rigid and cold) experimental surrounding to isolate, modify and analyse chemical systems while minimizing external disturbances [1]. Ultraviolet (UV) light has enough energy to excite electrons in molecules to higher energy states thereby enabling energy transfer for photoisomerisation or breaking chemical bonds leading to photodissociation [2,3]. These mechanisms are crucial in various fields, including atmospheric chemistry, where UV light drives the breakdown of pollutants and the formation of ozone.

Infrared (IR) light is particularly effective at promoting vibrational excitations in molecules leading to changes in the molecular structure and dynamics [4-7]. In chemical reactions, IR-induced vibrational excitations can lower activation barriers, thereby accelerating reaction rates and enabling selective bond breaking or formation. Moreover, for chemistry in low temperature matrices UV- or IR-light can be used to promote molecular reorganisations leading to higher energy species or chemical intermediates which can be trapped and detected, leading to deeper insights of chemical reaction mechanisms – and finally to tailor chemical entities of research and even technological benefits.

References

1. L. Khriachtchev, (Ed.), *Physics and chemistry in low temperatures*, Jenny Stanford Publishing, 2011.
2. J. Lundell, M. Räsänen, *J. Phys. Chem.,* 97 (1993) 9657.
3. L. Khriachtchev, M. Pettersson, N. Runeberg, J. Lundell, M. Räsänen, *Nature* 406 (2000) 874.
4. M. Pettersson, J. Lundell, L. Khriachtchev, M. Räsänen, *J. Am. Chem. Soc.,* 119 (1997) 11715.
5. A. Olbert-Majkut, J. Lundell, M. Wierzejewska, *J. Phys. Chem. A*., 118 (2014) 350.
6. J. Ahokas, I. Kosendiak, J. Krupa, M. Wierzejewska, J. Lundell, *J. Raman Spectrosc*., 49 (2018) 2036.
7. J. Ahokas, T. Nikitin, J. Krupa, I. Kosendiak, R. Fausto, M. Wierzejewska, J. Lundell, *Photochem,* 3 (2023) 197.

Computational Vibrational Spectroscopy in the Era of Machine Learning

Marcus Meuwly
Department of Chemistry, University of Basel, Klingelbergstr. 80, CH-4056 Basel, Switzerland
m.meuwly@unibas.ch

Machine learning (ML) has been and will continue to profoundly change how certain problems in the molecular sciences will be approached. Vibrational spectroscopy is one of the areas where ML-based approaches can be applied successfully. In this contribution I will present recent efforts to train and apply machine learning-based energy functions in molecular simulations to probe vibrational degrees of freedom for systems in the gas phase and in solution. Furthermore, I will also report on efforts to bypass explicit molecular simulation entirely and train models for predicting particularly interesting parts of the vibrational spectra.

Simulation of Vibrational Signatures from the Mid Infrared (MIR) to the Vacuum Ultraviolet (VUV)

Małgorzata Biczysko
Faculty of Chemistry, University of Wroclaw, F. Joliot-Curie 14, 50-383 Wroclaw, Poland
malgorzata.biczysko@uwr.edu.pl

Quantum treatment of nuclear motion effects, considering either one or two potential energy surfaces (PES) within the Born-Oppenheimer (BO) approximation, allows to simulate different molecular spectra in the broad energy range [1, 2]. Approaches set within second-order perturbation theory (VPT2), accounting for the intensities of non-fundamental transitions are applied for the mid-Infrared (MIR) to near IR (NIR) range. The vibrational features determine also spectra related to the transitions between two PESs, from the visible to the higher excitation regions, which are simulated within the harmonic Franck-Condon (FC) models. The latter can be corrected for the anharmonicity employing VPT2 computations on initial and final PESs, leading to an improved agreement with experiment for the band positions.
Computational spectroscopy results will be tested against the available experimental data for systems of increasing size and complexity, from semirigid [3, 4, 6] to more flexible [5] molecules, and the spectra range from the MIR (20 μm) up to the VUV (100 nm) range.

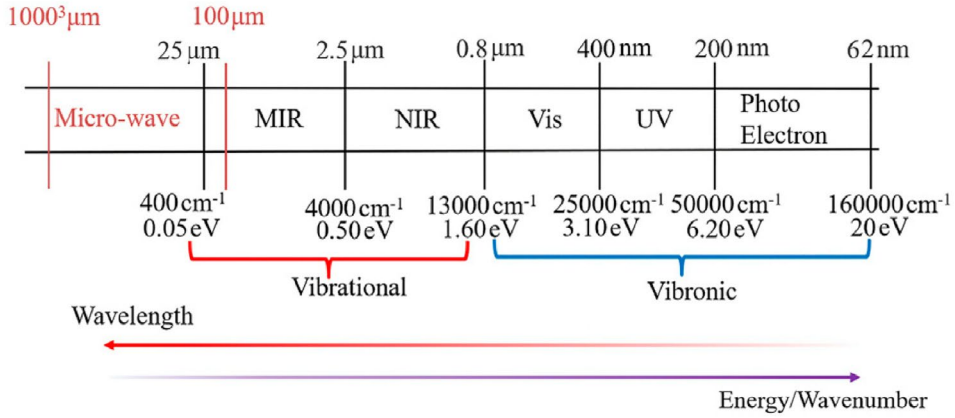


Figure 1 – The wavelength and energy range corresponding to vibrational and vibronic spectra simulations

References
1. V. Barone, S. Alessandrini, M. Biczysko, *et al.*, *Nat. Rev. Methods Primer* 1 (2021) 38.
2. J. Bloino, A. Baiardi, M. Biczysko, *Int. J. Quantum Chem.* 116 (2016) 1534.
3. Y. Zhao, M. Hochlaf, M. Biczysko, *Front. Astron. Space Sci.* 8 (2021) 757007.
4. Y. Xu, M. Biczysko, *Front. Chem.* 12 (2024).
5. R. Xu, Z. Jiang, Q. Yang, J. Bloino, M. Biczysko, *J. Comp. Chem.* 45 (2024) 1846.
6. R. Xu, Q. Yang, J. Bloino, M. Biczysko, *J. Phys. Chem. A* (2025) DOI: 10.1021/acs.jpca.5c02226.

Acknowledgements: The COST Action CA21101 "COSY–Confined molecular systems: from a new generation of materials to the stars" and computer resources provided by Wroclaw Centre for Networking and Supercomputing (http://wcss.pl) are acknowledged.

Near Infrared Spectroscopy in Food Science and Industry

Søren Balling Engelsen
Foodomics Group, Department of Food Science, University of Copenhagen, Rolighedsvej 26, DK -1958 Frederiksberg C, Denmark
se@food.ku.dk

In academia, NIR spectroscopy has not been considered serious due to strongly overlapping peaks with no baseline separations. On the industrial side, NIR spectroscopy has revolutionised quality control in practically all areas of primary food and feed production and has become the de facto standard for monitoring the quality of millions of samples including cereals, vegetables, milk, meat, wine, powders and tablets with unprecedented precision and speed and with practically no environmental fingerprint. NIR spectroscopy can thus be considered as the ugly duckling amongst spectroscopies that has turned into a swan and revolutionized quality control.
The key to this success of NIR spectroscopy is the extraordinary synergy that lies in the merging with the multivariate data technology. The combination of chemometrics and NIR spectroscopy is a most powerful cocktail, which is non-destructive and of observing nature and thus allow for a new level of inductive research, which in turn has led to a paradigm shift in the industry as well as in academia. Seen from a physical, chemical, and biological perspective, food systems are complex multifactorial systems containing mixtures of heterogeneous chemical mixtures of heterogeneous classes of molecules as well as complex physical structures such as amorphous solids, aqueous solutions, gels, macromolecules, macro-organelles, cells, crystals, pores, and cavities. Food systems are thus the perfect playground for developing new NIR and chemometric methods such as data pre-processing methods, data partition methods, data regression methods and data classification methods.
The potential of introducing real-time process monitoring through fingerprinting of complex process streams is enormous. In this setting, NIR spectroscopy represent a unique green analytical technology that will allow for controlling and optimizing processes toward increased sustainability - and there are practically no analytical alternatives [1].

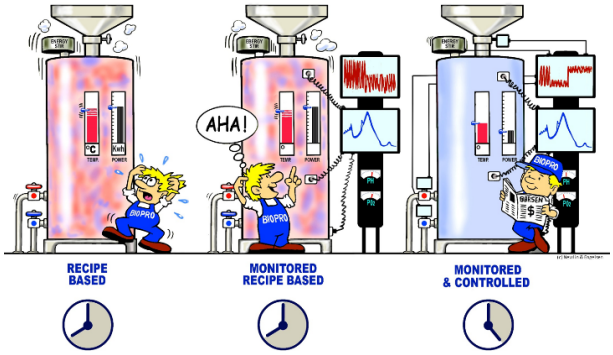


Figure 1 – The principle of monitoring batch processes by NIR spectroscopy. © Newlin & Engelsen

References

1. T.P. Czaja, S.B. Engelsen, *Spectrochim. Acta A,* 325 (2025) 125028.

Dielectric Spectroscopy in Solution Chemistry - Advantages and Pitfalls

Richard Buchner
Universität Regensburg, 93040 Regensburg, Germany
Richard.Buchner@chemie.uni-regensburg.de

Solutions, i.e. liquid multi-component systems, are ubiquitous in nature and technical processes and thus long in the focus of science. Key issue is to understand the delicate balance between solvent-solvent, solute-solvent and solute-solute interactions that govern solvation phenomena and solute aggregation processes as they determine macroscopic solution properties [1-4]. Spectroscopic techniques, such as NMR, Raman or time-resolved infrared spectroscopy, have provided valuable information here. However, these powerful methods are generally only sensitive to next-neighbour interactions and/or the reorientation dynamics of individual molecules. Accordingly, the important mesoscopic structural correlations and cooperative dynamic processes occuring in solutions often elude detailed investigation by these techniques. Here dielectric relaxation spectroscopy (DRS) can step in. DRS probes fluctuations of the macroscopic dipole moment and thus yields information on the cooperative and molecular dynamics of the sample on a timescale ranging in principle from $\sim 10^{-13}$ to 10^{3} s [5]. Processes relevant in solution chemistry are typically in the pico- to nanosecond range and encompass the reorientation and libration of permanent dipole moments (e.g. solvent molecules, ion pairs), intermolecular vibrations (e.g. of anions and cations relative to each other), and motions of counterions bound to micelles or polyions.
In this contribution a short introduction into the principles of dielectric relaxation spectroscopy will be given before proceeding to examples from our laboratory on applications of this technique in solution chemistry. The focus will be on the solvation and ion binding of electrolytes and non-electrolytes in aqueous and non-aqueous solutions, including ionic liquids and deep eutectic solvent. Aim is to highlight the merits of DRS in this field but also to pinpoint interpretation problems when used as „stand-alone" approach.

References

1. K.-I. Oh, C. R. Baiz, *J. Chem. Phys.*, 152 (2020) 190901.
2. K. P. Gregory, et al., *Phys. Chem. Chem. Phys*, 24 (2022) 12682.
3. Y.-L. Wang et al., *Chem. Rev.*, 120 (2020) 5798.
4. S. Kaur, M. Kunari, H. K. Kashyap, *J. Phys. Chem. B*, 124 (2020) 10601.
5. J. Hunger, R. Buchner, *Femto- to Nanosecond Dynamics in Ionic Liquids: From Single Molecules to Collective Motions*; in M. Paluch (Ed.), *Dielectric Properties of Ionic Liquids*, Springer International Publishing, Switzerland, 2016.

The Effect of Temperature on OH-stretching Bands of Hydrogen Bound Complexes

Henrik G. Kjaergaard
Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100, Denmark
hgk@chem.ku.dk

Hydrogen-bound complexes, in particular hydrated complexes, play important roles in the atmosphere, but are inherently difficult to study at relevant ambient temperatures [1]. Cold conditions of molecular jet favour complex formation and limits the number of thermally populated states. Based on our 12 dimensional vibrational model for water dimer, we reinterpreted a few cold vibrational transitions [2,3].
We present a conceptually simple model for understanding the significant changes that occur with temperature in the infrared spectra of complexes. We correctly predict spectral changes observed in the gas phase for the bound OH-stretch in methanol dimer from jet to room temperature (Figure 1) and corroborate this with experimental and theoretical results for the deuterated isotopologues [4]. The origin of the observed spectral features is explained based on a reduced-dimensional vibrational model, which includes the two high-frequency OH-stretches, the two methyl torsions and the six intermolecular low-frequency vibrations. Key to the success of the model is a new coordinate definition to describe the intrinsic large-amplitude curvilinear motion of the low-frequency vibrations. Despite the deceivingly simple appearance of the room temperature bound OH-stretching fundamental band, it consists of $\sim 10^7$ vibrational transitions. The model is applicable to the atmospherically relevant hydrated complexes.
Combining vibrational theory and experiments, we have also determined ΔG for a few hydrated complexes and for methanol dimer, trimer and tetramer [5,6].

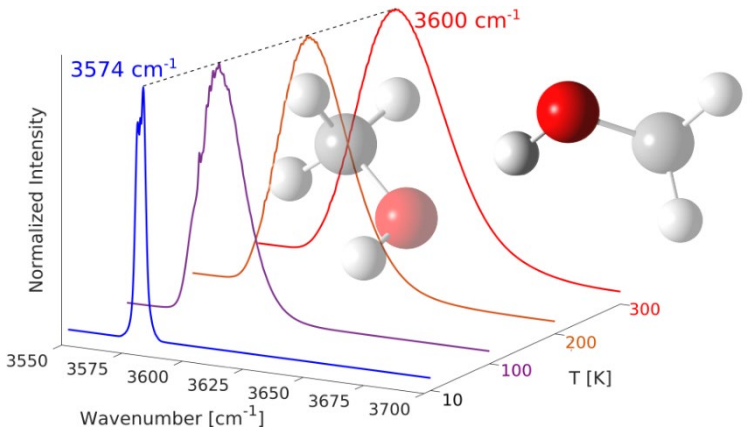


Figure 1 – The effect of temperature on the hydrogen bound OH-stretching vibration in methanol dimer

References
1. A.S. Hansen, E. Vogt, H.G. Kjaergaard, *Int. Review. Phys. Chem.*, 38 (2019) 115.
2. E. Vogt, H.G. Kjaergaard, *Annu. Rev. Phys. Chem.*, 73 (2022) 209.
3. E. Vogt, I. Simkó, A.G. Császár, H.G. Kjaergaard, *J. Phys. Chem. A*, 127 (2023) 9409.
4. E. Vogt, C.V. Jensen, H.G. Kjaergaard, *J. Phys. Chem. A*, 128 (2024) 392.
5. C.V. Jensen, E. Vogt, A.S. Poulsen, H.G. Kjaergaard, *J. Phys. Chem. A*, 128 (2024) 6382.
6. A. Kjaersgaard, D. Pal, E. Vogt, T.E. Skovbo, H.G. Kjaergaard, *J. Phys. Chem. A*, 129 (2025) 4438.

Enhancing Mid-IR Sensing Through Laser Technology and Integrated Photonics

Bernhard Lendl[a], Alicja Dabrowska[a], Daniela Tomasetig[a], Jesus Hernan Castro[a], Leopold Lindenbauer[a], Liam O'Faolian[b]
[a]*TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9, 1060 Wien, Austria*
[b]*Centre for Advanced Photonics and Process Analysis, Munster Technological University, T12 T66T Bishopstown, Cork, Ireland*
bernhard.lendl@tuwien.ac.at

The unique properties of mid-IR quantum lasers such as high-power, pulsed operation, coherence and inherent polarization allow to explore new sensing schemes for liquids, gases as well as imaging. In this presentation dispersion spectroscopy and photothermal spectroscopy will be introduced as new sensing modalities for liquid spectroscopy.
We use a bench-top Mach Zehnder Interferometer (MZI) coupled to a broadly tuneable External Cavity Quantum Cascade Laser to measure the refractive index spectrum of a liquid sample. Using this set-up we demonstrate measurement of enzymatic reactions in aqueous phase which are validated by established FTIR spectroscopy. We furthermore show latest results on waveguide based liquid sensing using a Germanium on Silicon platform and will introduce strategies and first results toward the development of chip based MZI.
Absorption of pulsed mid-IR laser radiation by a liquid sample causes an increase in temperature of the liquid, which induces changes to the refractive index of the liquid itself but also to the adjacent windows. In photothermal spectroscopy these refractive index changes are probed by a second visible laser. These techniques known as photothermal lens and photothermal mirror spectroscopy will be introduced and examples for trace detection of water in organic solvents shown. The final part of this presentation will report on resonant structures designed and realized via integrated photonic circuits (PICs), such as micro-ring-resonators can be used to probe refractive index changes.

References

1. A. Dabrowska, A. Schwaighofer, B. Lendl, *Applied Spectroscopy.* 78(9) (2024) 982.
2. A. Dabrowska, S. Lindner, A. Schwaighofer, B. Lendl *Spectrochim. Acta A,* 286 (2023) 122014.

Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols upon Photoexcitation

Piotr Piecuch,[a,b] Stephen H. Yuwono,[a,1] Ilias Magoulas,[a,2] Jun Shen[a]
[a] *Department of Chemistry, Michigan State University, East Lansing, Michigan 48824, USA*
[b] *Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA*
piecuch@chemistry.msu.edu

The development and characterization of reversible photoactivated reagents are key to the advancement of an important area of precision chemistry. This, in particular, applies to light-induced acid–base reactions, which require controlling the underlying excited-state proton transfer processes. This talk will be dedicated to a collaboration between our group and the experimental groups of Professors Gary Blanchard (synthesis and spectroscopy of interfaces), Babak Borhan (synthetic and bioorganic chemistry), Marcos Dantus (ultrafast science), and James Jackson (green and organic materials chemistry) from our department on a very strong super photobase, called **FR0**-SB, which upon photoexcitation exhibits a change in pK_a so large that the photoexcited **FR0**-SB* species extracts protons from alcohols [1–6]. We will discuss how modern methods of electronic structure theory based on the equation-of-motion coupled-cluster formalism, such as the rigorously size-intensive variant [7] of the completely renormalized triples correction to EOMCCSD [8], abbreviated as δ-CR-EOMCC(2,3) [7], can be used to explain the observed behavior of the photoactivated **FR0**-SB species in solution and help with the interpretation of experimental data. We will mainly focus on the results reported in Refs. [1–3], where our group's EOMCCSD and δ-CR-EOMCC(2,3) codes in GAMESS, combined with the embedding and implicit solvation models to account for solvent contributions and the carefully calibrated density functional theory and its time-dependent extension to excited states to determine geometries and reaction pathways, were used to accurately simulate the photoabsorption and photoemission spectra of **FR0**-SB in the gas phase and various alcohol solvents, to calculate its low-lying excited states and dipole moments that undergo a 3–4-fold increase upon photoexcitation, to explain the experimentally observed significance of steric factors in the excited-state proton transfer reactions involving **FR0**-SB* and alcohols, and to rationalize the up to ~60% increase in reactivity of **FR0**-SB* in two-photon experiments.

References

1. J. Lahiri, et al., *J. Phys. Chem. B* 123 (2019) 8448.
2. J. Lahiri, et al., *Phys. Chem. Chem. Phys.* 22 (2020) 19613.
3. J. Lahiri, et al., *J. Chem. Phys.* 153 (2020) 224301.
4. J. Lahiri, et al., *J. Phys. Chem. A* 125 (2021) 7534.
5. B.A. Capistran, et al., *J. Phys. Chem. B* 125 (2021) 12242.
6. B.A. Capistran, et al., *J. Phys. Chem. B* 125 (2021) 12486.
7. G. Fradelos, et al., *J. Chem. Theory Comput.* 7 (2011) 1647.
8. M. Włoch, et al., *Mol. Phys.* 104 (2006) 2149; 104 (2006) 2991 [Erratum].

Acknowledgements: Our collaboration with experiment was funded by a seed grant from DARPA and AMRDEC (W31P4Q-20-1-0001). The theoretical and computational work presented in this talk was funded by the U.S. Department of Energy (Grant No. DE-FG02-01ER15228 to P.P).

[1] Currently at Florida State University, Tallahassee, Florida 32306, USA.
[2] Currently at Emory University, Atlanta, Georgia 30322, USA.

A Kalejdoscopic View of Intramolecular Hydrogen Bonds

Poul Erik Hansen
Department of Science and Environment, Roskilde University, Universitetsvej 1, DK-4000, Denmark
Poulerik@ruc.dk https://thiele.ruc.dk/~poulerik/

Intramolecular hydrogen bonding can be of RAHB type as seen in its simplest form in Fig. 1 or it can be found e.g in proteins, as salt bridges. Intramolecular hydrogen bonding can occur both in the liquid and in the solid state.

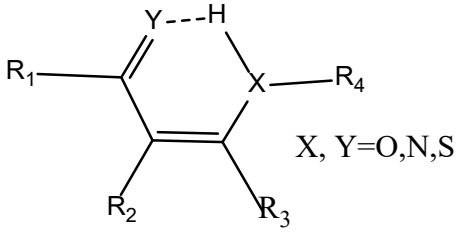
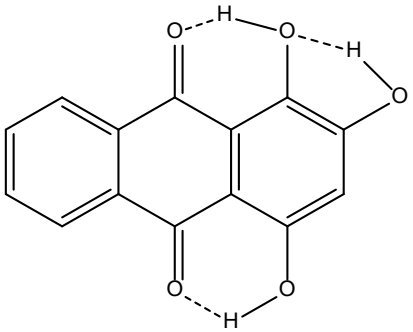


Figure 1

The structure in Fig. 1 invites to tautomerism and this will be discussed. The structure in Fig. 1 is simple. Often multiple hydrogen bonds are at play. Charged species both carbonium ions and anions may take part.
A number of cases will be discussed. Multiple hydrogen bonds of purpurin both neutral (Fig. 2) and as anion and of rifampicin.



Purpurin

Figure 2

The talk will also take a brief look at CH hydrogen bonds. Finally, salt bridges will be discussed in lysozyme and barnase.
Solid state spectra of *o*-hydroxySchiff bases will be discussed both in terms of hydrogen bonding and tautomerism.
The tools used in the study of multiple hydrogen bonds are chemical shifts, deuterium isotope effects on chemical shifts and DFT calculations of both.

From Alzheimer's Disease to Functional Nanomaterials: 100 Years of Advances in Vibrational Spectroscopy

Sylvia Turrell
LASIR, Université de Lille, 59655 Villeneuve d'Ascq, France
sylvia.turrelljones@gmail.com

The present-day panoply of tools used for vibrational spectroscopic studies seems all-powerful and infinitely adaptable. So simple have the techniques become, that it is very easy to forget that less than 200 hundred years ago, none of these things were even imaginable, much less in existence. And in the case of Raman spectroscopy, the conception dates to less than a hundred years ago.
The aim of this talk is to remind us of some of the genius researchers who led to the conceptions of vibrational spectroscopies, as well as to bring to mind some of the instrumentation and works which served as little thresholds obtained during the development of these fields.
From the initial instrumentation, we will watch techniques develop which will make possible the evolution of exploration into the domains of the very small and of very short-timed events. From small isolated molecules, studies gradually extended to those of complex inorganic systems and then to the numerous biological and medical systems. The technological evolutions allowed the possibilities of going out of the laboratory and to undertake "in-field" studies.
The experimental examples presented here will be both from work performed in my laboratories, as well as from numerous literature results from research laboratories around the world. Examples will include works on Alzheimer's disease, atmospheric pollution and Corona Virus contamination. Though not an exhaustive presentation, this review aims to highlight the scope and the extent of developments in vibrational spectroscopies over the past 100 years.

Figure 1 – a) Dispersive IR spectrometer 1968 b) In-field Raman spectrometer 2010

Oral Contributions

OC-1: Maria Rosa Lopez-Ramirez
OC-2: Anna Pieczara
OC-3: Halina Abramczyk
OC-4: Adriana Adamczyk
OC-5: Beata Brożek-Płuska
OC-6: Rares-Ionut Stiufiuc
OC-7: Andreas Barth
OC-8: Sylwester Mazurek
OC-9: Katarzyna Cieślik-Boczula
OC-10: Ewa Szczęsny-Małysiak
OC-11: Patrycja Dawiec
OC-12: Barbara Gieroba
OC-13: Marta Gordel-Wójcik
OC-14: Wiktoria Korona
OC-15: Jakub Dybaś
OC-16: Anna Kołodziej
OC-17: Vlada Pashynska
OC-18: Ahmad Salman
OC-19: Ivan Němec
OC-20: Thomas Golin Almeida
OC-21: Ružica Marković
OC-22: Piotr Najgebauer
OC-23: Nanna Falk Christensen
OC-24: Marek Drozd
OC-25: Václav Profant
OC-26: Natalia Piergies
OC-27: Przemysław Dopieralski
OC-28: Karolina A. Haupa
OC-29: Casper Vindahl Jensen
OC-30: Aleksandra Wesełucha-Birczyńska
OC-31: Vili-Taneli Salo
OC-32: Dhritabrata Pal
OC-33: Andrzej Teisseyre
OC-34: Sándor Góbi
OC-35: Tomasz Pawel Czaja
OC-36: Eva Kočišová
OC-37: Ali Muhieddine
OC-38: Szymon Smółka
OC-39: Vera Staun Hansen
OC-40: Andras Sun Poulsen
OC-41: Natalia Dutkiewicz
OC-42: Kazimierz Orzechowski
OC-43: Jacek Waluk
OC-44: Maciej Ptak
OC-45: Iwona Płowaś-Korus
OC-46: Eaindra Lwin
OC-47: Ivan Kopal
OC-48: Valerie Smeliková
OC-49: Karol Kułacz
OC-50: Agnieszka Sozańska
OC-51: Marek Procházka
OC-52: Justyna Grabska
OC-53: Aleksandra Szymańska
OC-54: Veranika Kuzmina
OC-55: Barbara Golec
OC-56: Alicja Dabrowska
OC-57: Shiva Ghasemi
OC-58: Jože Grdadolnik
OC-59: Rafał Szabla
OC-60: Roel van de Ven
OC-61: Anjali Sangwan
OC-62: Kamil Wojtkowiak
OC-63: Štěpán Jílek
OC-64: Galyna Dovbeshko

Highly Effective Core@shell AuAg Nanoparticles as Potential SERS Pubstrates

Maria Rosa Lopez-Ramirez[a], Lucas Olivares-Fernández[a], Arantxa Forte-Castro[b], Rafael Contreras-Cáceres[b]

[a]*Department. of Physical Chemistry, Faculty of Science, University of Málaga, 29071 Málaga, Spain*
[b]*Department of Chemistry and Physics. Faculty of Experimental Sciences. University of Almeria, 04120, Almería, Spain*
mrlopez@uma.es

A series of non-spherical bimetallic core@shell AuAg nanoparticles (NPs) were synthesized to improve surface-enhanced Raman spectroscopy (SERS) performance. The bimetallic AuAg NPs were fabricated by controlled Ag overgrowth onto two types of non-spherical Au NPs—nanooctahedra (Au NOc) and nanotriangles (Au NTs)—serving as seeds [1]. This process resulted in bimetallic nanocubes and nanopyramids, respectively. Transmission electron microscopy (TEM), energy-dispersive X-ray (EDX) and UV-vis spectroscopy was employed to characterized these nanoparticles.

Upon adsorption onto certain noble metals, p-aminothiophenol (PATP) undergoes a dimerization reaction to form 4,4′-dimercaptoazobenzene (DMAB) [2]. SERS measurements were conducted at a PATP concentration of 10^{-4} M using 532 nm and 785 nm laser wavelengths (Figure 1). Notably, the dimerization reaction was observed exclusively in the bimetallic nanostructures under 532 nm excitation. Furthermore, the extent of dimerization was found to be morphology-dependent.

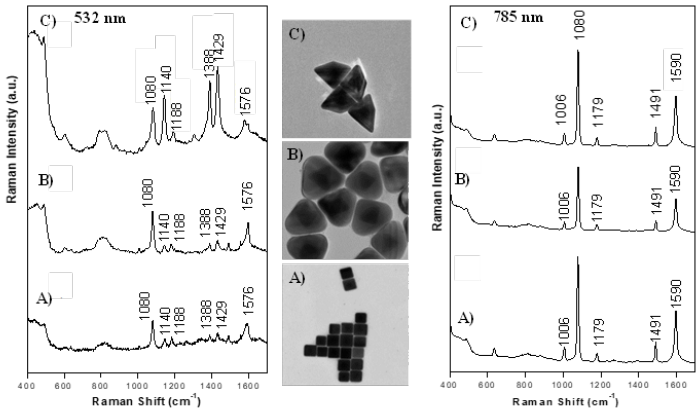


Figure 1 – SERS spectra of PATP on: A) AuAg NCs, B) AuAg NPyr R=8, and C) AuAg NPyr R=16 recorded at 532 nm (left) and 785 nm (right) excitation wavelengths

References

1. R. Contreras-Cáceres, I. Pastoriza-Santos, R. A. Alvarez-Puebla, J. Pérez-Juste, A. Fernández-Barbero, L. M. Liz-Marzán, *Chem. - A Eur. J.*, 16 (2010) 9462.
2. M. De la Cabeza Fernández, A. Alvear-Fernández, A. Forte-Castro, R. Contreras-Cáceres, M.R. López-Ramírez, *J. Raman Spectrosc.*, 55 (8) (2024) 855.

Acknowledgements: This work has been funded by the "Ramón y Cajal" fellowship from the Ministerio de Ciencia e Innovación, grant number RyC 2021-03447-I.

Raman-Based Biochemical Profiling of Adrenaline's Action on Lipid Metabolism in Endothelial Cells

Anna Pieczara, Jakub Machowski, Małgorzata Barańska
Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University, Bobrzynskiego 14, 30-348, Krakow
Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow
anna.pieczara@uj.edu.pl

Cellular responses to chemical compounds involve a wide range of modifications, including shifts in metabolism, protein expression, and organelle function. Understanding these changes is essential for unravelling how cells react to external stimuli, especially biologically active molecules such as hormones. Hormones initiate precise reactions in specific cells, tissues, and organs, orchestrating complex physiological processes like protein synthesis, metabolic regulation, and lipid mobilization. Due to their diverse and far-reaching effects, pinpointing the exact mechanism of action (MoA) of hormones remains a major scientific challenge[1,2].

In this study, we explored the impact of adrenaline on fatty acid metabolism in single live endothelial cells. To accomplish this, we developed a novel methodology combining isotope-labeled Raman microscopy with standard biological assays. Adrenaline was analyzed alongside four reference compounds with well-characterized effects on lipid metabolism and mitochondrial function, forskolin, niclosamide, oligomycin, and CCCP to define and compare their spectroscopic signatures.

Our semi-quantitative Raman analysis, based on key band intensity ratios, revealed that adrenaline shares a strikingly similar biochemical profile with forskolin and niclosamide. These spectroscopic findings were strongly supported by MTT assays, further validating the observed metabolic patterns. Together, these results highlight the potential of vibrational spectroscopy, especially when paired with targeted biological tests, as a powerful tool for dissecting the cellular mechanisms of hormone action at the single-cell level.

References
1. Ibrahim, N. Yucel, B. Kim, Z. Arany, *Cell Metab.*, 32 (2020) 309.
2. D. Zhang, Y. Wei, Q. Huang, Y. Chen, K. Zeng, W. Yang, J. Chen, J. Chen, *Molecules* 27 (2022) 1.

Acknowledgements: This research was funded in whole or in part by the National Science Center Poland (NCN), Maestro 2022/46/A/ST4/ 00054 to Malgorzata Baranska and Preludium 2023/49/N/ST4/03419 to Anna Pieczara.

A New Modality for Cancer Tracking-Raman Imaging, NanoIR Imaging, Fluorescence and AFM Studies Combined with AI Analysis

Halina Abramczyk, Monika Kopeć, Jakub Surmacki
Lodz university of Technology, Faculty of Chemistry, Institute of Applied Radiation Chemistry, Laboratory of Laser Molecular Spectroscopy, Wroblewskiego 15, 93-590 Lodz, Poland
halina.abramczyk@p.lodz.pl

This lecture explores the application of molecular spectroscopy and nanomechanical imaging in human brain, breast and lung cancers, including discussion on its capabilities in analysing both *in vitro* human cell lines, *in vivo* animal models and *ex-vivo* human tissues. The contribution also addresses current challenges and potential future applications of this technology in translational clinical applications. We will present a new modality for cancer tracking by using the multimode platform (R-IR-F-AFM): (Raman imaging-nano IR imaging-Fluorescence and AFM) that is in the Laboratory of Laser Molecular Spectroscopy at Lodz University of Technology, Poland. The approach has many advantages compared to conventional biology which needs cell disruption and release the cellular structures. Compared to the currently existing methods the platform (R-IR-F-AFM) shows an interesting alternative, which allows for a non-invasive monitoring of cellular processes. Since Raman method is label-free and does not involve any staining or antibody attachment for detecting cytochromes, DNA methylation (CpG methylation), phosphorylation, glycosylation, histone methylation, acetylation of proteins, and monitoring electron transport chain processes. Raman-driven methods offer straightforward sample handling over complex assays that must take into account the sensitivity and specificity to antibody. Our algorithms based on biochemical modifications in the cancerous cells that cover the entire Raman spectrum regions associated with glycans, lipids, nucleic acids, and proteins and using a machine-learning algorithm will be capable to classify different cells and tissue types and correlate the spectral signatures with different stages of malignancy. [1-4] We will show some examples of these applications, such as optical biopsy, Raman based histopathology, monitoring the future perspectives of therapeutic benefit of anti-cancer drugs in glioblastoma, the role of cytochrome c in mitochondrial metabolism of human oocytes or quantification of the human epidermal growth factor receptor-2 (HER2). We will show a broad range of breast cancer phenotypes to explore the potential utility of a novel immunodetection technique, using Raman imaging combined with artificial intelligence models. In the current lecture, we show the results for five breast cancer cell lines: MCF-10A, MCF-7, MDA-MB-231, HTB-30 (SK-BR-3) and AU-565 representing normal, non-tumorigenic epithelial cells, triple-positive breast carcinoma and triple-negative breast cancer cell lines. The correlations between Raman method and conventional HER2 testing methodologies (IHC and ISH) will be discussed. [5]

References

1. J. M. Surmacki, H. Abramczyk, *Sci. Rep.*, 13 (2023) 15049.
2. M. Kopec, A. Imiela, H. Abramczyk, *Sci. Rep.,* 9 (2019) 166
3. H. Abramczyk, A. Imiela, *Spectrochim. Acta A*, 188 (2018) 8-19
4. H. Abramczyk, J. M. Surmacki, *Cancers,* 15 (2023) 4535
5. H. Abramczyk, J. M. Surmacki, M. Kopeć, *J. Med. Chem.*, 67 (2024) 17629-17639.

Acknowledgements: This work was supported by the National Science Centre of Poland (OPUS, UMO-2021/43/B/ST4/01547)

A Spectroscopic Evaluation of the Erythroid Differentiation Process Induced by Drugs of Different Mechanisms of Action

Adriana Adamczyk[a], William Tipping[b], Duncan Graham[b], Małgorzata Barańska[a], Katarzyna Majzner[a]

[a]*Jagiellonian University in Krakow, Faculty of Chemistry, 2 Gronostajowa Str., 30-387, Krakow, Poland*
[b]*University of Strathclyde, Centre for Molecular Nanometrology, Department of Pure and Applied Chemistry, Technology and Innovation Centre, 99 George Str. G1 1RD, Glasgow, United Kingdom*
adriana.adamczyk@uj.edu.pl

Erythropoiesis is a tightly regulated multistep process in which erythroid precursors undergo morphological and phenotypic changes to transform into erythrocytes. Adequate erythrocyte function is crucial to the organism's functioning, so any changes associated with genetic mutations that lead to the uncontrolled proliferation of dysfunctional precursors require rapid diagnosis and treatment. Since isolation of erythroid precursors is an invasive method, *in vitro* studies of key players regulating this process are performed using human leukemic K562 cells treated with various pharmacological agents. Erythroid differentiation induced by drugs with different mechanisms of action is associated with changes in morphology and phenotype, even at the level of individual organelles, in particular mitochondria involved in iron metabolism and haem biosynthesis [1]. Therefore, Raman (RS) microscopy [2] is the method of choice for following changes in cellular composition in a non-destructive manner. Here, we provide a comprehensive investigation of early (24 h) and late (72 h) erythroid differentiation induced by the tyrosine kinase inhibitor imatinib, the DNA intercalating agent doxorubicin, and hemin, which act via different biological mechanisms but all lead to haemoglobin expression in the cells. Applying multivariate analysis, we selected the mechanism of action-related spectroscopic markers as follows: 790 cm^{-1} for DNA, 850, 1236, 1487 cm^{-1} for proteins, 702 cm^{-1} for cholesterol, 1305 and 1440 for saturated lipids. Haemoglobin accumulation confirmed by the presence of bands 673, 753, 973, 1550, 1622 cm^{-1}.

Since iron metabolism and haem biosynthesis occur in mitochondria [1], we introduced a mitochondrial-accumulating Raman probe, MitoBADY. Thanks to its positively charged triphenylphosphonium group, it can provide insight into the mitochondrial membrane potential, while the presence of -C≡C- groups in its molecular structure can be easily detected at 2220 cm^{-1} [2]. Therefore, we verified a previously developed method [3] to classify and monitor doxorubicin-induced differentiation of erythroid precursors into erythrocyte-like cells based on cell MB accumulation in imatinib- and hemin-induced differentiation. These findings demonstrate the feasibility of translating Raman-based techniques to high-speed stimulated Raman scattering microscopy, paving the way for future applications in clinical diagnostics.

References

1. A. Gonzalez-Ibanez, et al., *Cell Dev. Biol*., 8 (2020) 592035.
2. E. Matuszyk, et al*., Spectrochim. Acta Part A Mol. Biomol. Spectrosc*., 255 (2020) 119658.
3. A. Adamczyk, et al., *ChemRxiv* (2025).

Acknowledgements: This work was funded by National Science Centre (Poland), project PRELUDIUM—No. UMO-2021/41/N/ST4/03069 and NAWA BEKKER program No.BPN/BEK/2023/1/00221

Exploring The Therapeutic Molecules Effects in Colon Cells Using Integrated Raman Imaging-AFM-Femtosecond Laser Spectroscopy

Beata Brożek-Płuska, Karolina Beton-Mysur
Lodz University of Technology, Faculty of Chemistry, Institute of Applied Radiation Chemistry, Laboratory of Laser Molecular Spectroscopy, Wroblewskiego 15, 93-590 Lodz, Poland
beata.brozek-pluska@p.lodz.pl

CRC is one of the leading causes of cancer-related morbidity and mortality worldwide. Up to 47.2% of CRC patients experienced anxiety, while depression affected as many as 57%.[1] Antidepressants, such as SSRIs, are the cornerstone of treatment, with citalopram (CIT) being one of the most commonly prescribed drugs. Recently, CIT has raised interest in the broader scope of its effects on cellular metabolism beyond the brain. Understanding the fate of CIT in the intestinal environment is crucial for assessing its effects, especially in the gut-brain axis and the metabolic reprogramming observed in cancerous cells. Our study aims to explore the metabolic alterations induced by CIT in human gut cells, both normal and cancerous, by Raman imaging (RI).[2] Common treatment options for CRC include invasive surgery, chemotherapy, and radiotherapy. However, these modalities often fall short of providing a complete cure due to their invasive nature, side effects, and toxicity. Photodynamic therapy (PDT) emerges as a promising anti-tumor approach for CRC. PDT is well-tolerated for repeated dosing and demonstrates greater efficacy than traditional CRC treatments. The goal of the presented work was to expand the current knowledge of the potential of $AlPcS_4$ in PDT, with a particular focus on the localization and selective accumulation in the substructures of human colon cells using RI, both in the presence and absence of DTAC micelles. The presented results illustrate the innovative applications of RI, electronic absorption spectroscopy, fluorescence spectroscopy, and transient absorption spectroscopy to determine the distribution of PS in the human colon cells and the dynamic properties of PS's aqueous solutions.

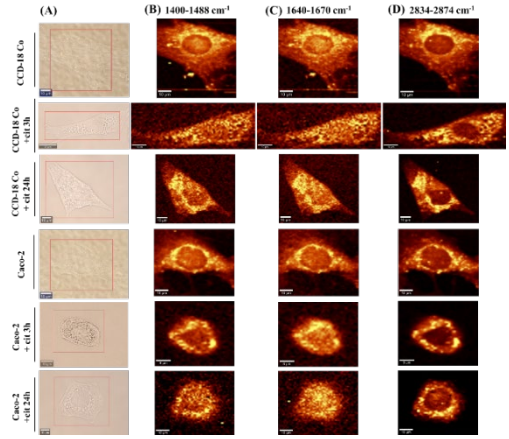


Figure 1 – Microscopic images (A), Raman images of the distribution of lipids (1400-1488 cm^{-1})(B), proteins (1640-1670 cm^{-1}) (C), and lipids& proteins (2834-2874 cm^{-1})(D)

References

1. Y.N. Peng, et al., *Int J Environ Res Public Health*, 16 (2019).
2. B. Brożek-Płuska, et al., *Spectrochim. Acta A*, 343 (2025) 126464.

The Role of Spectroscopic Liquid Biopsy in Early Disease Detection

Valentin Toma[a], Anca Onaciu[a], Rareș-Mario Borșa[a], Septila Renata[b], Brîndușa Drăgoi[b,c], Gabriela Știufiuc[d], Rares-Ionut Stiufiuc[a,b]

[a]*Department of NanoSciences, MEDFUTURE—Institute for Biomedical Research, "Iuliu Hatieganu" University of Medicine and Pharmacy, 4-6 Pasteur Street, 400349 Cluj-Napoca, Romania*

[b]*Nanotechnology Laboratory, TRANSCEND Department, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot, 700483 Iași, Romania*

[c]*Faculty of Chemistry, Alexandru Ioan Cuza University of Iași, 11 Bd. Carol I, 700506 Iași, Romania*

[d]*Faculty of Physics, "Babeș-Bolyai University", 1 M. Kogălniceanu Street, 400084 Cluj-Napoca, Romania*

rares.stiufiuc@umfcluj.ro

Spectroscopic analysis of biofluids has emerged as a powerful, non-invasive technique for biomedical diagnostics, disease monitoring, and biomarker discovery. Various spectroscopic methods, including infrared (IR), Raman, fluorescence, and nuclear magnetic resonance (NMR) spectroscopy, provide molecular-level insights into the biochemical composition of biofluids such as blood, urine, saliva, and cerebrospinal fluid. These techniques enable the identification and quantification of metabolites, proteins, and other biomolecules, facilitating early disease detection and personalized medicine. Advanced data processing approaches, such as chemometric analysis and machine learning, enhance spectral interpretation, improving diagnostic accuracy and clinical utility.

In this talk I will discuss about the possibility of employing ultrasensitive vibrational spectroscopy techniques such as Surface Enhanced Raman Spectroscopy (SERS) for the analysis of different biofluids in order to develop new (bio)medical applications. I will start with a short state of the art analysis of the results present in the scientific literature [1] and then I will emphasize the major achievements and obstacles we have encounter in our research group in the last decade since we have started to perform such studies on blood plasma & serum [2], urine [3], saliva [4,5], DNA [6,7]. Since SERS is a surface technique, the role of the plasmonic substrate employed for vibrational analysis of biofluids will be also addressed.

References

1. V. Moisoiu, S.D. Iancu, A. Stefancu, T. Moisoiu, B. Pardini, M.P. Dragomir, N. Crisan, L. Avram, D. Crisan, I. Andras, D. Fodor, L.F. Leopold, C. Socaciu, Z. Bálint, C. Tomuleasa, F. Elec, N. Leopold, *Colloids Surf. B Biointerfaces.*, 112064 (2021) 208.
2. G.F. Știufiuc, V. Toma, M. Buse, R. Mărginean, G. Morar-Bolba, B. Culic, R. Tetean, N. Leopold, I. Pavel, C.M. Lucaciu, R.I. Știufiuc, *Nanomaterials (Basel),* 10(6) (2020) 1212.
3. B.A. Buhas, V. Toma, J.B. Beauval, I. Andras, R. Couți, L.A. Muntean, R.T. Coman, T.A. Maghiar, R.I. Știufiuc, C.M. Lucaciu, N. Crisan, *Int J Mol Sci*, 25(7) (2024) 3891.
4. R.M. Borșa, V. Toma, M.T. Năsțuțiu, A. Onaciu, I.M. Colceriu-Șimon, G. Băciuț, S. Bran, C.M. Dinu, F. Onișor, G. Armencea, C. Culic, M.C. Hedeșiu, R.I. Știufiuc, M.F. Băciuț, *Sensors*, 24(24) (2024) 8021.
5. R.M. Borșa, V. Toma, A. Onaciu, C.S. Moldovan, R. Mărginean, D. Cenariu, G.F. Știufiuc, C.M. Dinu, S. Bran, H.O. Opriș, S. Văcăraș, F. Onișor-Gligor, D. Sentea, M.F. Băciuț, C.A. Iuga, R.I. Știufiuc, *Int. J. Mol. Sci.*, 24(15) (2023) 12125.
6. A. Onaciu, V. Toma, C. Moldovan, A.B. Țigu, D. Cenariu, C. Culic, R.M. Borșa, L. David, G.F. Știufiuc, R. Tetean, C. Tomuleasa, R.I. Știufiuc, *Sensors (Basel)*, 23(1) (2022) 346.
7. L. David, A. Onaciu, V. Toma, R.M. Borșa, C. Moldovan, A.B. Țigu, D. Cenariu, I. Șimon, G.F. Știufiuc, E. Carasevici, B. Drăgoi, C. Tomuleasa, R.I. Știufiuc, *Biosensors (Basel)*, 14(1) (2024) 41.

Acknowledgements: Part of this work was supported by a H2020 grant – ERA-Chair, no 952390.

The Structure of Amyloid-β Oligomers Studied by Experimental and Computational Isotope-Edited Infrared Spectroscopy

Faraz Vosough, Simon M. Carstensen, Cesare M. Baronio, Andreas Barth,
Dept. Biochem. Biophys., Stockholm University, Svante Arrhenius väg 16C, 106 91 Stockholm, Sweden
barth@dbb.su.se

Oligomers of the amyloid-β (Aβ) peptide are thought to be one of the causes of Alzheimer's disease but are difficult to study with common structural biology methods. To elucidate their structure, we therefore use a combination of Fourier transform infrared spectroscopy, site-specific ^{13}C,^{15}N-labeling, and spectrum calculations. We labeled (i) one residue per peptide to determine the local secondary structure of the amide group that contains the carbonyl group of the labeled residue and (ii) two residues per peptide to detect three-dimensional contacts. Isotope dilution experiment enabled us to distinguish between intra- and intermolecular contacts and the spectrum calculations guided our interpretation.
We investigated three types of oligomers of the 42-residue variant of Aβ, Aβ42 [1], termed large (~110 kDa), medium (~60 kDa), and small (~20). The large oligomers incorporate V18, F20, A30 and I32 in β-sheets, but the medium and small oligomers only A30 and I32. This shows that the local secondary structure at V18 and F20 is different for different oligomers.
Contacts between the two sections of the peptide were probed for the large oligomers using V18*A30*-Aβ42, F20*A30*-Aβ42, and F20*I32*-Aβ, where the star indicates the labeled residues. We found intramolecular contacts between the labeled residues of the former two peptides and an intermolecular contact between those of the latter. From these results we propose a new model for the β-hairpin structure of the Aβ molecules in the large oligomers.

References

1. F. Vosough, A. Barth, *ACS Chem. Neurosci.*, 12 (2021) 473.

Acknowledgements: We are indebted to Eeva-Liisa Karjalainen for our program for calculating the amide I spectrum. We also thank Oleksandra Kurysheva for her assistance with experimental work. This work was supported by the Swedish Research Council (2021-04595), Hjärnfonden (FO2019-0127), Olle Engkvists stiftelse (211-0051), and Magn. Bergvalls stiftelse (2020-03624).

Carotenoid Profile of Bee Pollen Fractions Based on Raman Spectra

Sylwester Mazurek[a], Sonia Pielorz[a], Joanna Kolniak-Ostek[b], Roman Szostak[a]
[a]*Department of Chemistry, University of Wrocław, 14 F. Joliot-Curie, 50-383 Wrocław, Poland*
[b]*Department of Fruit, Vegetable and Plant Nutraceutical Technology, Wrocław University of Environmental and Life Sciences, 37 Chełmońskiego, 51-630 Wrocław, Poland*
sylwester.mazurek@uwr.edu.pl

Bee pollen is a complex natural product, and its chemical composition depends on botanical and geographical origin [1]. Carotenoids are an important group of biologically active compounds identified in pollen grains. Multiple conjugated double bonds present in their molecules are responsible for intense, characteristic spectral features in the Raman spectra of these pigments. That allows for easy identification of carotenoids, even in the case of their low concentration in the analyzed material [2].
Results obtained by ultraperformance liquid chromatography (UPLC) for bee pollen fractions, combined with their Raman spectra, were used to construct calibration models enabling total carotenoids (TC) and individual carotenoids quantification. Multivariate calibration models were built by applying the partial least squares (PLS) method. Spectral variables used for modeling were selected by the interval PLS (iPLS) algorithm. Calibration models for TC determination, present in the studied samples in the 1-55 ppm range, were characterized by the root mean square error (RMSE), varying from 2.3 to 3.2 ppm; β-carotene, the most abundant carotenoid in the analyzed samples, was quantified with RMSE in the 0.9-1.5 ppm range. This error was even smaller for other carotenoids. For example, for 13-cis-antheraxantin, with content in the 0.04-2.4 ppm range, PLS modeling resulted in the RMSE errors of 0.03 ppm. Obtained results indicate an exceptional potential of Raman spectroscopy in analysis of carotenoids, in complex matrices of natural origin.

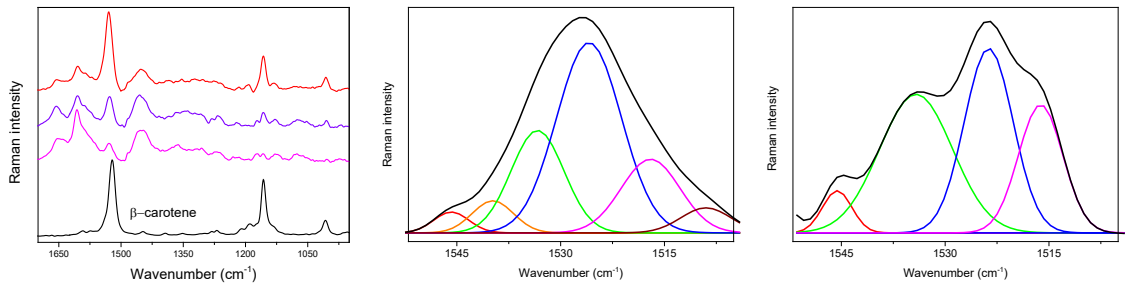


Figure 1 – Raman spectra for selected bee pollen grains and decomposition of the ν(C=C) band in spectra of green and yellow fractions

References

1. J.A.G. Sattler, et al., *Food Res. Int.*, 77 (2015) 82.
2. A. Krähmer, et al., *Food Chem.*, 212 (2016) 495.

FTIR Studies of the Structure of Lipid Membrane Models for Protein/Peptide-Lipid Matrix Interaction and for Carriers in the Transport of Biologically Active Substances

Katarzyna Cieślik-Boczula[a], Karolina Musiał[a], Mirosław Czarnecki[a], Anna Grygier[b], Magdalena Rudzińska[b]

[a]*Faculty of Chemistry, University of Wrocław, F. Joliot Curie 14, 50-383 Wrocław, Poland*
[b]*Department of Food Technology of Plant Orgin, Faculty of Food Science and Nutrition, Poznan University of Life Sciences, Wojska Polskiego 28, 60-637 Poznan, Poland*
katarzyna.cieslik-boczula@uwr.edu.pl

It is well known that mutual interaction in protein/peptide-lipid membrane systems plays a crucial role in many biological processes [1]. The main outstanding problem is that such systems are complex and multi-component systems, in which protein folding may not be a one-step process and phase separation may occur in the lipid membrane structure. Furthermore, liposomes are vesicles that are surrounded by a double lipid layer. Among their many positive features is that they are innovative and highly effective carriers for various biologically active substances. They ensure targeted delivery of active substances in hostile environments, stabilize biodegradable active compounds protecting them from oxidation and/or digestion. Due to the fact that liposomes can be applied to the body through multiple delivery routes, they have found applications in many industries, such as food, cosmetics and pharmaceuticals [2].

FTIR spectroscopy is known to be one of the most powerful methods for studying the secondary structure of proteins and peptides as well as many different structural properties of lipid membranes [3,4]. It will be shown how we can improve the quality of obtained spectroscopic results and increase the structural information about the protein/peptide-lipid membrane systems under study by using chemometric methods such as PCA, MCR-ALS, 2D COS and mowing window 2D COS. The *trans/gauche* isomerisation in the hydrophobic core of liposomal membranes will be discussed as a factor that determines the rigidity and permeability (tightness) of the lipid walls of liposome carriers.

References

1. T. Paulina, K. Cieślik-Boczula, *Spectrochim. Acta Part A – Mol. Biomol. Spectr.* 227 (2020) 117563/1.
2. T.M. Allen, P.R Cullis, *Adv. Drug Deliv. Rev.* 65 (2013) 36.
3. K. Cieślik-Boczula, P. Trombik, *Int. J. Biol. Macromol.* 125 (2019) 630.
4. J. Szwed, K. Cieślik-Boczula, B. Czarnik-Matusewicz, A. Jaszczyszyn, K. Gąsiorowski, P. Świątek, W. Malinka, *J. Mol. Struct.,* 974 (2010) 192.

Acknowledgements: This work was supported by National Science Centre, Poland, project OPUS 22 with decision number UMO-2021/43/B/NZ9/00345.

Monitoring of Cytochrome C Oxidation State in Live Cells with Resonance Raman Imaging

Ewa Szczęsny-Małysiak, Amanda Bartkowiak, Jakub Dybaś
Jagiellonian Centre for Experimental Therapeutics, Jagiellonian University, Kraków, Poland, 14 Bobrzynskiego St., 30-348 Krakow, Poland
ewa.szczesny@uj.edu.pl

Mitochondria of the living cell act not only as a powerplant providing life-supporting energy in the form of ATP, but also perform signalling duty and control many cellular processes [1]. One of the elements involved in mitochondrial signalling is cytochrome C (cytC). This heme protein resides in the mitochondrial intermembrane space and is a part of electron transport chain. CytC is redox-active, capable of free transition between ferrous (CytC-Fe^{II}) and ferric (CytC-Fe^{III}) state, what determines proper function of the respiratory chain [2]. Under specific conditions, i.e. upon its interaction with nitric oxide (NO) cytC becomes nitrosylated and may be released into the cytoplasm. Release and oxidation in turn can trigger activation of caspase and launch the process of apoptosis [3]. Therefore, tracking the oxidation state of CytC may help to assess mitochondrial dysfunction and apoptosis.
In the present work we have employed resonance Raman spectroscopy with 405 nm excitation to track molecular changes of CytC in response to nitric oxide in human endothelial cells. Human aortic endothelial cells (HAECs) were treated with agents capable of nitric oxide synthase stimulation (A23187, VEGF, bradykinin) or an external NO donor (DEA-NONOate) in order to evoke CytC-Fe^{II} to CytC-Fe^{III} transition. Other agents, like nitric oxide synthase inhibitor (L-NAME), superoxide scavenger (PEG-SOD) or specific mitochondrial $ONOO^-$ and ROS scavenger (NecroX-5) were employed to confirm the involvement of oxidative stress-related molecules, i.e. O_2^- and $ONOO^-$ in the process. Classic methods of molecular biology, i.e. fluorescent microscopy and flow cytometry were used to confirm the results obtained with use of resonance Raman spectroscopy.
Our findings demonstrate the utility of resonance Raman imaging for real-time monitoring of CytC redox state. Induction of NO production in the vascular endothelium entailed CytC-Fe^{II} to CytC-Fe^{III} transition. Moreover, the involvement of O_2^- and $ONOO^-$ in the process was confirmed. Although in the tested conditions apoptosis was not launched, disturbances in the mitochondrial membrane potential were observed. Thus, we can conclude that CytC oxidation can be an early marker of reversible mitochondrial stress.

References
1. M. Picard, O.S. Shirihai, *Cell Metab.*, 34(11) (2022)1620.
2. Y.L.P. Ow, D.R. Green, Z. Hao Z, T.W. Mak, *Nat. Rev. Mol. Cell Biol.*, 9 (2008) 532.
3. C.M. Schonhoff, B. Gaston, J.B. Mannick, J Biol Chem, 278 (2003) 18265.

Acknowledgements: This work was supported by the National Science Centre (UMO-2021/41/B/NZ3/04146).

Spectroscopic Profiling of Pharmacologically Induced Metabolic Shifts in Sensitive and Resistant Blood Cancer Cells

Patrycja Dawiec[a,b], Justyna Jakubowska[c], Marta Szewczyk[c], Olga Mazuryk[a], Agata Pastorczak[c], Kinga Ostrowska[c], Wojciech Młynarski[c], Małgorzata Barańska[a], Katarzyna Majzner[a]

[a]*Department of Chemical Physics, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2 St, 30-387 Krakow, Poland*

[b]*Doctoral School of Exact and Natural Sciences, Jagiellonian University, Łojasiewicza 11 St, 30-348 Krakow, Poland*

[c]*Medical University of Lodz, Department of Pediatrics, Oncology and Hematology, Czechoslowacka 4, 92-216, Lodz, Poland*

patrycja.dawiec@doctoral.uj.edu.pl

Drug resistance in blood cancers is a complex phenomenon and arises from multiple interrelated factors, including genetic alterations, epigenetic changes, molecular signaling pathways, and environmental factors. Cancer cells have a distinctive metabolism that allows them to adapt and develop new molecular mechanisms, which enables them to resist standard treatment therapies. In the face of these challenges, the importance of moving towards rapid and sensitive monitoring of treatment response using imaging techniques, biomarker analysis, and other methods cannot be overstated. Early identification of resistance could enable the development of more effective treatment strategies by allowing clinicians to modify therapies promptly. This approach could improve patient outcomes and enhance the efficacy of targeted treatments in managing hematological malignancies.

This research aims to utilize label-free and single-cell spectroscopic imaging to assess the biochemical and metabolic status of both sensitive and resistant hematologic cancer cells after treatment with standard drugs, including tyrosine kinase inhibitors, venetoclax, and PARP inhibitors. In this study, we treated several drug-sensitive and drug-resistant lymphoma and leukemia cell lines. After treatment, cells were fixed and imaged using Raman and FT-IR spectroscopy. By applying chemometric methods we identified distinct spectroscopic patterns for each studied drug, that distinguish sensitive cells from those exhibiting resistance.

Our findings indicate that each type of cancer cell responds differently by altering its use of lipids, proteins, or DNA, or by changing mitochondrial activity. We observed subtle metabolic shifts in cells with different levels of sensitivity to selected drugs, highlighting the distinct biochemical signatures of resistant hematological cancer cells compared to sensitive ones. Importantly, our spectroscopic approach effectively detects resistance across various tested drugs, providing valuable insights into the mechanisms that underlie drug resistance.

The use of Raman and/or FT-IR spectroscopy for rapid screening of drug-resistant cells presents a forward-thinking approach that is well-aligned with the shift towards more personalized and efficient diagnostic tools in oncology. By faster evaluation of new treatments approaches and facilitating the testing of new drugs, it holds significant potential for improving patient outcomes.

Acknowledgements: This research was funded by the program "Excellence Initiative – Research University" at the Jagiellonian University" and by the National Science Center Poland (NCN), PRELUDIUM 23 UMO-2024/53/N/ST4/03000. The „Label-free and rapid optical imaging, detection and sorting of leukemia cells" project is carried out within the Team-Net programme of the Foundation for Polish Science co-financed by the EU. POIR.04.04.00-00-16ED/18-00

Application of Fourier Transform Infrared Spectroscopy (FT-IR) in the Evaluation of Drug Release from Polysaccharide Matrices

Barbara Gieroba[a], Vladyslav Vivcharenko[b], Grzegorz Kalisz[a,b], Paulina Kazimierczak[c], Olena Mozgova[a,d], Maryna Khalavka[a], Liudmyla Nosach[c,e], Izabela S. Pięta[d], Robert Nowakowski[d], Agata Przekora[c], Anna Sroka-Bartnicka[a]

[a]*Independent Unit of Spectroscopy and Chemical Imaging, Medical University of Lublin, Chodźki 4a Street, 20-093 Lublin, Poland*

[b]*Department of Bioanalytics, Medical University of Lublin, Jaczewskiego 8b Street, 20-090 Lublin, Poland*

[c]*Department of Tissue Engineering and Regenerative Medicine, Medical University of Lublin, Chodźki 1 Street, 20-093 Lublin, Poland*

[d]*Institute of Physical Chemistry Polish Academy of Sciences, Kasprzaka 44/52 Street, 01-224 Warsaw, Poland*

[e]*Department of Amorphous and Structurally Ordered Oxides, Chuiko Institute of Surface Chemistry, NAS of Ukraine, 17 General Naumov St., 03164 Kyiv, UkraineFull authors' Addresses, one per line, including postal code*

barbaragieroba@umlub.pl

Modern medicine and pharmacy are increasingly emphasizing a personalized, patient-oriented approach to treatment, tailoring therapies to individual needs—especially in the context of chronic diseases and regenerative medicine [1]. Among the innovative materials explored in this regard, chitosan (CS)—a natural polysaccharide—stands out as a highly promising cationic polymer due to its biocompatibility, biodegradability, and antimicrobial properties [2]. The molecular weight of chitosan significantly influences its structural characteristics and interactions with therapeutic agents [3].

This study focused on the development of chitosan-based matrices: 2% (w/v) low molecular weight chitosan, 4% (w/v) low molecular weight chitosan, and 2% (w/v) medium molecular weight chitosan, all enriched with ibuprofen (IBU)—a widely used nonsteroidal anti-inflammatory drug (NSAID)—to enhance topical application and reduce systemic side effects associated with oral administration.

The physicochemical properties of crosslinked thin films were investigated, with particular emphasis on the molecular organization and drug release kinetics in phosphate-buffered saline (PBS). Using analytical techniques such as attenuated total reflectance Fourier-transform infrared spectroscopy (ATR FT-IR), contact angle measurements, and atomic force microscopy (AFM), the effect of ibuprofen incorporation on the structure and functional properties of chitosan films was evaluated.

The most suitable matrix for dermal application proved to be the 2% (w/v) medium molecular weight chitosan formulation, due to its favorable, slow release of ibuprofen. The results indicate that appropriately tailored chitosan formulations can effectively support drug delivery and enhance therapeutic outcomes, confirming the potential of personalized treatment strategies in clinical applications.

References

1. L.H. Goetz, N.J. Schork, *Fertil Steril* 109 (2018) 952.
2. A. Muxika, A. Etxabide, J. Uranga, P. Guerrero, K. de la Caba, *Int. J. Biol. Macromol.* 105 (2017) 1358.
3. I. Aranaz, A.R. Alcántara, M.C. Civera, C. Arias, B. Elorza, A. Heras Caballero, et al., *Polymers* 13 (2021) 3256.

Tailoring Diverse Light–Matter Interactions by Combining Plasmonic, Dielectric, and Quantum-Confined Nanostructures in Hybrid Nanosystems

Marta Gordel-Wójcik[a], Radosław Kołkowski[b], Marcin Nyk[c], Marek Samoć[c]
[a]*Faculty of Chemistry, University of Wrocław, 14.p F. Joliot-Curie Street, 50-383, Wrocław, Poland*
[b]*Department of Applied Physics, Aalto University, P.O.Box 13500, FI-00076 Aalto, Finland*
[c]*Institute of Advanced Materials, Faculty of Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, PL-50370, Wrocław, Poland*
marta.gordel-wojcik@uwr.edu.pl

We report on the design and characterization of a novel class of hybrid nanomaterials (Fig.1) exhibiting significantly enhanced nonlinear optical (NLO) responses. These materials are engineered by integrating silver sulfide quantum dots (Ag_2S QDs) [1] with silica and gold nanostructures, forming multifunctional colloidal systems. Using the femtosecond Z-scan technique across a broad spectral range (500–1600 nm), we investigated two-photon absorption (TPA) and saturable absorption (SA) behaviors in these hybrids. Embedding Ag_2S QDs within silica nanospheres results in a pronounced enhancement of TPA - up to a 16-fold increase in the figure of merit (σ_2/M) compared to isolated QDs. Further amplification, reaching up to a 73-fold increase, is achieved by coupling these QD-doped silica nanospheres with gold nanoparticles or gold nanoshells. These architectures also exhibit a competing SA effect, indicating a complex interplay between NLO processes. Intriguingly, QD-doped silica spheres encapsulated in a continuous gold shell display an unconventional saturation of extinction in the near-infrared region, with an intensity dependence that points to two-photon absorption as the activation mechanism. [2]
These findings underscore the potential of combining quantum-confined, plasmonic, and dielectric components to tailor and amplify light–matter interactions at the nanoscale, opening new avenues for advanced NLO applications.

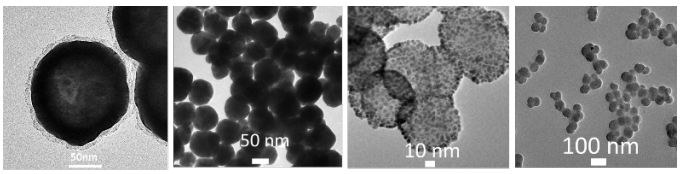


Figure 1 – TEM images of hybrid nanostructures

References
1. M. Gordel-Wójcik, M. Malik, A. Siomra, M. Samoć, M. Nyk, *J. Phys. Chem. Lett.,* 14 (2023) 11117.
2. M. Gordel-Wójcik, R. Kołkowski, M. Nyk, M. Samoć, *ACS Appl Mater Interfaces* 17 (2025) 28484.

Acknowledgements: This work was supported by the project No. UMO-2021/43/D/ST5/02249, SONATA 17, funded by National Science Center Poland (NCN).

A New Approach to Spectral Analysis of Lipid Pathways in Cancer Cells Using Labeled Raman and O-PTIR Technique

Wiktoria Korona[a,b], Anna Nowakowska[a], Barbara Orzechowska[a], Anna Pieczara[a], Małgorzata Barańska[a]
[a]*Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387, Krakow, Poland*
[b]*Jagiellonian University, Doctoral School of Exact and Natural Sciences, Losiajewicza 11., Krakow, Poland*
wiktoria.korona@doctoral.uj.edu.pl

Cellular metabolism forms a highly intricate web of biochemical processes that cannot be effectively studied without specialized tools. Spectroscopy offers a powerful tools of exploring cellular function at the molecular level. Recent advancements have introduced promising strategies—such as multiplexed labeling and multimodal imaging integration—that significantly improve the spectroscopic investigation of metabolism [1]. However, a major limitation persists: many current methods fail to fully address the complexity of metabolic systems, where multiple pathways are tightly interconnected.
This study introduces an innovative methodology that utilizes the vibrational tags, e.g. ^{13}C, $-N_3$, C≡C, emitting distinct and well-resolved signals within the spectral silent window. These probes enabled simultaneous detection of several lipid pathways at the single-cell level, allowing for the parallel assessment of structural and functional changes. The approach further integrated Raman imaging (RS) with the emerging O-PTIR technique to map critical cellular components that serve as indicators of biological activity and disease states. This presentation introduces an innovative strategy for the morphological analysis of cancer cells by harnessing OPTIR's capabilities in a novel context. Single-channel O-PTIR imaging was employed to achieve precise delineation of key cellular components—specifically, the lipid droplets—which are regarded as essential indicators of cellular function and pathology. By correlating signals from RS and O-PTIR, this combined strategy offers deeper and more reliable insights into the metabolic landscape of cancer cells.

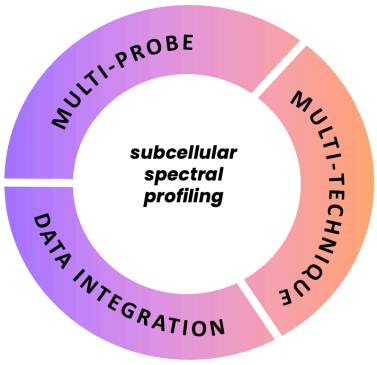


Figure 1 – Towards integrated strategy for subcellular spectral profiling using multi-probe, multi-technique, and data integration approaches.

References
1. X. Liu, L. Shi, Z. Zhao, et al. *Nat Methods* 21 (2024) 501.

Acknowledgements: This research was funded by the National Science Center Poland (NCN), Maestro 2022/46/A/ST4/ 00054 to Malgorzata Baranska. This publication was founded by the program Excellence Initiative – Research University at the Jagiellonian University.

Spectroscopic Analysis of Biochemical Composition of Red Blood Cells in Polycythemia Vera Patients

J. Dybaś[a], W. Lebowa[b,c], E. Szczęsny-Małysiak[a], A. Bartkowiak[a], M. Targosz-Korecka[d], T. Sacha[b,e], S. Chłopicki[a,f]

[a]*Jagiellonian Centre for Experimental Therapeutics, Jagiellonian University, 14 Bobrzynskiego St., 30-348 Krakow, Poland*

[b]*Department of Haematology, Jagiellonian University Hospital, 2 Jakubowskiego St., 30-688 Krakow, Poland*

[c]*Doctoral School of Medical and Health Sciences, Jagiellonian University Medical College,16 Sw. Lazarza, 31-530 Krakow, Poland*

[d]*Faculty of Physics, Institute of Astronomy and Applied Computer Science, Jagiellonian University, 11 Lojasiewicza St., 30-348 Krakow, Poland*

[e]*Chair of Haematology, Faculty of Medicine, Jagiellonian University Medical College, 12 Sw. Anny St., 30-008 Krakow, Poland*

[f]*Chair of Pharmacology, Faculty of Medicine, Jagiellonian University Medical College, 16 Grzegorzecka St., 31-531 Krakow, Poland*

jakub.dybas@uj.edu.pl

Polycythemia vera (PV) is a myeloproliferative neoplasm characterized by an excessive production of red blood cells (RBCs), increased hemoglobin (Hb) level and hematocrit [1], what in turn promotes increased blood viscosity. This burdens PV patients with an increased cardiovascular and all-cause mortality [2]. However, the functional alterations of RBCs in PV have not been fully characterized.

In this study a wide range of spectroscopic methods, comprising 532 nm Raman Spectroscopy, 405 nm resonance Raman spectroscopy, Fourier-transform infrared spectroscopy (FTIR), UV-VIS and EPR spectroscopy was used to investigate changes in hemoglobin structure. Blood was collected from 17 (11 females and 6 males) adult patients diagnosed with PV and 16 (11 females and 5 males) healthy controls. The experiments were performed on either intact RBCs or isolated RBC membranes.

Changes in the secondary and quaternary Hb protein structure revealed with use of FTIR were identified as the cause of an increased Hb concentration and a tendency for Hb aggregation in PV patients. This was followed by 532 nm Raman spectroscopy results showing an increase in Hb deposited on cell membranes. Resonance Raman spectroscopy with 405 nm excitation revealed elevated ferrous (Fe^{II})-to-ferric (Fe^{III}) Hb ratio in RBCs, discriminating higher level of deoxyhemoglobin. Moreover, in UV-VIS absorption-based reoxygenation assay an impaired Hb affinity for oxygen was shown in PV. The use of nitric oxide (NO) donor (DEA-NONOate) in EPR spectroscopy studies enabled to connect altered affinity for oxygen with weaker oxygen-iron binding, since NO is preferentially bound by deoxyhemoglobin. Other, non-spectroscopic methods of biological analysis, namely atomic force microscopy and flow cytometry revealed a tendency for increased stiffness of the cells and disturbances in the surface protein expression.

Taken together, our results uncover structural and functional alteration in RBCs of PV patients, of significant pathophysiological relevance, since the observed alterations in Hb structure and impaired ability of Hb to bind oxygen may contribute to chronic fatigue in PV patients.

References

1. A. Tefferi, T. Barbui, *Am. J. Hematol.*, 98(9) (2023) 1465.
2. Gruppo Italiano Studio Policitemia. *Ann. Intern. Med.*, 123(9) (1995) 656.

Acknowledgements:

This work was supported by the National Science Centre (UMO-2021/41/B/NZ3/04146).

Spectroscopic Study of Magnetic Composites Modified with Hydroxyapatite for Regenerative Medicine Applications

Anna Kołodziej[a], Małgorzata Świętek[b], Małgorzata Rachwał[a], Daniel Horak[b], Aleksandra Wesełucha-Birczyńska[a]
[a]*Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*
[b]*Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského Sq. 2, 162 06 Prague 6, Czech Republic*
anka.kolodziej@uj.edu.pl

One of the bone tissue engineering (BTE) strategies to address critical bone defects is to implement a biomaterial scaffold that promotes tissue regeneration. The main objective of the presented research is to design a bioactive group of materials with potential applications in BTE by integrating the properties of components such as poly(ε-caprolactone) (PCL) as a polymer matrix with modifying additives like nano/micro-hydroxyapatite (n-HAp /μ-HAp), oleic acid, and magnetic nanoparticles (MIONs, coated with oleic acid). MIONs were produced by the co-precipitation method and transferred into an organic solvent (DCM) through OA-mediated phase transfer. TEM images, TGA analysis and ATR-FTIR spectroscopy confirmed the presence of OA on the surface of iron oxide nanoparticles, which have the diameter of 10-15 nm. Spectroscopic measurements (FTIR, Raman) indicated that the obtained MIONs consist mainly of magnetite with a small presence of maghemite. Nanocomposite membranes were fabricated using the solvent casting method. The improvement of hydroxyapatite dispersion due to OA addition to the membrane was clearly observed by visual evaluation, further confirmed by Raman mapping and TEM analysis. SEM images indicated a high level of MIONs dispersion as well. Raman spectroscopy revealed a decrease in the PCL crystallinity influenced by the incorporation of MIONs into the polymeric matrix.

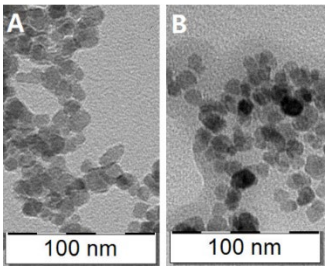


Figure 1 – TEM images of MIONs: (A) before and (B) after water -> DCM phase transfer

References
1. J. W. Jang, K. E. Min, C. Kim, J. Shin, J. Lee, S. Yi*, Int. J. Precis. Eng. Manuf.,* 24 (2023) 511.
2. S. Park, K. A. Rahaman, Y. C. Kim, H. Jeon H. S. Ha,. *Bioact Mater*., 40 (2024) 345.

Acknowledgements: The research has been supported by a grant from the Faculty of Chemistry under the Strategic Programme Excellence Initiative (Young Labs competition - Edition 4 and 5) at Jagiellonian University. This work was funded by the National Science Centre, Poland (Project 2024/08/X/ST4/01426 to A.K.) The study was carried out using research infrastructure funded by the European Union in the framework of the Smart Growth Operational Programme, Measure 4.2; Grant No. POIR.04.02.00-00-D001/20, "ATOMIN 2.0 – Center for materials research on ATOMic scale for the INnovative economy".

Molecular Interactions Between Anticancer Drugs and Ascorbic Acid: Insights into Drug Activity Modulation

V. Pashynska[a], Gy. M. Tokaji[b], B. Fiser[b,c,d], B. Minofar[b,c], A. Gomory[e], L. Drahos[e]
[a] *B. Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, 47 Nauky Ave., Kharkiv, 61103, Ukraine*
[b] *Institute of Chemistry, University of Miskolc, Miskolc-Egyetemváros 3515, Hungary*
[c] *Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland*
[d] *Ferenc Rakoczi II Transcarpathian Hungarian College of Higher Education, Beregszász 90200, Ukraine*
[e] *Institute of Organic Chemistry, HUN-REN Research Center for Natural Sciences, Budapest, Hungary*
vlada.pashynska@gmail.com

Molecular interactions of anticancer drugs with supporting medicines or biologically active compounds, such as vitamins or antioxidants (which often are co-administered in the medical practice) can influence significantly on the drugs` activity. In particular, vitamin C (ascorbic acid, ASC), which is widely used as a supporting agent in antitumor treatment or is affiliated with the patients` nutrition, can substantially reduce the doxorubicin (DOX) therapeutic efficiency [1]. To predict or prevent the modulatory effects of ASC on the drugs` activity it is important to examine the molecular basis of such effects. Our previous studies of the biologically significant molecular interactions of drugs with the supporting medicines allowed us to develop an effective approach combining electrospray ionization (ESI) mass spectrometry (MS) method and computer simulations for examination of the interactions which potentially can modulate the drugs` activity [2, 3].

In the current study this approach was used to probe paired model systems containing an anticancer drug (DOX, or 6-thiopurine (TP), or 2-thioadenine (TA)) and ASC with a 1:1 molar ratio dissolved in the polar solvents. In the ESI mass spectra of the model systems in methanol, peaks corresponding to noncovalent complexes of each antitumor agent (DOX, or TP, or TA) with ASC were observed, indicating the probability of stable noncovalent complexation between these anticancer drugs and vitamin C in a polar solvent media. Such molecular interactions between DOX (or TP, or TA) and ASC can inhibit the activity of these anticancer agents even at the administration stage if they co-administered with vitamin C. The obtained experimental ESI MS data about the formation of noncovalent complexes between the studied drugs and ASC were confirmed by molecular dynamics (MD) simulations. The MD calculations were performed by using the GROMACS package with a 2 fs time step at 300 K. The simulations were conducted by solvating 10 molecules of each selected anticancer drug with 10 molecules of ASC in the simulation box, resulting in an approximate concentration of 0.0170 M. The modeling indicated the formation of well-structured and strong to medium noncovalent interactions between the drug molecules and ASC in the modeled solutions (water and saline). Among the studied drugs, DOX exhibited the most structured and strongest interactions with vitamin C. Interestingly, the addition of NaCl in the model pair systems (saline conditions) promoted stronger complexation between the anticancer drugs and ASC compared to pure water.

References

1. M. Heaney, J. Gardner, N. Karasavvas, and others, *Cancer Res.*68 (2008) 8031.
2. V. Pashynska, S. Stepanian, A. Gomory, K. Vekey, L. Adamowicz, *Chem. Phys.*, 455 (2015) 81.
3. V. Pashynska, S. Stepanian, A. Gomory, L. Adamowicz, *J. Mol. Structure,* 1232 (2021) 130039.

Rapid Infection Diagnosis Using Infrared Microscopy, Peripheral Blood Tests, and an Expert System in Febrile Pediatric Oncology

Uraib Sharaha[a,b], Yotam D. Eshel[c], Dima Bykhovsky[d], Mahmoud Huleihel[a], Hagit Miskin[c], Itshak Lapidot[e,f], Shaul Mordechai[g], Joseph Kapelushnik[c], Ahmad Salman[h]

[a]*Department of Hematology and Oncology, Saban Pediatric Medical Center Soroka University Medical Center and Faculty of Health Sciences, Beer-Sheva, 84105, Israel.*

[b]*Department of Biology, Science and Technology College, Hebron University, Hebron P760, Palestine.*

[c]*Department of Microbiology, Immunology and Genetics, Faculty of Health Sciences, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel.*

[d]*Electrical and Electronics Engineering Department, SCE-Sami Shamoon College of Engineering, Beer-Sheva 84100, Israel*

[e]*Department of Electrical and Electronics Engineering, Afeka Tel-Aviv Academic College of Engineering, Tel-Aviv 69107, Israel.*

[f]*LIA Avignon Université, 339 Chemin des Meinajaries, Avignon 84000, France*

[g]*Department of Physics, Ben-Gurion University, Beer-Sheva 84105, Israel.*

[h]*Department of Physics, SCE-Sami Shamoon College of Engineering, Beer-Sheva 84100, Israel.*

ahmad@sce.ac.il

Infectious diseases, a leading cause of mortality, often present with similar clinical symptoms despite distinct immune responses to bacterial and viral pathogens. Timely and accurate identification of infection etiology in febrile pediatric oncology patients is critical to optimize treatment and reduce unnecessary antibiotic use. Current diagnostic methods can take 2–4 days, often leading clinicians to rely on non-specific biomarkers such as C-reactive protein (CRP), white blood cell (WBC) count, and absolute neutrophil count (ANC). Using antibiotics without knowing the exact cause can lead to several problems, including harmful side effects, changes in the body that make it easier for other infections to take hold, and an increased risk of antibiotic-resistant and multidrug-resistant (MDR) bacteria.The CDC's 2013 Threat Report estimated that up to 50% of antibiotic use is unnecessary.

In this study, we evaluated the diagnostic performance of these clinical measures, achieving approximately 70% accuracy in distinguishing bacterial from viral infections. We then applied machine learning algorithms to infrared (IR) spectra of isolated white blood cells (WBCs), achieving a classification accuracy of 97%. This builds upon our prior work demonstrating the effectiveness of IR spectroscopy in immune response monitoring [1–3]. Integrating IR spectral data with CRP, WBC, and ANC values increased diagnostic accuracy to 98.6%.

The dataset included 50 bacterial, 21 viral, and 39 control cases for clinical markers, and 59 bacterial, 29 viral, and 92 control cases for IR analysis. Our results demonstrate that combining IR spectroscopy with standard blood tests enables rapid (~1 hour) and highly accurate infection diagnosis, offering a promising tool for improving clinical decision-making and reducing antibiotic overuse in this vulnerable population.

References

1. A. H. Agbaria, G. Beck, I. Lapidot, et al., *Analyst*., 145 (21) (2020) 6955.
2. A. H. Agbaria, G. Beck, I. Lapidot, et al., *Anal. Chem.*, 90 (13) (2018) 7888.
3. Y. D. Eshel, U. Sharaha, G. Beck, et al., *Talanta*, 270 (2024) 125619.

Acknowledgements: This research was supported by the ISRAEL SCIENCE FOUNDATION (grant No. 1087/20).

Combined Spectroscopic and Structural Study of Promising NLO Crystals Based on 2D Molecular Building Units

Ivan Němec[a], Irena Matulková[a], Ivana Císařová[a], Róbert Gyepes[a], Petr Němec[b]
[a]*Charles University, Faculty of Science, Hlavova 8, Prague 2, 128 40, Czech Republic*
[b]*Charles University, Faculty of Mathematics and Physics, Ke Karlovu 3, Prague 2, 120 00, Czech Republic*
ivan.nemec@natur.cuni.cz

Molecular crystals represent one group of promising compounds in a broad family of materials with potential for applications in nonlinear optics (NLO). These crystals contain selected organic molecules/cations, which act as carriers of NLO properties, hydrogen-bonded to suitable cocrystalization partners. Hydrogen bonding in these materials assists in the self-assembly of building units, leading to proper symmetry of crystalline phases, and positively influences their thermal stability and overall optical properties. Studied molecular crystals can be used in a wide range of technical applications based on numerous existing NLO effects including SHG - Second Harmonic Generation, THG - Third Harmonic Generation, cascaded self-frequency doubling and tripling, and the processes associated with Stimulated Raman Scattering (SRS) [1,2]. The applications include generation of new laser frequencies, signal processing, optical communications, all-optical switching, optical power limiting and image manipulation.

This contribution is focused on the detailed characterisation of selected examples of hydrogen-bonded molecular crystals containing 2D organic moieties, particularly guanidinium(1+), aminoguanidinium(1+) and 2-aminopyrimidinium(1+) cations. The presented characterisation includes a combination of experimental (e.g. FTIR and Raman spectroscopy, X-ray diffraction, temperature-dependent SHG measurements and calorimetry) and theoretical (solid state quantum-chemical calculations) methods. Priority attention will be given to monitoring and the explanation of the observed phase transformations. Moreover, linear and nonlinear optical properties of the promising materials will be discussed.

References

1. L. Bohatý, P. Becker, E. Haussuhl, I. Němec, O. Lux, H.J. Eichler, H. Yoneda, A. Shirakawa, A.A. Kaminskii, *Zeitschrift für Kristallographie - Crystalline Materials*, 230 (2015) 639.
2. A.A. Kaminskii, P. Becker, H. Rhee, O. Lux, A. Kaltenbach, H.J. Eichler, A. Shirakawa, H. Yoneda, I. Němec, M. Fridrichová, L. Bohatý, *Physica Status Solidi B*, 250 (2013) 1837.

Acknowledgements: **A**dvanced **M**ultiscale **M**aterials for **K**ey **E**nabling **T**echnologies (**AMULET**) project, supported by the Ministry of Education, Youth, and Sports of the Czech Republic (project No. CZ.02.01.01/00/22_008/0004558) is gratefully acknowledged.

Atmospheric Oxidation Reaction Kinetics of Ethanolamines Employed in Carbon-Capture

Thomas Golin Almeida[a], Kristian H. Møller[b], Henrik G. Kjaergaard[a]
[a]*Department of Chemistry, University of Copenhagen, 2100 Copenhagen, Denmark*
[b]*Department of Weather Research, Danish Meteorological Institute, 2100 Copenhagen, Denmark*
tga@chem.ku.dk

Post-combustion carbon-capture technologies were developed in recent years, with the goal of limiting CO_2 emissions from large-scale combustion systems. Many such technologies employ amine-based solvents, which are able to act as CO_2 filters.[1] During their usage, these amines can escape to the atmosphere, with a potentially detrimental effect on the local air quality.[2] While simple amines are only weakly toxic, their breakdown upon atmospheric photo-oxidation can yield notably carcinogenic products, such as nitroamines or nitrosamines.[3] Furthermore, previous work revealed that tertiary amines are prone to undergo autoxidation, process in which successive O_2-addition and intramolecular H-transfer reactions produce highly-functionalized low-volatility compounds, contributing to the formation and growth of aerosol particles.[4] In this study, we employ quantum chemistry and theoretical reaction kinetics to explore the OH radical-initiated atmospheric oxidation mechanism of three tertiary amines (Figure 1), dimethyethanolamine (DMEA), methyldiethanolamine (MDEA), and triethanolamine (TEA). The last two amines are used as solvents in carbon-capture plants.

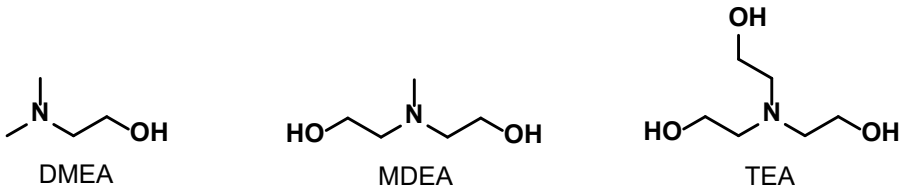


Figure 1 – Ethanolamines investigated in this study.

Preliminary results indicate that autoxidation reaction channels are especially favourable during oxidation of the investigated ethanolamines, when compared to simpler amines such as trimethylamine and diethylamine. We find that the presence of hydroxyl groups in the organic substrate is critical for this observation, stabilizing the transition state of H-shift reactions via intramolecular H-bonds. In addition, despite displaying complex and branched oxidation mechanisms, reaction pathways appear to converge to the formation of just a few highly-functionalized hydroperoxides.

References

1. Z.H. Liang, et al., *Int. J. Greenh. Gas Control*, 40 (2015) 26.
2. L. Zhu, et al., *Environ. Sci. Technol.,* 47 (2013) 14306.
3. S. Ravnum, et al., *Regul. Toxicol. Pharmacol.*, 69 (2014) 250.
4. K.H. Møller, et al., *Environ. Sci. Technol.*, 54, 18 (2020) 11087.

Vibrational Spectroscopy of Monohydrated Radical Cation Complexes

Ružica Marković, Henrik Grum Kjærgaard
Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark
ftq203@alumni.ku.dk

In neutral bimolecular clusters, the hydrogen bond is the strongest possible intermolecular interaction. It is well-studied with techniques such as infrared spectroscopy, due to the typically high intensity of the bonded OH-stretching vibration. In charged radical complexes, the hemi bond represents an additional binding motif with a bond strength comparable to that of the hydrogen bond. The vibrational spectroscopy of hydrated radical cation complexes is explored using non-linear techniques such as photodissociation spectroscopy, and quantum chemical calculations aid heavily in the interpretation of these, sometimes, complicated spectra. The competition between the hydrogen and hemi bond is explored for the monohydrated radical cation complexes $(H_2O\text{-}X)^+$ with X = Ar, N_2, CO_2 and N_2O. The vibrational spectra are calculated using second-order vibrational perturbation theory (VPT2) and a more advanced local mode model (LM). The VPT2 and LM models predict redshifts of the bonded OH-stretch in hydrogen-bonded charged complexes that are an order of magnitude larger than their neutral counterparts, which can be attributed to the increased binding energies in the charged complexes. The spectra of the hemi-bonded isomers resemble the spectrum of an isolated H_2O^+ pointing to minimal perturbation by the hemi-bonding partner molecule (Figure 1).

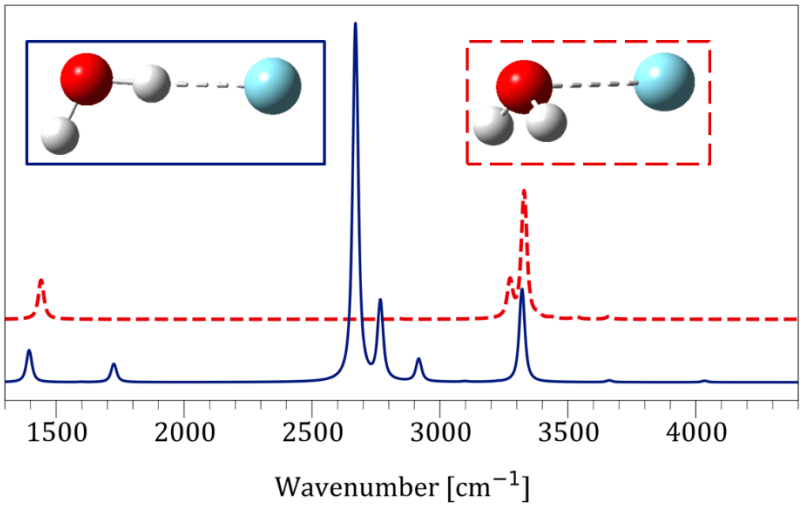


Figure 1 – Comparison of VPT2 calculated spectra for hydrogen-bonded (full line) and hemi-bonded (dashed-line) $(H_2O\text{-}Ar)^+$

References
1. M. Kominato, A. Fujii, *Phys. Chem. Chem. Phys.*, 25 (2023) 14726.

Acknowledgements: The authors thank Emil Vogt of Center for Free-Electron Laser Science (Hamburg), for helpful discussions regarding the project.

Molecular Modeling of Non-Covalent Interactions Between Orellanine and Graphene Oxide Models

Piotr Najgebauer, Monika Staś-Bobis, Teobald Kupka
Faculty of Chemistry and Pharmacy, University of Opole, Oleska 48 Street, 45-052 Opole, Poland
122217@student.uni.opole.pl

It is a known fact that some mushrooms contain toxins. One of such mushroom specimen is *Cortinarius orellanum*, which contains orellanine[1]. It is a dangerous nephrotoxine, that acts with a delay[2-3].
In order to enable orellanine detection with a chemical sensor, we decided to investigate interactions between orellanine and potential material for such sensor – graphene oxide (GO). We studied such systems, with and without implicit solvents (water, methanol and chloroform) using subsequent GFN2/GBSA and DFT/PCM calculations. Sample of our results, with phenol as GO model is shown below in Figure1.

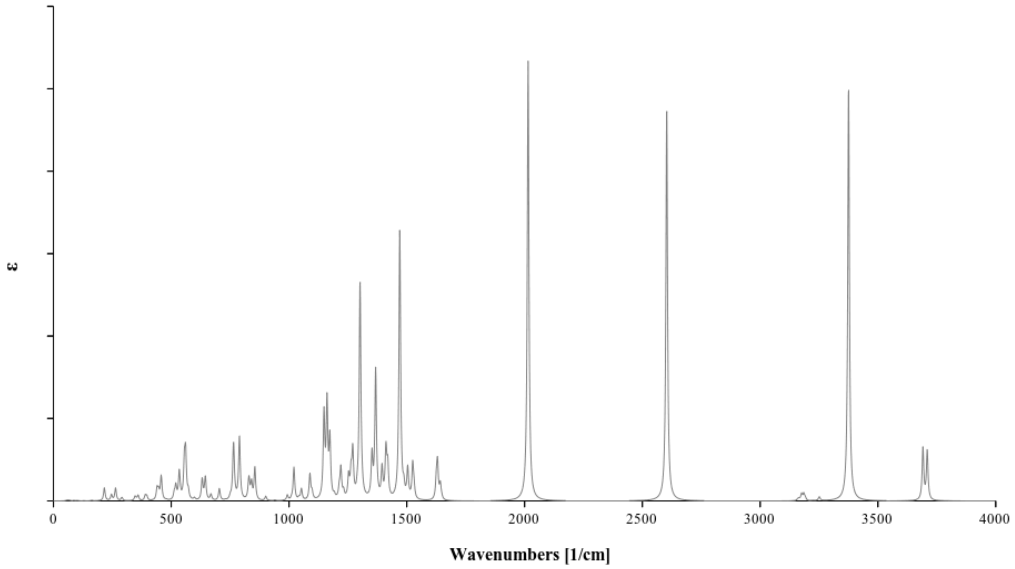


Figure 1 – Calculated at B3LYPD3/6-311++G** level of theory IR spectrum of derived non-covalent complexes of phenol and orellanine in chloroform

References
1. V. C. Danel, P. F. Saviuc, D. Garon, *Toxicon.*, 39 (2001) 1053.
2. M. Rohrmoser, M. Kirchmair, E. Feifel, A. Valli, R. Corradini, E. Pohanka, A. Rosenkranz, R. Piider. *J. Toxicol. Clin. Toxicol., 35* (1997) 63.
3. H. Hedman, J. Holmdahl, J. Mölne, K. Ebefors, B. Haraldsson J. Nyström, *BMC Nephrol.,* 18 (2017) 121.

Acknowledgements: The authors thank for resources provided by Wroclaw Centre for Networking and Supercomputing (https://wcss.pl) and for partial financial support provided by University of Opole.

Calculated Absorption Cross Sections and Photolysis Rates of Ketohydroperoxides

Nanna Falk Christensen, Henrik G. Kjaergaard
Department of Chemistry, University of Copenhagen, Universitetsparken 5, 2100, Copenhagen Ø, Denmark
nfc@chem.ku.dk

Ketohydroperoxides are a class of transient organic compounds frequently formed in the atmosphere from oxidation of emitted volatile organic compounds.[1,2] One key example, is hydroperoxymethyl thioformate (HPMTF), formed in the oxidation of dimethyl sulfide,[3,4] the largest component of the global biogenic sulfur emission.[5] We have used a nuclear ensemble approach to calculate the electronic absorption cross section of HPMTF and selected ketohydroperoxides, to estimate their atmospheric photolysis rates. We compare these photolysis rates with rates obtained using structure-activity relationship approaches. We find that photolysis is likely only a minor loss path for HPMTF and for ketohydroperoxides with oxygen or nitrogen in the α-position, photolysis is insignificant, due to strong heteroatom effects in this position.

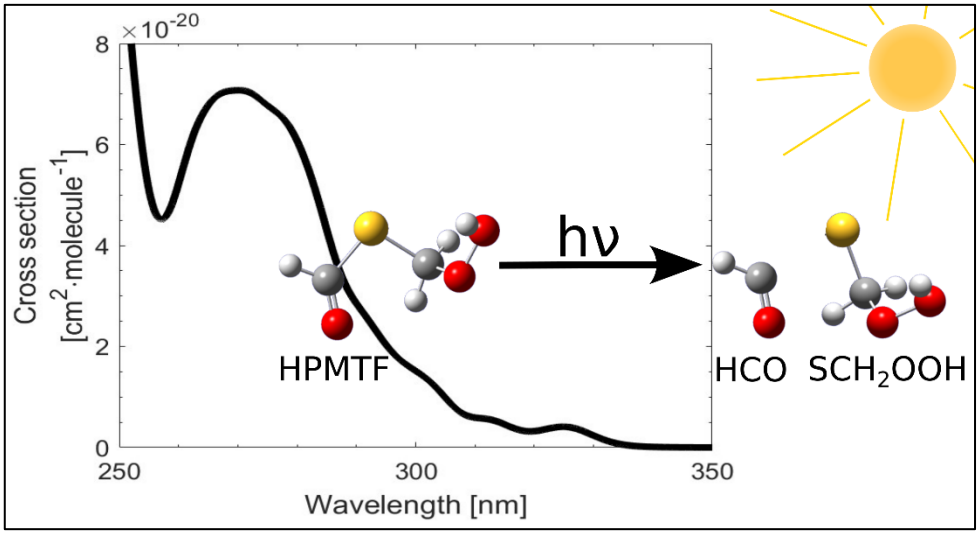


Figure 1 – Simulated electronic absorption cross section of HPMTF

References
1. K. H. Møller, T. Berndt, H. G. Kjaergaard, *Environ. Sci. Technol.* 54 (2020) 1108.
2. R. Wu, S. Wang, L. Wang, *J. Phys. Chem. A* 119 (2015) 112.
3. P. R. Veres, J. A. Neuman, T. H. Bertram, E. Assaf, G. M. Wolfe, C. J. Williamson, B. Weinzierl, S. Tilmes, C. R. Thompson, A. B. Thames, *PNAS*, 117 (2020) 4505.
4. M. P. Vermeuel, G. A. Novak, C. M. Jernigan, T. H. Bertram, *Environ. Sci. Technol.* 54 (2020) 12521.
5. C. L. Lee, P. Brimblecombe, *Earth-Sci. Rev.* 160 (2016) 1.

About Metamaterials and Other Second Harmonic Generators

Marek Drozd
Institute of Low Temperature and Structure Research, PAS, 2, Okolna Str., 50-950 Wroclaw, Poland
m.drozd@intibs.pl

The first NLO experiment was performed by Franken and coworkers in 1961. During the use of a laser with a 694 nm wavelength with a quartz crystal, a completely new signal at 347 nm was observed. In linear optics, a light wave acts on a molecule, which vibrates and then emits its own light wave that interferes with the original light wave. In nonlinear media, the polarisation density P responds nonlinearly to the electric field E of the light. Nonlinear optical effects include phenomena like second-harmonic generation (frequency doubling), third-harmonic generation, and optical parametric amplification. These effects are crucial for various applications in fields like telecommunications, medical imaging, and laser technology.

Nowadays, some methods of creating NLO materials (especially second-order generators) are being developed. From the fundamental science point of view are important common attributes of the mentioned groups of NLO materials are noticed. Firstly, all SHG crystals should be non-centrosymmetric. The question of how to enforce the crystal structure of noncentrosymmetric without chiral molecules still seems to be open, but sometimes the creation of weak chemical interactions, such as hydrogen bonds, can be decisive about the symmetry of prepared crystals.

During this lecture, three fundamental groups of SHG material will be presented. The first very promising materials belong to organic perovskites, which are solid compounds with a perovskite structure. They have potential applications in solar cells, lasers, light-emitting diodes, photodetectors, radiation detectors, scintillators, magneto-optical data storage and hydrogen production. The next SHG materials based on organic-inorganic hybrid compounds, which can be created with simple small molecules. These materials generally high NLO response (organic part of the crystal) and nice physical properties (inorganic part). The many examples of compounds based on the guanidinium cation will be shown. Last but not least, the phase-matched second-harmonic generation (SHG) from three-dimensional metamaterials consisting of stacked metasurfaces will be presented. The development of these materials connects the best from chemistry and physics.

References

1. T. Stolt, J. Kim, S. Héron, A. Vesala, Y. Yang, J. Mun, M. Kim, M. J. Huttunen, R. Czaplicki, M. Kauranen, J. Rho, P. Genevet*, Phys. Rev. Lett.*, 126 (2021) 033901.
2. M. Drozd, M. Daszkiewicz*, J. Mol. Struct.*, 1161 (2018) 383.
3. M. Mączka, A. Gagor, J.K. Zaręba, D. Stefanska, M. Drozd, S. Balciunas, M. Šimėnas, J. Banys, A. Sieradzki*, Chem. Mater.* 32 (2020) 4072.

Terahertz Raman Optical Activity as a New Window into Supramolecular Chirality

Štěpán Jílek[a], Lucia Ďuríšková[a], Martina Valášková[a], Josef Kapitán[b], Václav Profant[a]
[a]*Institute of Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Prague 2, Czech Republic*
[b]*Department of Optics, Faculty of Science, Palacky University Olomouc, 17. Listopadu, 771 46 Olomouc, Czech Republic*
vaclav.profant@matfyz.cuni.cy

Chiroptical spectroscopies are invaluable tools for probing absolute molecular configuration and supramolecular organization due to their intrinsic sensitivity to molecular chirality. Among these, vibrational chiroptical techniques – such as Vibrational Circular Dichroism (VCD) and Raman Optical Activity (ROA) – offer uniquely rich structural information but are fundamentally limited by weak signal intensities. Enhancing these signals to shorten acquisition times and improve spectral quality remains a major challenge in the field.[1]
In this contribution, we demonstrate that ROA, a differential form of Raman scattering sensitive to optical activity, exhibits striking signal enhancement in the terahertz (THz) frequency range (< 200 cm^{-1}) upon supramolecular aggregation. Using guanosine-5′-monophosphate (5′rGMP) as a model system forming mononucleotide G-quadruplexes (mG4), we observe up to a two-order-of-magnitude increase in ROA intensity in the low-frequency region. These spectral features are highly sensitive to structural variations mediated by different stabilizing cations. The enhanced THz-ROA signals originate from long-range chiral interactions and are characteristic of specific stacking arrangements within mG4 assemblies.[2] Notably, the THz-ROA signal is virtually background-free, providing a powerful new spectroscopic window into the emergence of chirality in molecular and biomolecular systems that fold into ordered supramolecular structures.

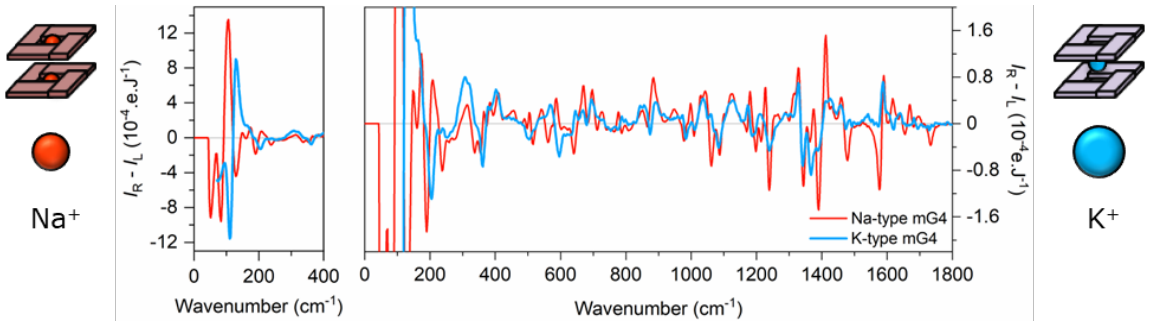


Figure 1 – ROA spectra of Na- (red) and K-type (blue) of mG4. The low-wavenumber (THz) regions of ROA spectra are shown once more on the left due to their much higher intensity

References
1. V. Profant, Š. Jílek, *Appl. Spectrosc. Rev.,* (2025) 1-37. DOI: 10.1080/05704928.2025.2500349
2. M.S.P. Kkadan, Š. Jílek, V. Profant, J. Kapitán, J. Kessler, P. Bouř, *Chem. Eur. J.,* 30 (2024) e202403245.

Acknowledgements: This research was supported by the Charles University Grant Agency (GA UK) project no. 298123.

Stability of Drug–Metal Nanoparticle Conjugates as a Key Determinant of Their *In Vitro* Efficacy

Natalia Piergies[a], Magdalena Oćwieja[b], Monika Szczepanek–Dulska[a], Agnieszka Panek[a], Katarzyna Pogoda[a]

[a]*Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland*

[b]*Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Niezapominajek 8, PL-30239 Krakow, Poland*

natalia.piergies@ifj.edu.pl

Metal nanoparticles are appealing for their unique properties and easy functionalization, enabling controlled surface modifications. Spectroscopic methods (Raman, FTIR, SERS, SEIRA) and AFM–SEIRA provide detailed insight into these modifications at the nanoscale.[1,2]

This study explores the adsorption of tyrosine kinase inhibitors erlotinib and afatinib on gold nanoparticles (AuNPs) using SERS and AFM–SEIRA. Time-resolved SERS spectra (Fig. 1A, B) show that erlotinib forms more stable conjugates than afatinib, which desorbs significantly within 6 hours. This differential stability is also evident in cellular environments. Microscopic and chemical imaging of H1299 cell line treated by the two type of conjugates, respectively, are shown in Fig. 1C–F. The Raman signature of erlotinib on AuNPs internalized by H1299 cells after 24 hours post treatment is clearly visible (Fig. 1D), whereas only characteristic AuNP bands are observed for afatinib:AuNPs (Fig. 1F), with no detectable afatinib signals. These findings correlate with MTS cytotoxicity assays, where erlotinib:AuNPs demonstrate higher cytotoxicity relative to afatinib:AuNPs, suggesting a stability-dependent therapeutic efficacy.

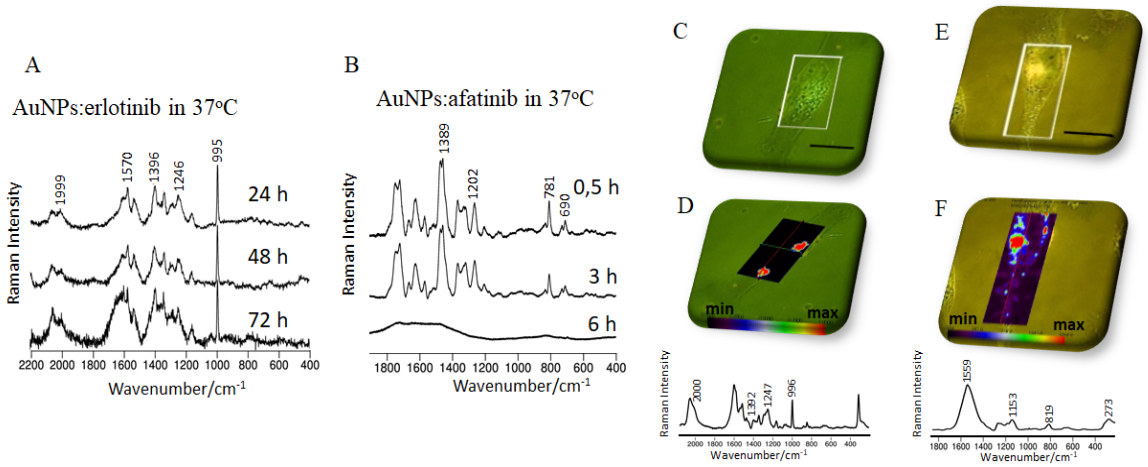


Figure 1 – Desorption kinetics of erlotinib and afatinib from AuNPs, monitored by SERS at 37 °C over time (A, B). Images of H1299 cells after 24 h treatment with AuNPs:erlotinib and AuNPs:afatinib conjugates (C, E), along with intracellular distribution of nanosystems revealed by Raman-based cluster analysis and representative spectral profiles (D, F).

References

1. N. Piergies, M. Oćwieja, C. Paluszkiewicz, W.M. Kwiatek, *Applied Surf. Sci.* 537 (2021) 147897.
2. N. Piergies, A. Dazzi, A. Deniset-Besseau, J. Mathurin, M. Oćwieja, C. Paluszkiewicz, W.M. Kwiatek, *Nano Res.* 13 (2020) 1020.

Impact of Water on the Nanomechanical Degradation of Functionalized Gold Surface

Przemysław Dopieralski[a], Martin Zoloff Michoff[b], Dominik Marx[c]
[a]*Faculty of Chemistry, Univeristy of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław*
[b]*Facultad de Ciencias Quimicas, Univesidad Nacional de Cordoba, Cordoba, Argentina*
[c]*Lehrstuhl fuer Theoretische Chemie, Ruhr-Universitaet Bochum,44780 Bochum, Germany*
przemyslaw.dopieralski@uwr.edu.pl

The mechanochemical detachment of a PEGylated divalent thiolate-gold interface was investigated by means of *ab initio* molecular dynamics simulations [1] in an explicitly water solvated environment. Pure mechanical stress produces two different rupture channels in the high force regime: one leading to a 6-membered cyclic gold complex; and another in which the final detachment takes place through the rupture of a S-Au bond. Interestingly, solvation of the interface turned out to be a key factor into determining the fate of the hybrid Au-S interface. Additionally, OH^- assisted detachment of the molecule, mediated by the facilitation of a S-Au bond rupture was also explored in the low force regime. Unexpectedly, the activation free energy for this process **is higher** for the more stressed S-Au bond.

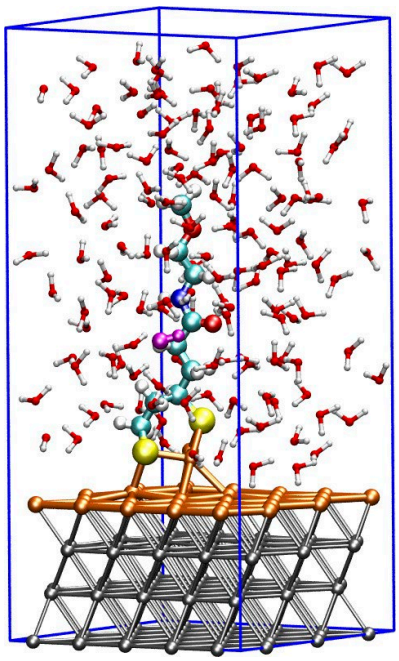


Figure 1 – Initial structure used for the MD simulations, as obtained from the isotensional pulling simulation at 1.6 nN in vacuum and then solvated with 148 water molecules

References
1. D. Marx, J. Hutter, *Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods,* Cambridge University Press, Cambridge, 2009.

Acknowledgements: We gratefully acknowledge financial support via the National Science Centre of Poland - NCN - (2020/37/B/ST4/00423) as well as additional computational support by Wroclaw Supercomputer Center (WCSS).

Spectroscopy for Sustainability: The Role of FTIR in Green Technologies

Karolina A. Haupa
Bruker Optics GmbH and Co. KG, Rudolf-Plank-Str. 27, 76275 Ettlingen, Germany
karolina.haupa@bruker.com

FTIR spectroscopy is playing an increasingly important role in the development of sustainable technologies by providing detailed molecular insights into materials and processes. This talk offers an overview of how FTIR supports research in key areas such as energy storage, hydrogen technologies, and fuel cells, helping to analyze interfaces, monitor degradation, and improve material performance.
In catalysis, advanced FTIR methods like operando and iso-potential DRIFTS are used to study reaction mechanisms in real time. FTIR also contributes to the design of materials for passive radiative cooling by enabling precise emissivity measurements. Its role in the development of renewable fuels and sustainable heat management solutions will also be highlighted.
Environmental applications include greenhouse gas monitoring, detection of micro- and nanoplastics using emerging techniques like NEMS-FTIR, and agricultural uses such as soil and crop analysis. FTIR is further applied in the optimization of solar panels and semiconductors, particularly for characterizing thin films and surface properties.
Together, these examples show how FTIR spectroscopy is helping to advance cleaner technologies, optimize performance, and support the transition to a more sustainable future.

Figure 1 – Applications of FTIR in GreenTech

Resonance Tuning of the Water-Trimethylamine Complex in Three Different Experimental Media

Casper Vindahl Jensen, Eaindra Lwin, Dhritabrata Pal, (…), Henrik G. Kjaergaard
Universitetsparken 5, 2100 KBH O, Denmark
CVJ@chem.ku.dk

☒ I am applying for the **Bruker Customer Excellence Award**

Hydrogen bound complexes have been shown to exhibit large spectroscopic changes with temperature. These include a widening and a blueshift of the OHb-stretching band with increased temperature. These effects can be accounted for by considering population of low-frequency intermolecular vibrations. Water-trimethylamine is one of the strongest bound hydrated bimolecular complexes. The room temperature spectrum shows rich complexity which can only be accounted for by considering resonance coupling between the OHb-stretch, the HOH-bend and intermolecular motion. By probing the water-trimethylamine complex with FTIR techniques in three different media (room temperature gas phase, He-jet expansion and Ar-matrix) we can fine-tune the transition frequency of the OHb-stretch and thereby its resonance coupling to other modes.

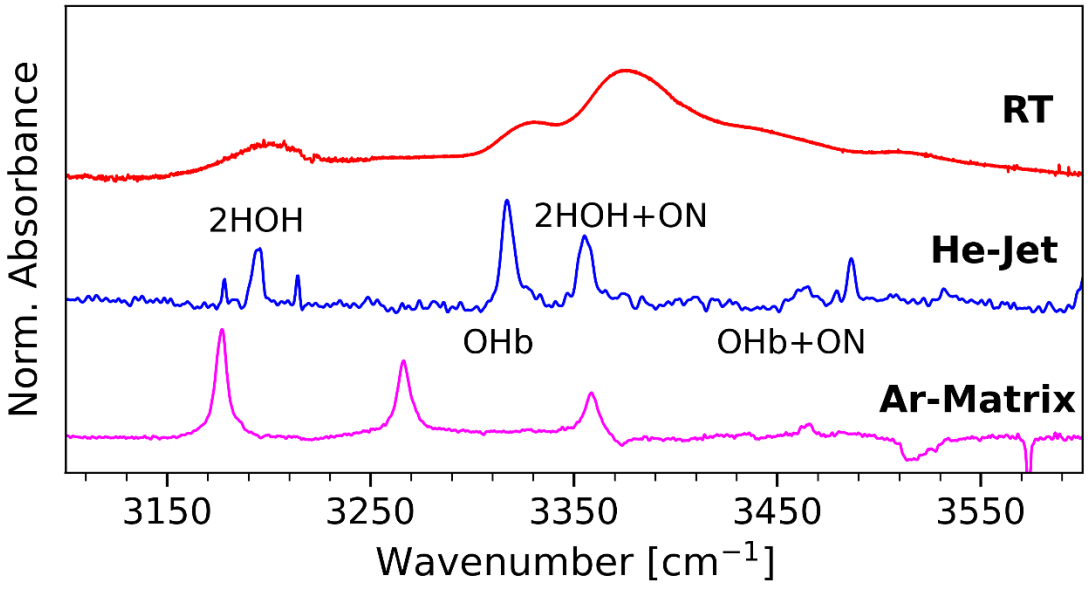


Figure 1 – Water-trimethylamine complex in three media. The bright OHb-stretch shares intensity to resonance partners based on coupling element and energetic proximity

References
1. T. Fischer, C. Jensen, et al., *Phys. Chem. Chem. Phys.*, (2025).
2. E. Vogt, C. Jensen, H. Kjaergaard, *J. Phys. Chem. A*, 128(2) (2024) 392.
3. A. Hansen, et al., *J. Phys. Chem. A*, 38(1) (2019) 115.

Acknowledgements: The authors thank the additional contributors in the project Taija Fischer and Martin Suhm and thank Emil Vogt for helpful discussions.

Raman and Nanomechanical Studies of Polymer Mats with Carbon Nano-additives

Aleksandra Wesełucha-Birczyńska[a], Maria Pajda[b], Anna Kołodziej[a], Małgorzata Świętek[c], Elżbieta Długoń[d], Marta Błażewicz[d]
[a]*Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, Kraków 30-387, Poland*
[b]*Technolutions, ul. Wiejska 7, Łowicz 99-400, Poland*
[c]*Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského Sq. 2, 162 06 Prague 6, Czech Republic*
[d]*Faculty of Materials Science and Ceramics, AGH-University of Science and Technology, Mickiewicza 30, Kraków 30-059, Poland*
birczyns@chemia.uj.edu.pl

Polymer nanocomposites formed as PCL/MWCNTs and PCL/MWCNTs-f, PCL/ESCNFs and PCL/ESCNFs-f, PCL/GO or PCL/rGO membranes were studied, containing the same amount of nanoadditive relative to the weight of the polymer in each material. Synthetic membranes are currently widely used in the areas of energy production and environmental protection, they are used in fuel cells and batteries [1].
Raman spectroscopy enabled the evaluation of the PCL matrix ordering, as a result of introducing different types of carbon nanoparticles. The parameters defining the degree of organization of carbon nanoparticles were estimated, which are the position of D- and G-bands and their half-width (FWHH), the intensity ratio D/G (R1 coefficient) and the integral intensity ratio D/(G + D) (R2 coefficient) [2]. The G' (2D) band present in the second-order region of the Raman spectrum was also analyzed, which can be correlated with the mechanical properties of the material [3].
In order to check the functionality of the tested polymer mats, their wear tests were carried out on a micro scale, in linear, reciprocating motion using a nanotribometer in order to calculate the static and dynamic friction coefficient. The surface topography of materials was estimated by the non-contact method of interferometric profilometry. The optical profilometer was used to illustrate the surface of the samples after the nanotribometer test. In this way, the abrasion paths and their surfaces were estimated and compared for the tested polymer mats.

References
1. H. Lin, Y. Ding, *J. Polym. Sci*., 58 (2020) 2433.
2. O. Beyssac, B. Goffe, J.-P. Petitet, E. Froigneux, M. Moreau, J.-.N. Rouzaud, *Spectrochim. Acta* A 59 (2003) 2267.
3. M Pajda, A. Wesełucha-Birczynska, A. Kołodziej, M. Swietek, E. Długon, M. Ziabka M. Błażewicz, *J. Mol. Struct*. 1264 (2022) 133305.

Acknowledgements: The study was carried out using research infrastructure funded by the European Union, Poland, in the framework of the Smart Growth Operational Programme, Measure 4.2; Grant No. POIR.04.02.00-00- D001/20, "ATOMIN 2.0 – Center for materials research on ATOMic scale for the INnovative economy". This study was supported by the subsidiary research part of Jagiellonian University Faculty of Chemistry, Krakow, Poland from the Ministry of Science and Higher Education, Poland.

Kinetics of Atmospheric Oxidation of Ammonia

Vili-Taneli Salo, Henrik G. Kjaergaard
H. C. Ørsted Institute, Department of Chemistry, Universitetsparken 5, 2100 Copenhagen, Denmark
vili@chem.ku.dk

The atmospheric oxidation of ammonia begins by a reaction with an OH radical, yielding an aminyl radical (NH_2). So far it has been thought that the NH_2 radical reacts further bimolecularly with the various atmospheric trace gases, such as NO_x and ozone, to yield N_2, N_2O, and NO as final products.[1] The reaction of NH_2 with the most prevalent atmospheric radical, molecular oxygen, has been deemed to be too slow to compete.[2] This is in contrast with carbon- and sulfur-centered radicals, which predominantly add molecular oxygen to give the corresponding peroxyl radicals, whose central role in various atmospheric reaction pathways is well-known.

In this work,[3] we looked into the apparent lack of aminoperoxyl radical (NH_2O_2) formation in the reaction between NH_2 and O_2 (Figure 1) by using state-of-the-art computational methods, such as multireference electronic structure methods, variational transition state theory, and master equation simulations for obtaining pressure and temperature dependent reaction rate coefficients. We found that the reaction actually occurs, and fast. In atmospheric reaction conditions it is by far the predominant reaction of NH_2, but the reason NH_2O_2 has eluded direct observations is that it is very unstable with respect to dissociating back to reactants. Both the formation and the dissociation reactions of NH_2O_2 are so fast that an equilibrium is established before other bimolecular reactions, which would consume either the NH_2 or the NH_2O_2, start to occur. We modelled this equilibrium in various conditions and found out that NH_2O_2 formation is favoured under cold temperatures and high O_2 concentrations. The NH_2O_2 reaches appreciable equilibrium fractions in various atmospherically relevant conditions, suggesting that its currently overlooked further chemistry should be investigated more thoroughly.

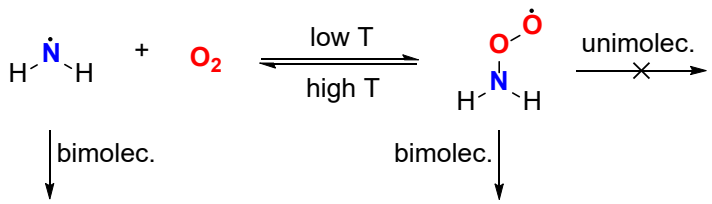


Figure 1 – The temperature-dependent equilibrium between NH_2 and NH_2O_2 radicals determines the fate of NH_3 oxidation

References
1. S.J. Pai, C.L. Heald, J.G. Murphy, *ACS Earth Space Chem.,* 5 (2021) 1674.
2. R. Atkinson, et al., *Atmos. Chem. Phys.,* 6 (2006) 3625.
3. V.-T. Salo, J. Chen, H.G. Kjaergaard, *Manuscript in review.*

Dimethyl Ether-Water Hydrogen Bond Complex: Room Temperature Gas-Phase Detection and Determination of Formation Gibbs Energy

Dhritabrata Pal[a], Alexander Kjaersgaard[a], Emil Vogt[a,b], Tine Elmelund Skovbo[a], Henrik G. Kjaergaard[a]

[a]*Department of Chemistry, University of Copenhagen, DK-2100 Copenhagen, Denmark*
[b]*Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany*
dp@chem.ku.dk

☒ I am applying for the **Bruker Customer Excellence Award**

Hydrated complexes are of general interest for understanding atmospheric nucleation processes, where water is abundant; however, the extent to which water enhances or inhibits nucleation remains uncertain. Water dimer, $(H_2O)_2$, is one of the most studied bimolecular complexes[1], and it is of profound importance in the atmospheric chemistry. The formation constant of water dimer has been the subject of several elaborate experimental and theoretical studies, and the room temperature equilibrium constant is estimated to be in the range of about 0.04−0.06 [2−6]. The complex of H_2O and dimethyl ether (CH_3OCH_3, DME), $H_2O{\cdot}$DME, is similar to water dimer, although significantly easier to detect experimentally, due to the high vapor pressure of DME. We have recorded the Fourier transform infrared absorption spectrum of the water-dimethyl ether bimolecular complex in the gas phase at room temperature and in the cold matrix isolation condition. All the IR spectra were recorded using VERTEX 70 FTIR spectrometer from Bruker. Four distinct bands are observed and assigned. The equilibrium constant of complex formation is determined from the experimental integrated absorbance of the bands and the corresponding calculated intensities. The calculated band intensities are obtained with a 9D reduced-dimensional variational local mode model with the CCSD(T)-F12a/cc-pVDZ-F12 potential energy and dipole moment surfaces. A similar equilibrium constant for a majority of the observed bands is obtained, with an average value of 0.042 ± 0.003 at T = 298 K. The water-dimethyl ether complex studied here is similar to the water dimer, and our determined equilibrium constant may serve as a reasonable estimate for that of water dimer, which is especially relevant in the atmospheric chemistry.

References

1. E. Vogt, H. G. Kjaergaard, *Annu. Rev. Phys. Chem.*, 73 (2022) 209.
2. Y. Scribano, N. Goldman, R. Saykally, C. Leforestier, *J. Phys. Chem. A,* 110 (2006) 5411.
3. C. Leforestier, *J. Chem. Phys*., 140 (2014) 074106.
4. L. Curtiss, D. Frurip, M. Blander, *J. Chem. Phys.*, 71 (1979) 2703.
5. B. Ruscic, *J. Phys. Chem. A*, 117 (2013) 11940.
6. I. V. Ptashnik, K. M. Smith, K. P. Shine, D. Newnham, *Q. J. R. Meteor. Soc.*, 130 (2004) 2391.

Acknowledgements: The authors thank the Novo Nordisk Foundation, grant numbers NNF22OC0080193 for financial support and the High Performance Computer Centre at the University of Copenhagen for computer time.

The Inhibitory Effects of Genistein and Resveratrol on Voltage-Gated Potassium Channels in Cancer Cells – Putative Role in Anti-Cancer Activity

A. Teisseyre, A. Uryga, K. Środa-Pomianek, A. Palko-Łabuz
Department of Biophysics and Neurobiologuy, Wrocław Medical University, ul. Chałubińskiego 3, 50-368 Wrocław, Poland
andrzej.teisseyre@umw.edu.pl

Genistein and resveratrol are plant-derived compounds, which share numerous biological activities including various anti-cancer actions. The compounds are also known as modulators of many types of potassium channels. Our previous studies have shown that both compounds are effective inhibitors of voltage-gated potassium channels Kv1.3 in human T lymphocytes [1].

Kv1.3 channels are encoded by the KCNA3 gene. The channels are widely present among tissues, both normal and cancer [1]. The channels' activity plays a significant role in a regulation of proliferation and apoptosis of Kv1.3 channel-expressing cells [1]. Inhibitors of the channels may putatively find clinical application in therapy of various diseases, including some cancer disorders characterized by an over expression of Kv1.3 channel, such as melanoma, pancreatic ductal adenocarcinoma (PDAC), multiple myeloma and B-type chronic lymphocytic leukaemia (B-CLL) [1].

It is known that some lipophilic small-molecule organic inhibitors of Kv1.3 channels may exert anti-proliferative and pro-apoptotic activity on Kv1.3 channel-expressing cancer cells, selectively eliminating them while sparing the normal ones [1].

To the group of lipophilic small-molecule organic inhibitors of Kv1.3 channels in cancer cells belong also some compounds from the groups of flavonoids, chalcones and statins [1,2]. The inhibitory effect on the channels may significantly be augmented upon a co-application of the flavonoids and chalcones with the statins: simvastatin and mevastatin [3]. The augmented inhibitory effect on the channels may be co-related with an improved pro-apoptotic activity of these compounds, applied in a combination, on Kv1.3 channel-expressing cancer cells Jurkat T [3,4].

This study reports an inhibitory effect of genistein and resveratrol on Kv1.3 channels in cancer cells – human leukemic Jurkat T cell line. Obtained data provide evidence that an application of both compounds at micromolar concentrations caused a dose-dependent inhibition of the channels. The inhibitory effect of the compounds on the channels was reversible. The inhibitory effect of both compounds was significantly augmented upon a co-application with the statins: mevastatin and simvastatin. The inhibition of Kv1.3 channels may be involved in anti-cancer activities of these compounds on Kv1.3 channel- expressing cancer cells, especially upon a co-application with the statins [3,4].

References
1. A. Teisseyre, A. Palko-Łabuz, K. Środa-Pomianek, K. Michalak, *Front. Oncol.*, 9 (2019) 933.
2. A. Teisseyre, A. Uryga, K. Michalak. *J. Mol. Struc.*, 1230 (2021) 129905.
3. A. Teisseyre, M. Chmielarz, A. Uryga, K. Środa-Pomianek, A. Palko-Łabuz. *Molecules* 27 (2022) 3227.
4. A. Teisseyre, K. Środa-Pomianek, A. Palko-Łabuz. *J. Mol. Struc.*, 1307 (2024) 137967.

Acknowledgements: This study was supported Polish Ministry of Research and University Education funds for Wrocław Medical University.

Hydrogen-Atom-Assisted Thione–Thiol Tautomerization of Thiourea Derivatives in *para*-H_2 Matrix

Sándor Góbi[a], Barbara Keresztes[a,b], Anita Schneiker[a,b], György Tarczay[a,c]
[a]*Laboratory of Molecular Spectroscopy, Institute of Chemistry, ELTE, H-1518 Budapest, Hungary*
[b]*Hevesy György PhD School of Chemistry, Institute of Chemistry, ELTE, H-1518 Budapest, Hungary*
[c]*Centre for Astrophysics and Space Science, ELTE, H-1518 Budapest, Hungary*
sandor.gobi@ttk.elte.hu

In the past several years, a lot of experimental and theoretical effort has been dedicated to the investigation of thioureas and related thioamides in low-temperature conditions. In these experiments, the samples are examined in (amorphous) ice phase as well as in cryogenic matrices, and are exposed to numerous different radiation sources (laser UV, Lyman-α, H atoms, energetic electrons).[1–5] The experiments are conducted using the state-of-the-art VIZSLA (Versatile Ice Zig-Zag Sublimation Setup for Laboratory Astrochemistry) setup.[6]

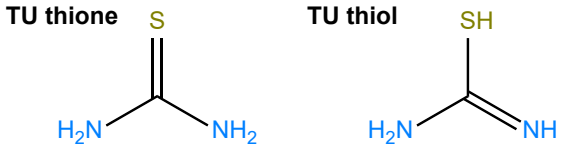


Figure 1 – TU thione (left) and thiol (right) tautomers

The present study focuses on the thione–thiol tautomerization of thiourea (TU) and its *N*-methylated derivative, *N*-methyl thiourea (NMTU).[7] The measurements were carried out in the exotic *para*-H_2 matrix at 3.2 K, in which H atoms can be conveniently and efficiently generated. When exposed to H atoms in this unique environment, the more stable thione tautomeric forms (which are exclusively found in the matrix after deposition) are shown to undergo tautomerization and the presence of thiols can be undoubtedly proven. Based on this and earlier results, the tautomerization of tioamides in the presence of H atoms takes place in a facile way, without any external energy sources (*e.g.*, UV irradiation), which process is ubiquitous and independent on the media (cryogenic matrix or amorphous ice).

References

1. S. Góbi, I. Reva, G. Tarczay, R. Fausto, *J. Mol. Struct.*, 1220 (2020) 128719.
2. S. Góbi, B. Keresztes, A. Schneiker, G. Ragupathy, G. Tarczay, *J. Chem. Phys.*, 160 (2024) 024310.
3. S. Góbi, B. Keresztes, A. Schneiker, G. Tarczay, *Phys. Chem. Chem. Phys.*, 26 (2024) 9963.
4. S. Góbi, B. Keresztes, A. Schneiker, G. Tarczay, *Phys. Chem. Chem. Phys.*, 26 (2024) 21589.
5. S. Góbi, I. Reva, G. Ragupathy, R. Fausto, G. Tarczay, *J. Phys. Chem. C*, 128 (2024) 21691.
6. G. Bazsó, I. P. Csonka, S. Góbi, G. Tarczay, *Rev. Sci. Instrum.*, 92 (2021) 124104.
7. S. Góbi, B. Keresztes, A. Schneiker, G. Tarczay, *J. Chem. Phys.*, 162 (2025) 174306.

Acknowledgements: The Hungarian Scientific Research Fund (No. OTKA K143196) and the Thematic Excellence Program of the Eötvös Loránd University (No. TKP2021-NKTA-64), both from the fund of the National Research, Development and Innovation Office (NKFIH), are acknowledged. S. G. was supported by the "Bolyai" scholarship of the Hungarian Academy of Sciences (MTA) B. K. was also supported by the "DKÖP-23 Doctoral Excellence Program" of the Ministry for Culture and Innovation (KIM) from the source of NKFIH. A. S. was also supported by the "EKÖP-24 University Excellence Scholarship Program" of KIM from the source of NKFIH.

Using ASCA to Study Sampling in Spectroscopy

Tomasz Pawel Czaja[a], Klavs Martin Sørensen[b], Morten Arendt Rasmussen[a], Søren Balling Engelsen[a]
[a] *Department of Food Science, University of Copenhagen, 1958 Frederiksberg C, Denmark*
[b]*FOSS Analytical A/S, Nils Foss Allé 1, 3400 Hillerød, Denmark*
tomasz.czaja@food.ku.dk

As the demand for sustainable agriculture and green technologies grows, non-destructive and rapid analytical methods like Near Infrared Spectroscopy (NIRS) are becoming essential tools in plant phenotyping and precision breeding. However, their performance is often challenged by sampling variability—particularly when working with transmission spectroscopy of heterogeneous food samples such as single seeds, where orientation, thickness and internal structure can significantly influence the measured spectra [1].
To systematically investigate these sources of variation, ANOVA Simultaneous Component Analysis (ASCA)—a method that combines analysis of variance with multivariate decomposition—can be applied to partition and quantify the effects of experimental factors on spectral data in a design of experiment [2].
This study analyzes 2184 short-wavelength Near Infrared (SW-NIR) transmission spectra collected from individual wheat kernels. The experimental design includes 7 kernels from 13 wheat varieties, measured in 2x4 orientations (germ up/down, furrow up/down/left/right), with three replicate measurements per orientation. Protein content was determined for each kernel as a chemical reference posterior spectral measurements. The results show that ASCA can clearly separate the contributions of kernel orientation, variety, and individual differences to spectral variance, providing a detailed understanding of sampling effects. This insight is key to improving the accuracy and robustness of high-throughput sorting systems for grain quality traits, particularly protein content, and supports the development of environmentally friendly agricultural technologies.

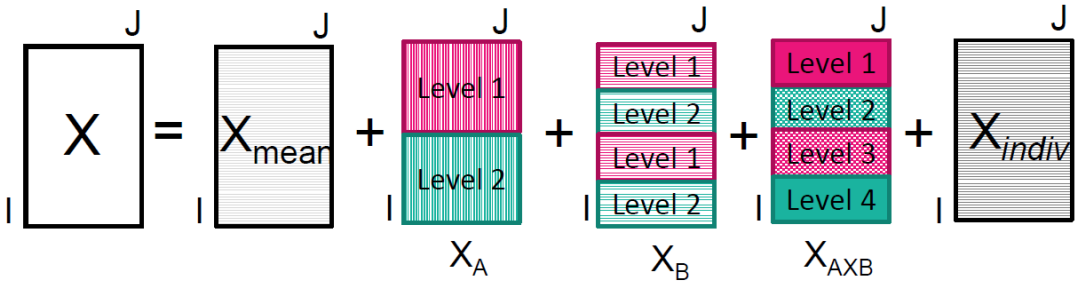


Figure 1 – Schematic overview of the ASCA approach

References

1. T.P. Czaja, S.B. Engelsen, *Spectrochim. Acta A*, 303 (2024) 125028.
2. A.K. Smilde, J.J. Jansen, H.C.J. Hoefsloot, R.-J.A.N. Lamers, J. van der Greef, M.E. Timmerman, *Bioinformatics*, 21 (2005) 3043.

Metal Oxides and Metal Oxides/Metal Nanostructures for Surface-Enhanced Raman Scattering (SERS) Spectroscopy

Eva Kočišová, David Novák, Šimon Kapusta, Marek Procházka, Ondřej Kylián
Charles University, Faculty of Mathematics and Physics, Institute of Physics, 121 16 Prague 2, Czech Republic; Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, 180 00 Prague 8, Czech Republic
eva.kocisova@matfyz.cuni.cz

While metal oxides alone represent non-plasmonic substrates suitable for SERS spectroscopy, providing good spectral sensitivity and reproducibility, stability and photoactivity [1], their performance may be further enhanced when combined with metals. In this contribution, we focused on metal oxides (V_2O_5 and Nb_2O_5) in combination with noble metals (Ag or Au) prepared by plasma-assisted techniques. Methylene blue (MB) was chosen as a SERS probe. The V_2O_5/metal substrate proved to be the best for SERS performance, demonstrating the synergy of the chemical (charge-transfer) and electromagnetic SERS mechanisms. The maximum enhancement (1200×) of the SERS signal was achieved for V_2O_5 films decorated with a metal (Figure 1), while considerably lower enhancement was observed for metal-decorated V_2O_5 nanoparticles [2]. We obtained remarkable spectral reproducibility with an RSD of the SERS signal of 10%. For Nb_2O_5/metal, we observed the efficient cleaning of the substrates using UV radiation and their possible reusability [3].

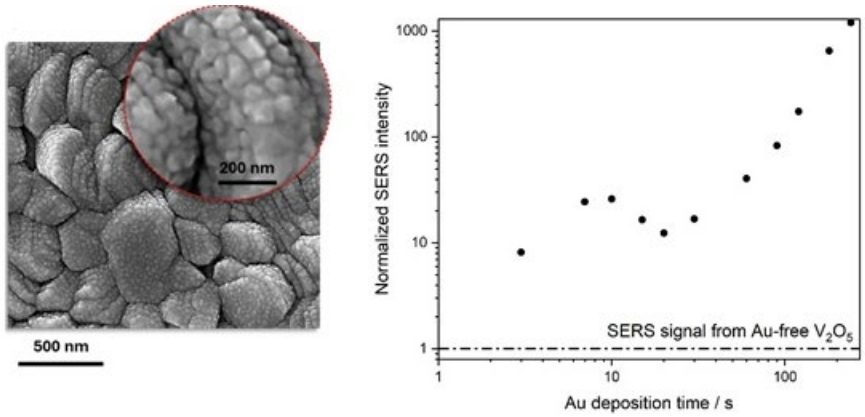


Figure 1 – Left: SEM image of thin V_2O_5 decorated with Au for 240 s Au deposition time. Right: Normalized SERS intensity of 6.7×10^{-6} M MB on smooth V_2O_5/Au substrate *versus* Au deposition time

References
1. E. Kočišová, O. Kylián, M. Procházka, in *Surface- and Tip-enhanced Raman scattering spectroscopy - Bringing theory and applications,* (M. Procházka et al. eds.), Springer, 2024, p. 219-247.
2. M. Procházka, D. Novák, E. Kočišová, O. Kylián, W. Ji, Y. Ozaki, *J. Phys. Chem. C*, 128 (2024) 11732.
3. M. Pavlovič, N. Khomiakova, E. Kočišová, M. Procházka, O. Kylián, *Mat. Lett.,* 388 (2025) 138308.

Acknowledgements: The authors thank the Czech Science Foundation (grant No. 25-14402L) for financial support.

Photodetachment of Cooled Deprotonated Chlorophyll Pigments in the Gas Phase

Ali Muhieddine, Benoît Soep, Satchin Soorkia, Michel Broquier, Niloufar Shafizadeh
Institut des sciences moléculaires d'Orsay, UMR 8214, France, 91400
alimuhydine@gmail.com

☒ I am applying for **Bruker Customer Excellence Award**

For a better understanding of the photosynthesis mechanism, it is important to precisely determine the vibrational and vibronic structure of various chlorophyll pigments in the gas phase. To achieve this, we perform electron photodetachment spectroscopy on cooled anions. The properties of these anions are characterized by measuring the kinetic energy of the ejected electrons after photoexcitation. We have built a new experimental setup Figure 1, coupling a nonoelectrospray, a cooled ion trap with a photoelectron detection.

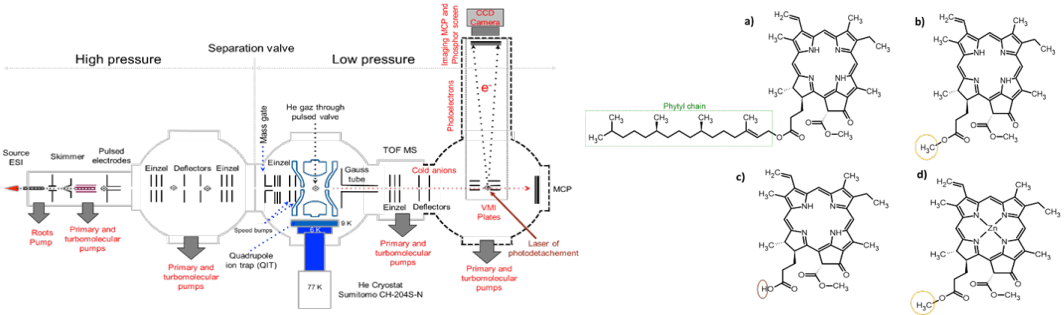


Figure 1–At the left experimental setup. At the right structures of a) pheophytin b) methylpheophorbide c) pheophorbide d) zinc methylpheophorbide

The first step of this work is to determine the most stable deprotonation sites of several chlorophyll pigments in gas phase by determining the photodetachment threshold. In this talk, I will show our first results on different pigments: pheophytin, zinc methyl pheophorbide, pheophorbide, and methylpheophorbide (Figure 1, right). These latter two molecules are identical to a pheophytin where the phytyl chain $C_{20}H_{39}$ has been replaced by a hydrogen atom or a methyl group, respectively. These comparisons allowed us to correlate the values of the photodetachment threshold energies with the deprotonation sites of the molecule. In this aim, we have succeeded in recording the action spectra of the first two allowed electronic states of deprotonated pheophorbide, methyl pheophorbide and zinc methyl pheophorbide (transitions Qx and Qy). The action spectra were obtained by monitoring, as function of wavelength, the intensity of photoelectrons resulting from the absorption of two photons. The Q_x and Q_γ transitions were accessed by the first absorbed photon. Our high-resolution measurements revealed several identical vibrational modes across the different species. The assignment of these vibrational modes is based on comparison with unique fluorescence excitation spectra obtained by Rebane[1] in matrix-isolated experiments at low temperature.

References

1. R. Avarmaa, K. Rebane, *Spectrochim. Acta A,* 41 (1985) 1365.

Physicochemical Properties and Phase Transition Mechanisms of Lead Halides Comprising Small Organic Cations in the Structure: Novel Perovskites with Tunable Optoelectronic Properties

Szymon Smółka, Mirosław Mączka, Maciej Ptak
Institute of Low Temperature and Structure Research Polish Academy of Sciences, Wrocław, Poland
s.smolka@intibs.pl

Hybrid lead halide perovskites incorporating small organic cations exhibit diverse structural architectures and dimensionalities, which enable broad tunability of their optoelectronic properties[1,2]. We investigated five hybrid lead halide perovskites incorporating imidazolium cations, comprising three bromide-based compounds and two chloride analogues, differing in halide type, stoichiometry, and structural dimensionality. These variations result in distinct inorganic frameworks ranging from 1D to 3D architectures, enabling a systematic exploration of structure–property relationships in this class of materials.

By examining these systems, we addressed how temperature, pressure, and chemical composition influence phase behavior and optoelectronic responses in hybrid lead halide perovskites with imidazolium cations. Through temperature- and pressure-dependent Raman and infrared spectroscopy, supported by X-ray diffraction measurements, we revealed that octahedral distortions — induced by external or internal factors — play a central role in structural phase transitions, which significantly modulate properties such as band gap, dielectric response, and emission characteristics. The coupling between organic cation dynamics and the inorganic framework plays a central role in these phenomena.

In systems incorporating disk-shaped cations such as imidazolium, phase transitions are often associated with a gradual reduction in orientational freedom and the formation of hydrogen bonds, which induce octahedral distortions that alter the symmetry and electronic structure. Our findings highlight the importance of lattice dynamics and cation ordering in shaping structure–property relationships in hybrid perovskites, with implications for the development of tunable optoelectronic materials.

References

1. S. Smółka, M. Mączka, D. Drozdowski, D. Stefańska, A. Gągor, A. Sieradzki, J. K. Zaręba, M. Ptak, *Inorg. Chem.*, 61 (2022) 15225.
2. X. Li, J. M. Hoffman, M. G. Kanatzidis, *Chem. Rev.*, 121 (2021) 2230.

Absorption Cross-Section of Gas-Phase Isoprene in the Entire JWST Region

Vera Staun Hansen, Casper Vindahl Jensen, Sofie Markussen, Anisha Iyer, Henrik G. Kjaergaard
Department of Chemistry, University of Copenhagen, Universitetsparken 5, Copenhagen Ø, DK-2100, Denmark
vsh@chem.ku.dk

☒ I am applying for **Bruker Customer Excellence Award**

We have recorded the gas phase absorption spectrum of isoprene at room temperature from the mid-infrared range and into the visible range (600 cm^{-1} to 17050 cm^{-1}) using Fourier transform infrared, conventional dispersion ultraviolet-visible-near-infrared, and cavity ring-down spectroscopy with a resolution comparable to that of the instruments on the James Webb Space Telescope.[1]

We have assigned the CH-stretching fundamental and overtone bands corresponding to the Δv_{CH} = 1-6 transitions based on anharmonic vibrational calculations using normal mode and local mode models, for the lower- and higher-energy regions, respectively. We have determined accurate absolute intensities of the observed CH-stretching regions and compare with existing experimental values [2,3] and with theoretical results. Our spectrum can facilitate the detection and possibly quantification of isoprene in planetary atmospheres.

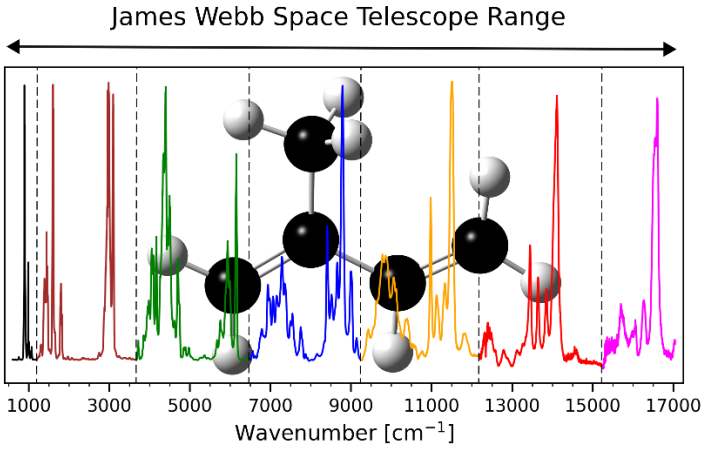


Figure 1 – Spectrum of isoprene recorded in the entire JWST region. Each section of the spectrum is scaled with a scaling factor increasing about one order of magnitude for each section

References

1. C.V. Jensen, V.S. Hansen, S. Markussen, A. Iyer, H.G. Kjaergaard, *Spectrochim.. Acta. A Mol. Biomol. Spectrosc.,* 330 (2025), 125667
2. C.S. Brauer, T.A. Blake, A.B. Guenther, S.W. Sharpe, R.L. Sams, T.J. Johnson, *Atmos. Meas. Tec*h. 7 (2014) 3839.
3. I. Gordon, L. Rothman, R. Hargreaves, R. Hashemi, E. Karlovets, F. Skinner,E. Conway, C. Hill, R. Kochanov, Y. Tan, et al., *J. Quant. Spectrosc. Radiat. Transfer* 277 (2022) 107949.

Generation and Consideration of Trioxyl Radical

Andras Sun Poulsen
Universitetsparken 5, 2100 KBH O, Denmark
ansp@chem.ku.dk

☒ I am applying for **Bruker Customer Excellence Award**

The microwave discharge products of water in an argon matrix have been investigated, showing a wide range of products assigned to radicals and radical-water complexes. The assigned peaks for the hydroxyl, hydroperoxyl, and hydrotrioxyl radicals are in good agreement with the literature [1,2]. The concentrations of these radicals are investigated further. Here it is shown that the concentration of the hydrotrioxyl radical is growing upon annealing, whereas the concentration of the hydroxyl and hydroperoxyl are decreasing.

References

1. T. Svensson, B. Nelander, G. Karlström, *Chem. Phys.,* 265.3 (2001) 323.
2. B. Nelander, A. Engdahl, T. Svensson, *Chem. Phys. Lett.,* 332.3 (2000) 403.

Porphyrin-acene Dyads for Controlled Singlet Oxygen Generation and Depletion

Natalia Dutkiewicz[a], Maciej Majdecki[b], Barbara Golec[c], Ireneusz Wielgus[d], Przemysław Gaweł[b], Aleksander Gorski[a]
[a]*Institute of Physical Chemistry, Polish Academy of Sciences, 01-224 Warsaw, Poland*
[b]*Institute of Organic Chemistry, Polish Academy of Sciences, 01-224 Warsaw, Poland*
[c]*Faculty of Mathematics and Science, Cardinal Stefan Wyszyński University, 01-815 Warsaw, Poland*
[d]*Faculty of Chemistry, Warsaw University of Technology, 00-662 Warsaw, Poland*
ndutkiewicz@ichf.edu.pl

Molecular oxygen is the principal quencher of the triplet states of organic compounds in solution, directly influencing photoreaction yields. The quenching process predominantly leads to the formation of singlet oxygen ($^1O_2$). Due to its high reactivity, singlet oxygen plays a crucial role in numerous biomedical and catalytic processes.[1,2] Controlled generation and release of $^1O_2$ improves reaction efficiency and selectivity, contributing to more sustainable and cost-effective chemical processes.
An innovative approach to $^1O_2$ managing involves the use of bichromophoric compounds (Figure 1). These BCs are designed to generate $^1O_2$ at room temperature, store it for extended periods at lower temperatures, and release it upon warming within the biologically relevant temperature range. This unique capability positions BCs as promising candidates for applications in anticancer therapy, photocatalysis, and the development of energy upconversion materials.

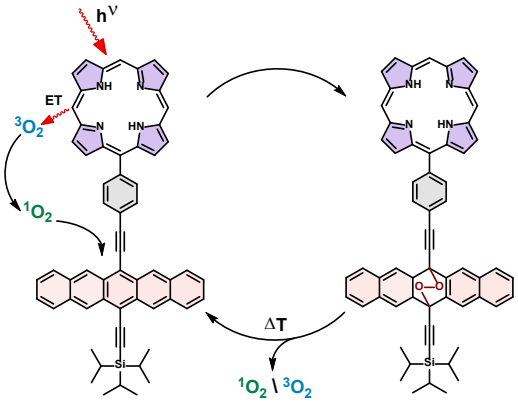


Figure 2 – Molecular design and working principle of porphyrin-acene dyads for $^1O_2$ storage and release

References
1. N. Singh, R. Sen Gupta, S. Bose, *Nanoscale*, 6 (2024) 3243.
2. A. A. Ghogare, A. Greer, *Chem Rev*, 116 (2016) 9994.

Acknowledgements: This work was supported by the Polish National Science Center grants no SONATA 2020/39/D/ST4/00560 and OPUS 2020/39/B/ST4/01956.

Dielectric Spectroscopy in Breast Cancer Imaging

Kazimierz Orzechowski[a,b], Marek Rząca[b,c], Stanisław Baj[b]
[a]*Faculty ocf Chemistry, University of Wroclaw, Joliot-Cureie Str. 50-383 Wroclaw, Poland*
[b]*Onco Scanner Ltd, Kasztanowa 3a Str, 53-125 Wroclaw, Poland*
[c]*Specialistic Regional Hospital, Kamieńskiego 100 Str,*
kazimierz.orzechowski@uwr.edu.pl

The application of X-ray or ultrasonic wave absorption and dispersion, nuclear magnetic resonance (NMR), and positron annihilation spectroscopy are well-established methods for breast cancer imaging. These techniques are considered the gold standard in cancer diagnosis at every stage of the disease.
Electromagnetic wave-based methods also offer effective and precise tools for this purpose. Infrared (IR) and Raman spectroscopy, which utilize short-wavelength electromagnetic radiation (2.5–25 μm), provide valuable molecular-level information. Alternatively, dielectric spectroscopy, which uses much longer wavelengths (ranging from 300 m to 3 mm), presents a promising approach for cancer imaging.
In this talk, I will present a method designed to verify the absence of cancerous tissue at surgical margins during breast cancer surgery — commonly referred to as the "clean margins" issue. The technique involves measuring the dielectric properties of breast tissue removed from the operative site. Significant differences between cancerous and normal breast tissue have been recognized since the 1930s. However, only recently have we resolved the challenges associated with conducting dielectric measurements in the long-wavelength (LW) range in the presence of highly conductive biological fluids such as blood and lymph. I will present both the physical principles and clinical results supporting this method.
An intraoperative breast cancer detection probe has been developed and patented, and a startup company, **Onco Scanner Ltd**, has been established to bring this innovation to clinical practice.

References
1. K. Orzechowski, M. Rudowski and M. Rząca, *Physiol. Meas.* 29 (2008) S321.
2. M. Rząca, K. Orzechowski, A. Wolny, M. Sitarska, *NOWOTWORY Journal of Oncology,* 67 (2017) 108.
3. A. Wolny, K. Orzechowski, M. Rudowski, *Results in Physics,* 6 (2016) 288.

Photostability: Proper Determination and Control

Barbara Golec[a,b], Aleksander Gorski[a], Idaresit Mbakara[a], Agnieszka Gajewska[a], Arkadiusz Listkowski[a,b], Jacek Waluk[a]

[a]*Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, Warsaw, Poland*
[b]*Faculty of Mathematics and Science, Cardinal Stefan Wyszyński University, Dewajtis 5, 01-815 Warsaw, Poland*
jwaluk@ichf.edu.pl

Photostability, a parameter expressing the number of photons a molecule can absorb before it photobleaches, is arguably the most important factor to consider in applications based on light-matter interactions.

Photodegradation quantum yield is determined as N_{pr}/N_{abs}, where N_{pr} is the number of product molecules formed upon irradiation and N_{abs} is the number of photons absorbed in the photoreaction. This simple formula is somewhat deceiving, since the correct determination of the above ratio is experimentally challenging and prone to errors.

In this talk, results of photostability measurements will be discussed for various experimental regimes, including molecular ensembles[1-5] and single molecules[6,7] in different environments. It will be shown how stability can be altered and controlled by appropriate substitution, suitable choice of solvent, formation of hydrogen bond, presence of triplet quenchers, or varying the amount of oxygen in the sample. Some pitfalls in the determination of photostability will also be pointed out. Finally, the validity of the assumption, usually taken for granted, that, for a given sample, photodegradation quantum yield remains constant during the experiment will be critically analysed.

References

1. B. Golec, K. Nawara, A. Gorski, J. Waluk, *Photochem. Photobiol. Sci*., 22 (2023) 2725.
2. B. Golec, A. Gorski, R.P. Thummel, M. Sierakowski, J. Waluk, *Photochem. Photobiol. Sci*., 22 (2022) 333.
3. B. Golec, M. Kijak, V. Vetokhina, A. Gorski, R.P. Thummel, J. Herbich, J. Waluk, *J. Phys. Chem. B*, 119 (2015) 7283.
4. J. Ostapko, A. Gorski, J. Buczyńska, B. Golec, K. Nawara, A. Kharchenko, A. Listkowski, M. Ceborska, M. Pietrzak, J. Waluk, *Chem. Eur. J.*, 26 (2020) 16666.
5. M. Banaszek, B.Golec, R. Rybakiewicz-Sekita, J. Kowalski, P. Szczodry, N. Dutkiewicz, J. Waluk, A. Gorski, *J. Phys. Chem. B* (2025), https://doi.org/10.1021/acs.jpcb.5c02423.
6. H. Piwoński, A. Sokołowski, J. Waluk, *J. Phys. Chem. Lett.*, 6 (2015) 2477.
7. A. Bednarz, I. Kamińska, A. Jamrozik, K. Zielonka, A. Listkowski, J. Waluk, *Methods Appl. Fluoresc.*, 9 (2021) 035004.

Acknowledgements: This work was supported by the Polish National Science Center grant no. 2019/35/B/ST4/00297.

Mechanism of Phase Transition in Layered 2-Fluoroethylammonium Cadmium Chlorobromide

Maciej Ptak[a], Dorota Kowalska[a], Szymon Smółka[a], Mariusz Stefański[a], Julia Osmólska[a,b], Damian Szymański[a], Adam Sieradzki[c]
[a]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 5-422 Wrocław, Poland*
[b]*Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom*
[c]*Department of Experimental Physics, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*
M.Ptak@intibs.pl

The hybrid cadmium halides intercalated by ammonium cations form a group of multifunctional organic-inorganic hybrids. Because of the variety of structural motifs and dimensionality of the inorganic subnetwork, compounds of this class can form a wide range of crystal structures.
In this research, the structural, thermal, optical, and phonon properties of 2D hybrid crystals based on 2 fluoroethylammonium (FEA^+) cations were studied: the previously described $(FEA)_2CdCl_4$ [1] and the newly synthesized mixed-halide analogue $(FEA)_2Cd[Br_{2/3}Cl_{1/3}]_4$ [2]. The substituted compound exhibits a first-order phase transition at about 270 K from an ordered monoclinic $P2_1/c$ structure to a disordered orthorhombic *Cmce* phase. The mechanism of this transformation, exhibiting unusually high change in entropy, involves also displacements within the inorganic layers (see Figure 1).
Partial substitution of Cl^- by Br^- ions and the presence of highly polar C–F bonds cause changes in cation mobility and occurring phase transition. Understanding molecular dynamics allows defining the correlation between the fine-tuning of the properties of hybrid materials through structural modifications.

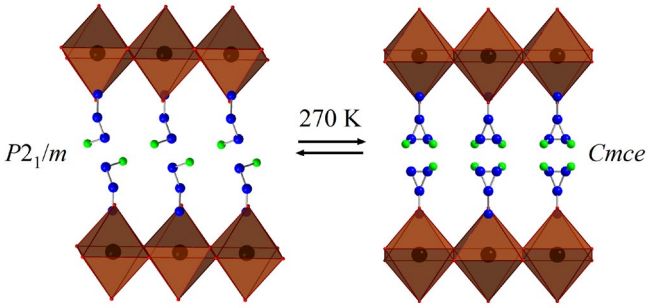


Figure 1 – Comparison of the ordered low-temperature phase $P2_1/c$ with the disordered high-temperature phase *Cmce*.

References
1. N. Song, S.-P. Chen, X.-W. Fan, Y.-H. Tan, W.-J. Wei, Y.Z. Tang, *ACS Omega*, 5 (2020) 6773.
2. M. Ptak, D. A. Kowalska, S. Smółka, M. Stefański, J. Osmólska, D. Szymański, A. Sieradzki, *in preparation*.

Acknowledgements: This research was funded in whole by the National Science Centre (Poland), project no. 2021/41/B/ST5/01684.

Molecular Dynamics and Interactions in Aqueous Solutions of Skin Care Ingredients

Iwona Płowaś-Korus[a], Mikołaj Wichrowski[b]
[a]*Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznan, Poland*
[b]*Faculty of Mechanical Engineering, Poznan University of Technology, Piotrowo 3, 60-965 Poznan, Poland*
iwplowas@ifmpan.poznan.pl

The cosmetics industry has been experiencing rapid growth, particularly in certain segments like natural and organic beauty, colour cosmetics as well as in clean and self-care beauty.
In cosmetics formulations, hydrogen bonds play a crucial role in ingredients interactions, most notably for humectants and other moisture-related ingredients. They help retain moisture by attracting water molecules to the skin. The most commonly used humectants in skincare are glycerine, hyaluronic acid, urea, and sugar alcohols.
On the other hand, there are many other cosmetics ingredients capable of forming hydrogen bonds, which belong to base ingredients. They are crucial for creating the desired texture, consistency, and stability of the product. For example, polyglyceryl-4-caprate, a non-ionic surfactant, is known for its emulsifying and skin-conditioning properties. Other popular non-ionic surfactant is Polysorbate-20, which is used as an emulsifier, stabilizer, and dispersing agent in cosmetics manufacturing.
The purpose of our studies is to obtain complete information on dynamics and intermolecular interactions in aqueous solutions of various type of skin care ingredients like polyglyceryl-4-caprate and Polysorbate-20 able to form hydrogen bonds and compare the results with our previous studies of sugar alcohols + water mixtures.[1,2] In order to maintain this, we have carried out measurements of the mixtures by using the broadband dielectric spectroscopy in the frequency range of 10 MHz to 50 GHz at 25 °C. Dielectric relaxation spectroscopy is a powerful tool for the investigation of liquid-state dynamics as it is especially sensitive to the cooperative motions in hydrogen-bonded systems. Goal of our investigations is to find out how the structure of the solutes affect their hydration and cooperative solution dynamics.

References

1. I. Płowaś-Korus, R. Buchner, *Phys. Chem. Chem. Phys.*, 21 (2019) 24061.
2. I. Płowaś-Korus, P. Korus, R. Buchner, *J. Phys. Chem. B* 129 (2025) 712−718.

Acknowledgements: The authors thank prof. Richard Buchner from the University of Regensburg for his support and mentorship, and also thank the Deutsche Forschungsgemeinschafthanks and the University of Regensburg for allowing the donation of prof. Richard Buchner's reflectometer setup to Iwona Płowaś-Korus upon his retirement.

The Universal Vibrational Dynamics of Water Bound to Tertiary Amines: More Than Just Fermi Resonance

Eaindra Lwin, Nils O. B. Lüttschwager, Martin A. Suhm
Georg-August-Universität Göttingen, Institut für Physikalische Chemie, Tammannstr. 6, 37077 Göttingen, Germany
eaindra.lwin@uni-goettingen.de

Tertiary amines are strong hydrogen bond acceptors towards an OH group of a water molecule. The hydrogen bonded OHb stretching vibration wavenumber is lowered and comes closer to the water bending overtone b2, which gives rise to anharmonic resonance with b2 and states building on it, or to combination transitions of OHb with low frequency intermolecular vibrations [1]. A combination of FTIR, Raman, isotope and chemical substitution spectroscopy in supersonic jet expansions establishes the existence, character and extent of the underlying anharmonic coupling for 8 tertiary amines. The observed resonance pattern is remarkably systematic, which allows to extract coupling constants that are relevant for the initial energy flow out of the excited OH oscillator. The coupling pattern for the weakest transition is still challenging, which invites detailed anharmonic quantum dynamic studies. The robust deperturbed positions of the uncoupled oscillators for 8 amine monohydrates are valuable for an experimental benchmarking database [2].

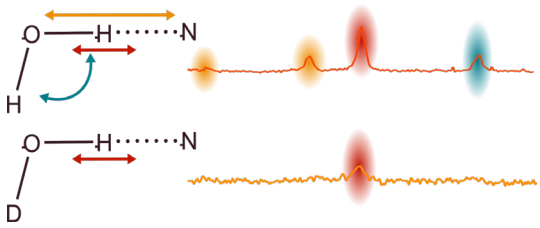


Figure 1 – Anharmonic resonances and how to remove them by isotope substitution

References
1. E. Lwin, T. L. Fischer, M. A. Suhm, *J. Phys. Chem. Lett.*, 14 (2023) 10194.
2. E. Lwin, N. O. B. Lüttschwager, M. A. Suhm, *Phys. Chem. Chem. Phys*., 27 (2025) 5808.

Acknowledgements: The authors thank the DFG-funded RTG2455 BENCh.

Underrated Surface Phenomena Influencing Surface-Enhanced Raman Scattering at Plasmonic Interfaces

Ivan Kopal[a,b], Valerie Smeliková[b,c], Matěj Kmetík[b,d], David Palounek[a], Marcela Dendisová[b], Marek Piliarik[a]

[a]*Institute of Photonics and Electronics, Czech Academy of Sciences, Chaberská 1014/57, Prague 8, 182 00, Czech Republic*

[b]*Department of Physical Chemistry, University of Chemistry and Technology Prague, Technická 5, Prague 6 160 00, Czech Republic*

[c]*J. Heyrovský Institute of Physical Chemistry, Czech Acadeny of Sciences, Dolejškova 2155/3, Prague 8, 182 00, Czech Republic*

[d]*Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 542/2, Prague 6, 160 00, Czech Republic*

kopal@ufe.cz

Although a significant period has passed since the first report of the enormous enhancement of Raman scattering from molecules deposited on plasmonic surfaces, researchers' interest in surface-enhanced Raman scattering (SERS) remains unrelenting to this day. Even though the main challenges — such as the description of enhancement mechanisms and observation of single-molecule signals — seem to have been overcome, the current focus on developing effective and reproducible substrates for analytical purposes can still be significantly improved by incorporating effects that are typically considered weak or negligible by the community.[1]

Here, we aim to apply a combined experimental and theoretical approach to extract additional information about these systems by examining subtle changes in the immediate vicinity of plasmonic surfaces — such as molecule–metal complex formation,[2] photo-/plasmon-mediated catalysis,[3,4] analysis of combination vibrational modes, or structural transformations of molecules trapped in well-defined hot spots.[5] We believe that integrating these aspects into standard methodology can lead to substantial improvements — not only enabling the detection and quantification of target species, but also allowing real-time monitoring of new substance formation, enhanced detection selectivity, and the extraction of quantum characteristics of single-hot-spot systems. This approach may prove especially valuable not only for the study of common molecular species such as dyes, but even more so for the analysis of biomolecules, where the use of certain high-efficiency substrates is limited due to analyte instability, and where chemical and/or geometrical transformations have a direct impact on biological function.

References

1. L. Langer, D. Jimenez de Aberasturi, J. Aizpurua, R., et al., *ACS Nano*, 14 (2020) 28.
2. V. Smeliková, I. Kopal, M. Člupek, M. Dendisová, M. Švecová, *Anal. Chem.*, 96 (2024) 5416.
3. I. Kopal, M. Švecová, M. Král, A. Michalcová, L. Lapčák, et al., *Coll. Surf. A*, 709 (2025) 136187.
4. I. Kopal, M. Švecová, V. Jeřábek, D. Palounek, A. Michalcová, et al., *ACS Omega*, 9 (2024) 6005.
5. D. Palounek, M. Vala, Ł. Bujak, I. Kopal, K. Jiříková, et al., *ACS Photonics,* 11 (2024) 3907.

Acknowledgements: The authors IK, DP, and MP acknowledge funding from the Czech Science Foundation (Project No. 23-07703S). The authors IK, VS, MK, and MD acknowledge institutional financial support from the University of Chemistry and Technology Prague (specific university research grant No. A1_FCHI_2025_001).

Treatment of MoS2 Monolayers by Atomic Deuterium

Valerie Smeliková[a,b], Michele Gastaldo[a], Jan Plšek[a], Martin Kalbáč[a]
[a]*J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences, Dolejškova 2155/3 182 00 Prague 8, Czech Republic*
[b]*Department of Physical Chemistry, University of Chemistry and Technology Prague, Technická 5, 160 00 Prague 6, Czech Republic*
valerie.smelikova@jh-inst.cas.cz

Two-dimensional materials, particularly transition metal dichalcogenides (TMDs), are known for their remarkable chemical and physical properties resulting from their atomic-scale thickness. The controlled introduction of defects or chemical dopants can enhance these properties.[1] In this study, we investigate both pristine and defect-engineered monolayers of molybdenum disulfide (MoS_2), a representative TMD, prepared by gold-assisted exfoliation in ultra-high vacuum conditions. The pristine and defective (He^+-treated) monolayers were subsequently exposed to atomic deuterium at low temperatures and then annealed.[2,3] This treatment induced a phase transition from the semiconducting 2H phase to the metallic 1T phase, with the degree of transformation strongly dependent on the defect concentration. The incorporation of deuterium into the MoS_2 lattice was also indicated by temperature-programmed desorption (TPD) combined with quadrupole mass spectrometry.[4] Structural and chemical modifications of the monolayers were analyzed using Raman spectroscopy, X-ray photoelectron spectroscopy, transmission electron microscopy, and X-ray diffraction.

References
1. E. Ascrizzi, M. Nalesso, N. L. Marana, G. Milotti, et al., *J. Phys. Chem. C*, 17 (2025) 8086.
2. F. Ozaki, S. Tanaka, W. Osada, K. Mukai, M. Horio, et al., *Appl. Surf. Sci.*, 593 (2022) 153313.
3. A. Baraldi, G. Comelli, S. Lizzit, G. Paolucci, R. Rosei, *Appl. Surf. Sci.*, 120 (1997) 219.
4. Y. Qu, H. Pan, C. Kwok, *Sci Rep 6*, (2016) 34186.

Acknowledgements: We gratefully acknowledge the assistance provided by the Advanced Multiscale Materials for Key Enabling Technologies project, supported by the Ministry of Education, Youth, and Sports of the Czech Republic. (Project No. CZ.02.01.01/00/22_008/0004558)

Complexity and Various Dynamic States of Interlayer Water in Nontronite: Insights from Dielectric Spectroscopy and TG–DSC Analysis

Karol Kułacz, Kazimierz Orzechowski
University of Wrocław, Faculty of Chemistry, ul. F. Joliot–Curie 14, 50–383 Wrocław, Poland
karol.kulacz@uwr.edu.pl

Nontronite is a smectite layered mineral composed of sheets organized into TOT layers (tetrahedral–octahedral–tetrahedral). The tetrahedral sheets are primarily built from SiO_4^{4-} units, while the nontronite octahedral sheet contains Al^{3+} and Fe^{3+} cations coordinated by oxygen and hydroxyl groups [1–3]. The structure exhibits a negative charge, which arises from structural vacancies as well as substitution effect, where higher–valent cations such as Al^{3+} are partially replaced by lower–valent cations like Mg^{2+}. This negative charge is equalized by the presence of interlayer cations: Na^+ or Ca^{2+}, located in the spaces between TOT layers. Furthermore, the interlayer spaces contain water molecules, which are stabilized by H–bonds with oxygen atoms from tetrahedral sheets and by ion–water interactions. Environmental conditions, humidity and temperature, strongly affect the amount of interlayer water [1]. At high humidity and room temperature, the interlayer spaces remain significantly hydrated. When humidity decreases or temperature increases, dehydration occurs. This results in shrinking of the interlayer spaces and leads to a decrease in the interplanar distance (d_{001}) [1].
Hydrated nontronite presents promising dielectric properties with the potential to reduce electromagnetic smog [2,3]. Its dielectric parameters strongly depend on the degree of hydration [1–3], which affects relaxation times (Fig. 1), dielectric increments and activation energies of relaxation processes. Additionally, TG studies have shown that dehydration proceeds in several parallel processes with kinetics determined by the activation energy, about 50 kJ/mol for weakly bound water (WBW) and 100 – 180 kJ/mol for strongly bound water (SBW).

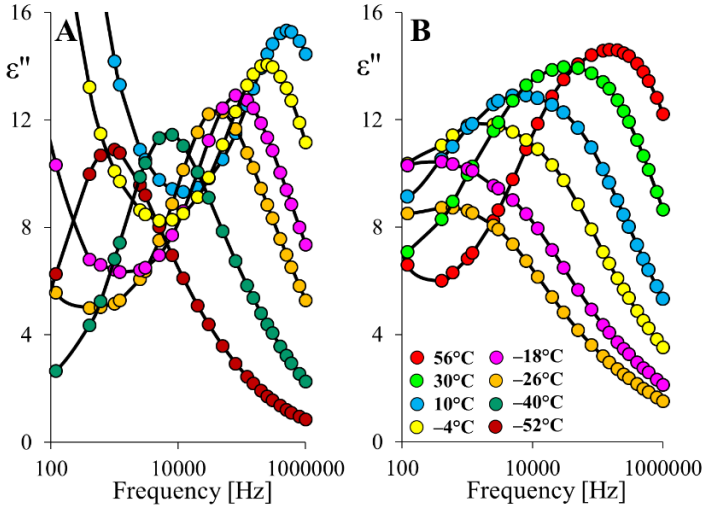


Figure 1 – The imaginary part of the electrical permittivity for samples containing A – 17% and B – 12% interlayer water, respectively

References
1. K. Kułacz, J. Waliszewski, S. Bai, L. Ren, H. Niu, K. Orzechowski, *Appl. Clay Sci.*, 202 (2021) 105952.
2. K. Kułacz, K. Orzechowski, B. Zsirka, J. Kristóf, *Appl. Clay Sci.*, 228 (2022) 106637.
8. K. Kułacz, K. Orzechowski, *Dalton Trans.*, 48 (2019) 3874.

Remote and *in situ* Sampling with the Virsa™ Raman Analyser

Agnieszka Sozańska
Spectroscopy Product Division, Renishaw
agnieszka.sozanska@renishaw.com

Raman spectroscopy has become a key analysis technique within wide range of applications including materials research, battery storage, drug development or medicine. It can retrieve detailed chemical information from samples in their endogenous, unaltered form. This makes Raman an effective method for assessing specific information about the form of the materials, their uniformity and quality, or in case of bio-samples about the disease state within biofluids, cells and tissues.
We will demonstrate the capabilities of the **Virsa™ Raman analyser**, discuss fundamentals of fiber optic probe design, Virsa™ imaging options and combine measurements possibilities which could enhanced analysis in thermal microscopy, electrochemistry, tribological testing, or the XRF elemental analysis technique.
The application of Renishaw's new **Virsa™ Raman analyser** for *in situ* SEM, and range of reactors, follow up by *in vivo* tissue analysis will be present, demonstrating the use of fiber-optic probes to give real-time *in situ* information.

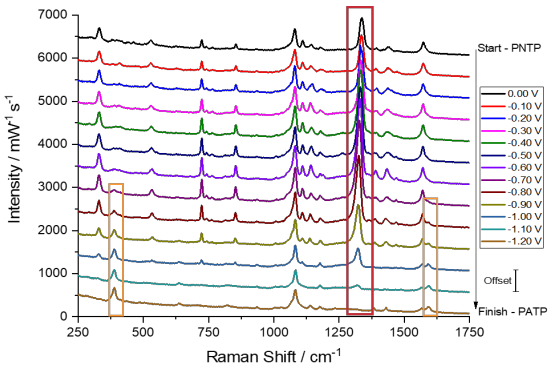


Figure 1 – Spectra of pNTP monolayer adsorbed on an Au SSV substrate, at potentials from 0.00 V to -1.20 V vs. Pt QRE Red highlighted region (C-N stretch of the nitro group) disappears

Surface-Enhanced Raman Scattering (SERS) Spectroscopy on Conductive Polymers and Hybrid Metal/Conductive Polymers Materials

Marek Procházka, Eva Kočišová, Jan Hanuš, Ondřej Kylián
Charles University, Faculty of Mathematics and Physics, Institute of Physics, 121 16 Prague 2, Czech Republic; Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, 180 00 Prague 8, Czech Republic
marek.prochazka@matfyz.cuni.cz

Recent studies have reported SERS spectroscopy on conductive polymers based on quaterthiophenes (4T) [1] or thiophenes [2], suggesting that the highly delocalized molecular orbitals of π-conjugated polymers facilitate efficient orbital overlap with the analyte molecule, thereby enabling intermolecular charge transfer (a chemical mechanism).
In this contribution, we tested poly(3,4-ethylenedioxythiophene) (PEDOT) in poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) films as efficient SERS-active substrates. We observed a significant enhancement (several orders of magnitude) for testing molecule methylene blue (Figure 1). Moreover, a combination of PEDOT:PSS with nanostructured noble metals (Ag, Au) significantly increased the SERS enhancement by the synergy of chemical and electromagnetic mechanisms, which paves the way for the design of novel highly SERS-active surfaces.

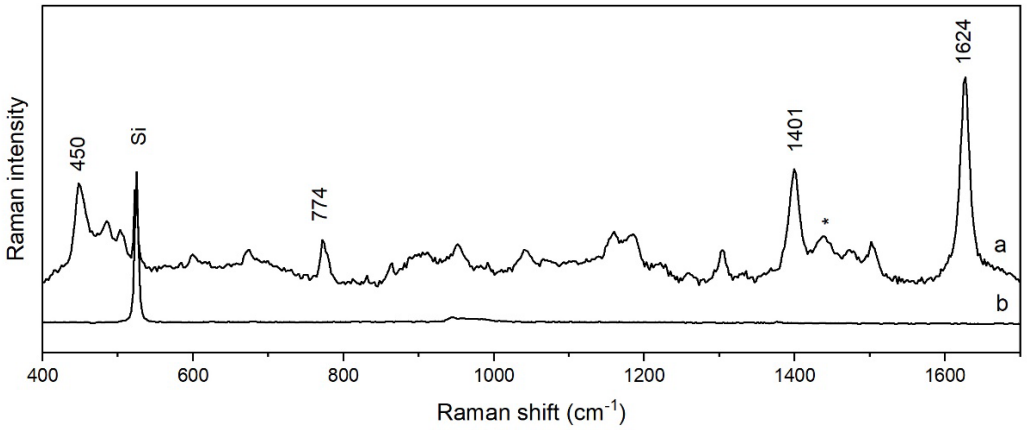


Figure 1 – Raman spectra measured from (PEDOT:PSS) films (a) and Si wafer (b) soaked in 1×10^{-5} M methylene blue aqueous solution for 2 hours. The strongest Raman bands of methylene blue and PEDOT:PSS are marked by numbers and by an asterisk, respectively. Excitation 632.8 nm

References

1. M. Yilmaz, E. Babur, M. Ozdemir, R. L. Gieseking, Y. Dede, U. Tamer, G. C. Schatz, A. Facchetti, H. Usta, G. Demirel, *Nat. Mat.*, 16 (2017) 918.
2. S. Guo, Y. Park, E. Park, S. Jin, L. Chen, Y. M. Jung, *Angew. Chem. Int. Ed.*, 62 (2023) e202306709.

Acknowledgements: The authors thank the Czech Science Foundation (grant No. 24-12197S) for financial support.

Integration of NIR Spectroscopy and Anharmonic Chemical Calculations for Applied Analysis

Justyna Grabska, Krzysztof B. Beć, Christian W. Huck
University of Innsbruck, Institute of Analytical Chemistry and Radiochemistry, Innrain 80-82, 6020 Innsbruck, Austria
Justyna.Grabska@uibk.ac.at

Near-infrared (NIR) spectroscopy has become a widely used analytical method in the research domain and industry due to its non-destructive, rapid measurement capability and its adaptability to both laboratory and on-site conditions [1]. The advent of miniaturized, portable NIR spectrometers has further broadened its utility, enabling on-site analyses in various applications [2]. However, the interpretation of NIR spectra remains challenging due to the presence of broad, overlapping overtone and combination bands, which complicate structural discrimination and compound identification.

To address these challenges, the integration of anharmonic quantum chemical calculations has emerged as a powerful complementary approach [3]. Theoretical NIR spectra enable the prediction of overtone and combination bands, allowing direct interpretation of spectral features based on underlying vibrational dynamics rather than relying solely on empirical correlations. This approach enhances the chemical specificity of NIR spectroscopy, which is one of the few significant limitations this technique has.

In an applied context, the integration of theoretical and experimental NIR data supports a more informed and targeted selection of spectral regions for chemometric modelling. The use of calculated spectra in model design helps interpret key variables, and improves the method understanding and transferability to various sample types or instruments [3]. We demonstrate how the theoretical insight can support informed variable selection and aid in the interpretation of spectral variance, contributing to more comprehensible analytical method.

References

1. K.B. Beć, J. Grabska, C.W. Huck In: *Molecular and laser spectroscopy - Advances and applications*. Vol. 3, Gupta, V.P. Ed.; Elsevier, 2022, pp. 141-188.
2. K.B. Beć, J. Grabska, C.W. Huck, *Chem. Eur. J.* 27 (2021) 1514.
3. K.B. Beć, J. Grabska, C.W. Huck, *Spectrochim. Acta A* 279 (2022) 121438.

Acknowledgements: This work was supported by **Austrian Science Fund (FWF): V1014-NBL.**

Seeing Red and Orange: Tailored Nanostructured SERS Substrates for Azo Dye Detection

Aleksandra Szymańska[a,b], Piotr Wróbel[b], Agata Królikowska[a]
[a]*University of Warsaw, Faculty of Chemistry, Pasteura 1, 02-093 Warsaw, Poland*
[b]*University of Warsaw, Faculty of Physics, Pasteura 5, 02-093 Warsaw, Poland*
a.szymanska40@uw.edu.pl

Azo dyes like methyl orange (MO) and methyl red (MR) are widely used as pH indicators and model compounds in industrial and laboratory settings. However, their chemical stability and toxicity raise serious environmental concerns, particularly when released into water systems via industrial discharge. This highlights a growing need for sensitive and reliable detection methods of these dyes in aqueous environments. While surface-enhanced Raman scattering (SERS) spectroscopy offers excellent sensitivity and molecular specificity, targeted studies on MO and MR remain limited. Core–Shell-Like Nanostructured (CSLN) SERS substrates offer a promising solution, with tunable geometry and plasmonic properties - engineered through controlled fabrication - for uniform, reproducible, and sensitive detection [1].
In this study, we investigate the influence of key experimental parameters - solvent type, adsorption mode and time, and solution pH - on the SERS performance of the MO and MR. Notably, efficient azo dyes adsorption on the SERS substrates is achieved without host-guest strategies. Additionally, we explore how the dyes' refractive indices affect SERS response of CLSN substrates, combining experiments with FDTD simulations. Our findings provide insights to optimize SERS protocols for more accurate and reproducible azo dyes detection.

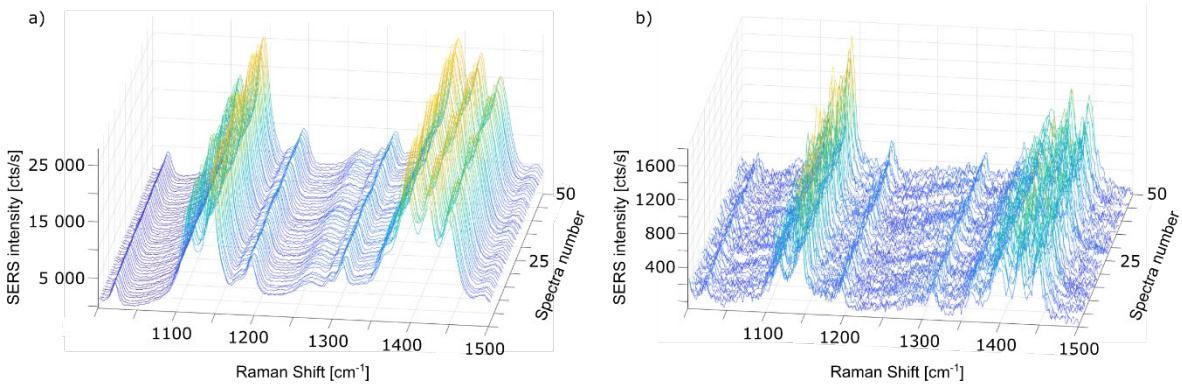


Figure 1 – Two sets of 50 SERS spectra (laser: 532 nm) of methyl orange for different adsorption time and solvent representing: a) perfectly tailored conditions and b) poorly tailored conditions.

References:
1. M.C. Suster, A. Szymańska, T.J. Antosiewicz, A. Królikowska, P. Wróbel, *ACS Appl. Mater. Interfaces* 17 (2025) 23076.

Acknowledgement: A.K. acknowledges support from the Excellence Initiative Research University program, via Project IDUB-622-316/2022 (University of Warsaw).

Insights into the Photochemical Behavior of Coumarin Derivatives via UV-Vis and NMR: From Reversible Rotation to Irreversible Photodegradation

Veranika Kuzmina, Mariusz Pietrzak, Jacek Waluk, Tomasz Ratajczyk
Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland
vkuzmina@ichf.edu.pl

Photochemical processes are crucial reactions attracting interest in their use due to the production of photoactive systems. Coumarins are among the most investigated photoactive molecules and have already been used in the testing of photoactive materials. [1]
Optical spectroscopy is commonly used to study photochemical processes. However, it does not provide detailed information on structural changes that occur during reactions. [2]
In this study, we employed UV-Vis spectroscopy, supported by NMR, to investigate the photochemistry of coumarin derivatives **A**–**D** (Fig.1). Illumination of **A**–**C** transformed them into respective isomers: **iso-A**, **iso-B** and **iso-C**. At -35°C (**A**, **C)** and -75°C (**B**), the conversion reached a steady state composition containing 80% of the isomer. Upon increasing the temperature, isomers reconverted to the original compounds and the activation energies of this process was experimentally determined. In the case of **D**, illumination led to its decomposition into at least two products, and no reconversion of these products to the original compound was observed.
Preliminary research suggests that introducing the $N(CH_3)_2$ group into the coumarins' molecular framework can profoundly alter their photochemical behavior and UV-Vis with NMR has proven to be a straightforward and effective method for determining these differences.

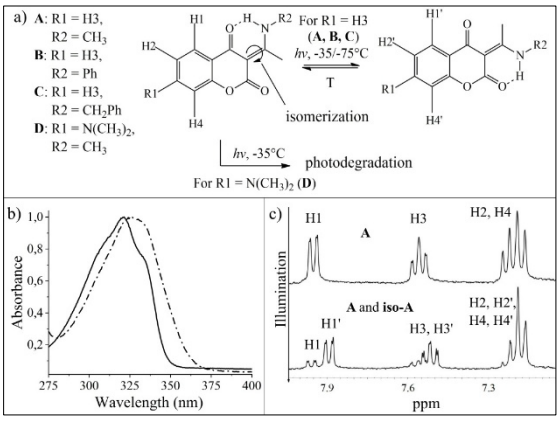


Figure 1 – Photoreaction of **A–D**. a) Products of illumination of **A–D**; b) absorption spectrum of **A** (solid) and a mixture of **A** and **iso-A** (dashed) measured in acetonitrile at -35°C; c) ^{1}H NMR spectrum of **A** (above) and a mixture of **A** and **iso-A** (below) measured in acetonitrile-d_3 at -35°C at 300 MHz at the region 8.10-7.10 ppm with signals of protons H1–H4 and H1'–H4' from the aromatic ring

References
1. K. B. Manjappa, D-Y. Yang, S-C. Fan, *Front. Chem.*, 11 (2023) 1295347.
2. Y. Ji, D. Dirocco, J. Kind, C. Thiele, R. Gschwind, M. Reibarkh, *ChemPhotoChem*, 3 (2019) 984.

Photostability of Azaaromatic Compounds

Barbara Golec[a,b], Aleksander Gorski[b], Jacek Waluk[b]
[a]*Faculty of Mathematics and Science, Cardinal Stefan Wyszyński University, 01-815 Warsaw, Poland*
[b]*Institute of Physical Chemistry, Polish Academy of Sciences, 01-224 Warsaw, Poland*
b.golec@uksw.edu.pl

Photochemical stability is one of the most important parameters that determine the usefulness of the organic dyes (fluorophores and photosensitizers) in different applications, e.g. fluorescence microscopy or photodynamic therapy, because the photodegradation limits the time scale of processes that can be followed and their efficiencies.
The photophysics and photostability of organic molecules can be strongly dependent on the environment: solvent (e.g., water, protic and aprotic organic solvents, micellar solutions) or oxygen content.
Here we present the results of our studies of the photodegradation of two groups of azaaromatic compounds: i) indole derivatives that can simultaneously act as hydrogen bond donors and acceptors and ii) porphyrins - commonly used as photosensitizers (Fig. 1).
Our investigations clearly show that the environment can drastically change the photostability of these molecules: from few to thousand times.[1-4]

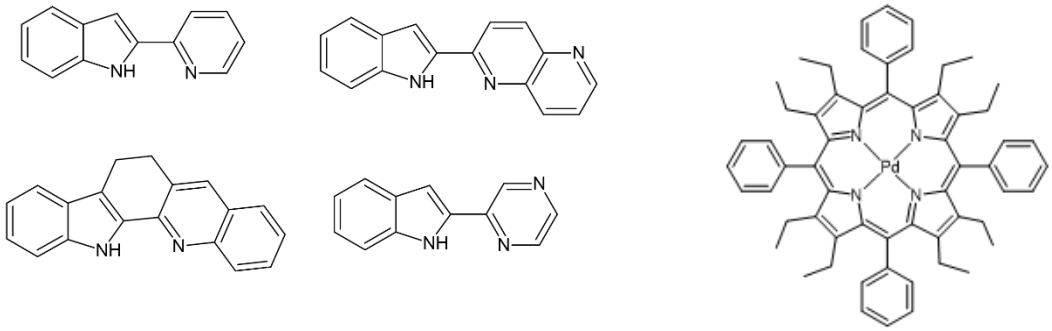


Figure 1 – The examples of the studied indole and porphyrin derivatives

References

1. B. Golec, A. Gorski, R.P. Thummel, M. Sierakowski, J. Waluk, *Photochem. Photobiol. Sci.* 22 (2022) 333.
2. B. Golec, K. Nawara, A. Gorski, R.P. Thummel, J. Herbich, J. Waluk, *Phys. Chem. Chem. Phys.* 20 (2018) 13306.
3. B. Golec, J. Buczyńska, K. Nawara, A. Gorski, J. Waluk, *Photochem. Photobiol. Sci.* 22 (2023) 2725.
4. M. Banaszek, B. Golec, R. Rybakiewicz-Sekita, J. Kowalski, P. Szczodry, N. Dutkiewicz, J. Waluk, A. Gorski, (2025). DOI:10.1021/acs.jpcb.5c02423

Acknowledgements: This work was supported by the Polish National Science Center grant no OPUS 2020/39/B/ST4/01956.

Towards on-Chip Mach-Zehnder Interferometer for Complex Refractive Index Sensing of Liquids in the Mid-Infrared

Alicja Dabrowska, Bernhard Lendl
Institute of Chemical Technologies and Analytics, Technische Universität Wien, Vienna, Austria
alicja.dabrowska@tuwien.ac.at

☒ I am applying for **Bruker Customer Excellence Award**

In the mid-infrared (mid-IR) region (400 – 4000 cm^{-1}), many molecules exhibit strong fundamental vibrations, making it a crucial spectral window for highly specific, non-invasive chemical analysis. Traditional absorption-based methods remain popular for qualitative and quantitative measurements, yet they provide only partial information about the sample's optical properties, specifically, the imaginary part of the refractive index. To obtain a complete picture, one must measure the complex refractive index, encompassing both the real part n and the imaginary part κ, denoted as $\bar{n} = n + i\kappa$. By combined data analysis of both dispersion and absorption features, more accurate identification of molecular species and quantification of their concentrations can be achieved, extending the scope of applications in various fields ranging from environmental monitoring to biochemical diagnostics.

In this work, we present our compact Mach-Zehner interferometer (MZI) setup, coupled with a tunable quantum cascade laser (QCL), for simultaneous measurement of both real and imaginary parts of the complex refractive index of liquid samples in the mid-IR region.[1] We further demonstrate the translation of this innovative benchtop MZI configuration into a chip-integrated platform utilizing the evanescent field within a Germanium (Ge)-on-Silicon (Si) waveguide to interact with liquid media. The Ge-on-Si sensing platform incorporates innovative coupling strategy, including monolithic microlenses embedded in the Si substrate and downward-coupling gratings facilitating free-space optical interfacing and alignment through the substrate.[2] An integrated microfluidic module with customizable dual-channels for the reference and sample arms of the MZI enables efficient sample handling and optimal path length selection, depending on the sample's absorption characteristics. Moreover, we showcase a signal processing method for extracting the refractive index components (n/κ data) from the recorded interference patterns, relying on in-phase (I) and quadrature (Q) components to form the complex signal $s = I + iQ$. From this complex signal, both the phase shift (arg(s)) and amplitude (|s|) can be accurately determined. Ultimately, the combined analysis of the extracted spectral data is expected to improve analyte identification when subjected to chemometric methods.

References

1. A. Dabrowska, S. Lindner, A. Schwaighofer, B. Lendl, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, 286 (2023) 122014.
2. https://www.menir-project.eu/

Acknowledgements: This research is part of the joint efforts of a consortium under the EU's Horizon M3NIR project (grant no. 101093008) to develop a modular sensing platform for the mid-IR region [2].

Chemometric Deconvolution of Raman Spectra in Multi-Doped Carbon Nanomaterials

Shiva Ghasemi, Reza Shorabadi
Department of Chemistry, Faculty of Science, Bu-Ali Sina University, Hamedan 6517838695, Iran
shivaghasemi805@gmail.com

Doping carbon-based nanomaterials with heteroatoms has emerged as a powerful strategy to tailor their electronic, optical, and catalytic properties. However, the Raman spectra of multi-doped carbon quantum dots (CQDs) often exhibit overlapping features that obscure accurate interpretation of structural and defect-related changes. In this study, we synthesized CQDs doped individually and combinatorially with nitrogen (N), sulfur (S), boron (B), iron (Fe), copper (Cu), and silver (Ag), and performed high-resolution Raman spectroscopy to investigate their vibrational behavior.

To resolve the complex spectral patterns, we applied advanced chemometric techniques including Principal Component Analysis (PCA), Partial Least Squares Regression (PLSR), and Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS). These tools enabled the deconvolution of overlapping D and G bands, isolation of dopant-specific vibrational modes, and identification of subtle shifts and intensity variations correlated with specific dopant elements. The chemometric results were further validated using complementary characterization methods such as X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM).

Our approach demonstrates how data-driven spectral analysis can reveal the underlying structural modifications induced by multi-element doping in carbon nanomaterials. This work provides a reproducible framework for interpreting complex Raman spectra and highlights the utility of chemometrics in the rational design of functionalized CQDs for optoelectronic and sensing applications.

References
1. S. Guo, J. Popp, T. Bocklitz, *Nat. protoc.* 16(12) (2021) 5426.
2. Y. Khristoforova, L. Bratchenko, I. Bratchenko. *arXiv:2210.10051* (2022).
3. C. Ruckebusch, L. Blanchet., *Analytica chimica acta,* 765 (2013) 28.
4. M.V. Kharlamova, Ch.Kramberger, *Nanomaterials,* 13 (2023) 640.

The Physical Origin of Hydrophobicity

Jože Grdadolnik, Barbara Zupančič
National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia
joze.grdadolnik@ki.si

Hydrophobicity plays a crucial role in numerous physicochemical processes, yet its fundamental origin remains unclear. There are two main opposing views on how small, purely hydrophobic (apolar) solutes — such as alkanes and noble gases — affect the hydration layer. The classical view, based on thermodynamic measurements of the dissolution of apolar solutes in water, suggests that a hydrophobic solute induces structural and dynamic changes in nearby water molecules by forming semi-ordered, transient clathrates ('icebergs'). This perspective assumes that water-water hydrogen bonding near a hydrophobic solute is enhanced, leading to the formation of more ordered and energetically stable water structures than those in bulk water. Such structural changes can arise from the strengthening and/or an increase in the number of water-water hydrogen bonds. This explanation accounts for the characteristic changes observed in the thermodynamic variables of hydrophobic hydration. According to the second view, a hydrophobic solute primarily slows down the dynamics of nearby water molecules by obstructing the jump mechanism, which is thought to be involved in rotational relaxation, while leaving their structure essentially unchanged. The main issue with both perspectives is the lack of direct experimental evidence for either the enhancement of hydrogen bonding and subsequent formation of semi-ordered clathrates in the hydration shell of small hydrophobic solutes or the jump mechanism of rotational relaxation in water molecules. We will present the application of redshifts and line shapes of the isotopically decoupled infrared O-D stretching mode of small, purely hydrophobic solutes in water as a means to study hydrophobicity at the most fundamental level. The first unequivocal, model-free experimental evidence for the presence of strengthened water hydrogen bonds near four hydrophobic solutes — matching those found in ice and clathrates — will be demonstrated. The water molecules involved in these enhanced hydrogen bonds exhibit extensive structural ordering, resembling that seen in clathrates. **Ab initio** molecular dynamics simulations further confirm that water molecules near methane form stronger, more numerous, and more tetrahedrally oriented hydrogen bonds than those in bulk water, while also experiencing restricted mobility. Our results provide strong support for the classical view of hydrophobic hydration.

References
1. J. Grdadolnik, F. Merzel, F. Avbelj, *PNAS USA,* 114 (2017) 322.
2. B. Zupančič, J. Grdadolnik, *J. Mol. Liq.,* 341 (2021) 1.
3. B. Zupančič, J. Grdadolnik, Water–hydrogen-bond network and hydrophobic effect. V: M.J. Wójcik, Y. Ozaki, *Spectroscopy and computation of hydrogen-bonded systems*. John Wiley & Sons, 2022. pages: 435-478.

Stacking and Chalcogen Bonding Enhance Photoinduced Electron Transfer in Nucleic Acids

Rafał Szabla, Mikołaj Janicki, Shivangi Garg
Faculty of Chemistry, Wroclaw University of Science and Technology, Poland
rafal.szabla@pwr.edu.pl

Photoinduced electron transfer (PET) is one of the most common consequences of the absorption of UV light by nucleic acids. It leads to the population of long-lived excited charge transfer (CT) states, which often involve several stacked nucleobases in a DNA strand. Recently, we also demonstrated that PET is the key step in the synthesis of RNA and DNA nucleosides under the conditions of early Earth [1,2]. In this talk, I will demonstrate that the efficiency of PET in DNA is strongly dependent on structural factors such as nucleobase stacking overlap [3]. I will also show that the efficiency of PET can be strongly influenced by chalcogen bonding interactions, the role of which has not been considered in photochemistry until recently [1,2,4]. My talk will be focused on our recent discoveries of productive photoredox reactions and on the mechanistic description of nonenzymatic self-repair of RNA and DNA, which can be used for predicting photoreactivity in related systems [5,6].

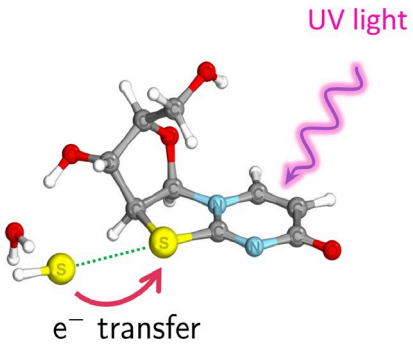


Figure 1 – Chalcogen bonding interactions support efficient photoinduced electron transfer

References
1. J. Xu, V. Chmela, N.J. Green, D.A. Russel, M.J. Janicki, R.W. Góra, R. Szabla, A.D. Bond, J.D. Sutherland, *Nature*, 582 (2020) 60.
2. M. Janicki, R. Szabla, *Angew. Chem. Int. Ed.*, 64 (2025) e202413498.
3. C.L. Kufner, S. Crucilla, D. Ding, P. Stadlbauer, J. Šponer, J.W. Szostak, D.D. Sasselov and R. Szabla, *Chem. Sci.*, 15 (2024) 2158 .
4. K.E. Szkaradek, P. Stadlbauer, J. Sponer, R.W. Góra, R. Szabla, *Chem. Commun.*, 56 (2020) 201.
5. R. Szabla, M. Zdrowowicz, P. Spisz, N.J. Green, P. Stadlbauer, H. Kruse, J. Šponer and J. Rak, *Nat. Commun.,* 12 (2021) 3018
6. R. Szabla, H. Kruse, P. Stadlbauer, J. Šponer, A.L. Sobolewski, *Chem. Sci.*, 9 (2018) 3131.

Acknowledgements: Support from the National Science Centre Poland (2020/37/B/ST4/04092 to R. S.) is gratefully acknowledged.

Finding a Needle in a Needle Stack: Leveraging Vibrational Spectra and Machine Learning to Guide Conformational Search

Roel van de Ven, Daria Ruth Galimberti
IMM, Radboud University, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands
roel.vandeven@ru.nl

The standard approach for identifying the conformer corresponding to an experimental infrared (IR) spectrum involves exploring the potential energy surface (PES), locating the minima and calculating the spectra of each conformation until a match is found. This sampling approach is highly inefficient because it requires numerous frequency calculations on structures that, in the end, are discarded. It becomes unfeasible for larger and larger molecules since the number of minima on the PES will increase exponentially with the number of atoms.
I will present a new methodology to cleverly direct the conformational search using molecular dynamics (MD) simulations informed by an on-the-fly machine learning (ML) model based on generated vibrational spectroscopy data during the search. Our program starts from a random position on the PES and the machine learning model learns on the fly how to modify the molecular conformation in a way to improve the spectral match until the correct conformation is found. The inputs of the ML model are the spectral similarity vectors, i.e., vectors describing the difference between the current and target spectra, and contain all information about intensity and frequency (mis)matches. The outputs of the ML model are proposed biases that should be applied in the next MD simulation to push the molecule to the desired conformer.
I will critically discuss the results we obtained on a test set of calculated spectra generated for the diphenylglycine molecule.

Formation of Ethanolamine-Mediated Surfactant-Free Microemulsions Using Hydrophobic Deep Eutectic Solvents

Anjali Sangwan, Siddharth Pandey
Department of Chemistry, Indian Institute of Technology Delhi, 110016, India
sipandey@chemistry.iitd.ac.in

Hydrophobic deep eutectic solvents (HDESs) are emerging as versatile, relatively benign, and inexpensive alternatives to conventional organic solvents in a diverse set of applications. In this context, the formation of microemulsions with HDES replacing the oil phase has become an area of active exploration. Because of recent reports on the undesirable toxicity of many common surfactants, efforts are under way to investigate the formation of surfactant-free microemulsions (SFMEs) using HDES as an oil phase. We present SFME formation using HDESs constituted of *n*-decanoic acid and five (5) structurally different terpenoids [thymol, l(−)-menthol, linalool, β-citronellol, and geraniol] at a 1:1 molar ratio as the oil phase and water as the hydrophilic phase. Ethanolamine (ETA) exhibited the best potential as a hydrotrope among several other similar small molecules. Results showed a drastic increase in water solubility within the HDESs in the presence of ETA. ETA exerted its hydrotropic action at different extent for each DES system via chemical interaction with the H-bond donor (HBD) constituent of the HDES. The optimum hydrotropic concentration (minimum hydrotrope and maximum water retention, X_{ETA}^{OPT}) assigned for each DES/ETA/water system and water loading are reported, and the trends are discussed in detail. Ternary phase diagrams are constructed using visual observation and the dye staining method. The area under the single- and multiple-phase regions (assigned in ternary phase diagrams) was estimated. "Pre-Ouzo" enforced by ETA was investigated using dynamic light scattering (DLS) of the DES/ETA/water systems at X_{ETA}^{OPT}. A systematic growth in nanoaggregates was observed with the subsequent addition of water in DES/ETA systems while continuously changing the existing microstructure. The presence of a core (oil)–shell (water)-like structure as indicated by the fluorescence response of Nile red in the "pre-Ouzo" region is speculated. We were able to prepare a homogeneous solution of $[K_3Fe(CN)_6]$ salt in "pre-Ouzo" mixtures with no apparent deviation in the Beer–Lambert law.

References
1. A. Sangwan, S. Pandey, *Langmuir* 40(4) (2024) 2254.

Acknowledgements: Author would like to thanks IIT Delhi for providing fellowship.

Theoretical Study of Selected Halogen-Bonded Complexes: Case of Methionine and Its Derivatives

Kamil Wojtkowiak
Faculty of Chemistry, University of Wrocław, F. Joliot Curie 14, 50-383 Wrocław, Poland
kamil.wojtkowiak2@uwr.edu.pl

Halogen bonds (XBs) alongside the famous hydrogen-bonds can be regarded as one of the most prominent noncovalent-interactions from the perspective of the stability of ligand molecules in the binding pockets of receptors. In fact, besides biochemistry, XBs are extensively used to tune the properties of chemical compunds in optoelectronics or in crystal engineering. In the biological systems, especially in the context of ligand-protein interactions, methionine seems to be an important electron density donor for the X-bond formation [1,2]. In this talk, I will present the results obtained from the quantum-chemical calculations of complexes of methionine and its derivatives with halogenomethanes. The geometrical, electronic, spectroscopic as well as dynamical properties of the examined models will be discussed. These findings will be placed in the context of interactions in the binding pocket of c-Jun N-terminal kinase with modified aminopyrimidines derivatives [3]. On the basis of the obtained results, I will try to explain intriguing differences between the observed tendencies and the standard chemical intuition regarding the polarizability of the halogen acceptors and the donation abilities of electron density donors.

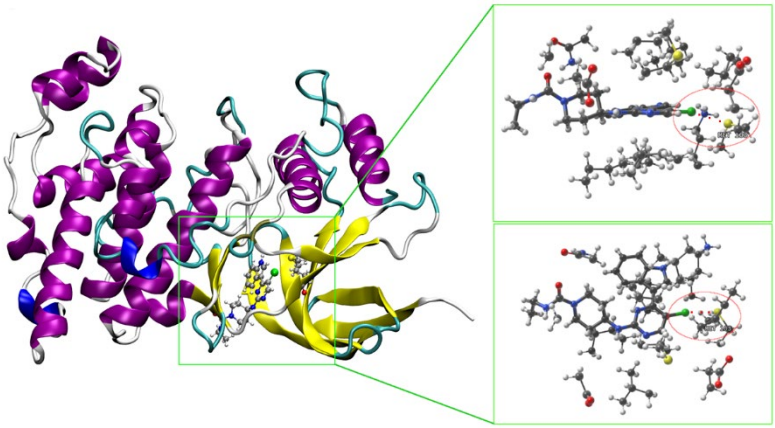


Figure 1 – Visualization of c-Jun N-terminal kinase structure with the native ligand (PDB deposit: 2P33) and its magnified binding pocket from two different perspectives

References
1. R. Wilcken, M.O. Zimmermann, et al., *Theory Comput.*, 7 (2011) 2307.
2. R. Wilcken, M.O. Zimmermann, et al., *J. Med. Chem.*, 56 (2013) 1363.
3. M. Alam, R.E. Beevers, et al., *Bioorg. Med. Chem. Lett.* 17 (2007) 3463.

Acknowledgements: The author thanks to the PL-Grid intrastructure in the Academic Cyfronet Center (Ares, LUMI), Wrocław Centre for Networking and Supercomputing as well as Poznan Supercomputing and Networking Center (PSNC) for providing computer facilities.

Investigation of the Structural Plasticity of Lithium Stabilized Mononucleotide G-Quadruplexes via Raman Optical Activity

Štěpán Jílek[a], Mohammed Siddhique Para Kkadan[a,b], Josef Kapitán[c], Václav Profant[a]
[a]*Institute of Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Prague 2, Czech Republic*
[b]*Institute of Organic Chemistry and Biochemistry, Academy of Sciences,Flemingovo náměstí 2, 16610 Prague, Czech Republic*
[c]*Department of Optics, Faculty of Science, Palacky University Olomouc, 17. Listopadu 12, 771 46 Olomouc, Czech Republic*
stepan.jilek@matfyz.cuni.cz

The self-assembly of guanosine-5′-monophosphate (5′-rGMP) into mononucleotide G-quadruplexes (mG4) via the formation of G-quartets and their subsequent stacking has attracted sustained interest due to its biological and physicochemical relevance. While sodium and potassium cations are known to stabilize distinct mG4 topologies, with K^+ typically inducing more stable structures than Na^+, a detailed atomistic understanding of the structural differences between Na- and K-stabilized mG4 remains elusive. Several structural models have been proposed, including variations in G-quartet stacking polarity (head-to-head for K^+ vs. head-to-tail for Na^+), but direct experimental evidence remains limited.
In this contribution, we focus on mG4 stabilized by lithium ions (Li^+), a significantly smaller cation that has received little attention in this context. Using Raman scattering and Raman Optical Activity (ROA)[1], particularly in the THz region (< 200 cm^{-1}) where sensitivity to supramolecular chirality is enhanced[2], we probe the temperature-dependent structural dynamics of Li-mG4. ROA spectra reveal a reversible three-state transition, suggesting multiple conformational populations and dynamic structural rearrangements.
QM calculations support our experimental findings, revealing that the structural transition in mG4 arises from modulation in the twist between stacked G-quartets, driven by a shift in Li^+ coordination from in-plane to inter-planar positions, rather than a change in G-quartet polarity. This reorganization involves alterations in glycosidic conformations, sugar puckering, and hydrogen bonding, highlighting the intrinsic structural plasticity of mG4.

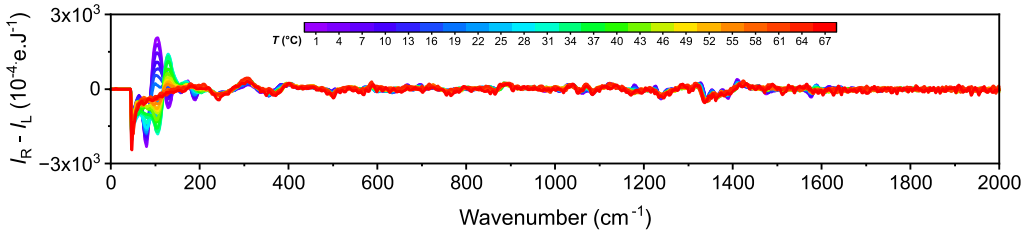


Figure 1 – ROA spectra of Li_2-5′rGMP at different temperatures. The color of each spectrum corresponds to the temperature scale in the upper part of the figure

References
1. V. Profant, Š. Jílek, *Appl. Spectrosc. Rev.*, (2025) 1-37.
2. M. S. P. Kkadan, Š. Jílek, V. Profant, J. Kapitán, J. Kessler, P. Bouř, *Chem. Eur. J.*, 30 (2024) e202403245.

Acknowledgements: This work was supported by the Charles University Grant agency (Project No. 298123).

Vibrational Markers of Model Metastatic Circulating Tumor Cells: FTIR, Raman, CARS Spectroscopy and Microscopy

G. Dovbeshko[a], O. Gnatyuk[a], M. Olenchuk[a], D. Komisar[b], O. Ilchenko[b,c], Z. Zhang[c], A. Boisen[c], G. Monastyrskyi[a], D. Kolesnyk[d], G. Solyanik[d]

[a]*Institute of Physics, Natl. Acad. of Sci. of Ukraine, Prospect Nauky, 46, UA-03028, Kyiv, Ukraine.*

[b]*Lightnovo ApS, Birkerød, Denmark.*

[c]*Technical University of Denmark, Department of Health Technology, Ørsteds Plads, Building 345C, DK-2800 Kgs. Lyngby, Denmark*

[d]*Laboratory of Molecular and Cellular Mechanisms of Metastasis, R.E. Kavetsky Institute of Exp erimental Pathology, Oncology and Radiobiology, Vasyl'kivs'ka St., 45, UA-03022, Kyiv, Ukraine.*

matinelli@gmail.com

Metastasis is a serious complication of cancer, which correlates with a negative prognosis for the patient. The early stage of the metastatic cascade is the detachment of metastatic cells and their migration beyond the primary tumor. Studying the biochemical and morphological characteristics of such cells is an extremely difficult task, since, entering the blood, most of them die due to apoptosis. However, a small part still survives and reaches another healthy organ, where secondary tumors (metastases) develop. That is why the determination of the biophysical and biochemical characteristics of circulating metastatic cells can give us a new concept for antimetastatic therapy.

In this study the FT-IR spectral features of Lewis lung carcinoma tumour cells were investigated. To model the process of metastasis, two methods of cell cultivation were used - adhesive and de-adhesive growth. To create stress conditions close to the presence of cells in the bloodstream, the drugs metformin and oxamate were used. Sodium oxamate as an inhibitor of glycolysis has the ability to stop the production of lactate by inhibiting lactate dehydrogenase [1]. Metformin is an inhibitor of oxidative phosphorylation, is an antidiabetic agent and affects glucose metabolism.

To study the spectral markers of cells, IR absorption spectra were recorded on an FTIRspectrometer INVENIO-R (Bruker, Germany) with a BioATR attachment. Raman spectra, mapping and imaging in different points of the cell were recorded at THOR S Raman Microscope with Cobolt Samba 05-01 532nm 1500mW laser (LightNovo, Denmark). Images of the studied cells at vibrational frequencies were also recorded using the CARS method. The work was carried out on a unique multifunctional microscope TCS SP8 CARS (Leica), equipped with a set of lasers.

The recorded spectral and morphological features correlate with changes in the functional activity of the biomolecules of the cell components, and changes in the intensity and contour of the bands corresponding to the protein and the nucleic acid components correlate with a decrease in cell survival and a decrease in their proliferative activity due to the inhibition of energy processes in the cell by the drugs.

References

1. O. Gnatyuk, D. Kolesnyk, T. Voitsitskyi, S. Karakhim, A. Nikolenko, A. Dementjev, G. Solyanik, G. Dovbeshko, *Spectrosc. J.*, 9 (2024) 306.

Acknowledgements: G. Dovbeshko, O. Gnatyuk,, D. Kolesnyk, G. Solyanik thank to NRFU project No 2021.01/0229.

Posters

P-1 Adriana Adamczyk
Investigating Differentiation Therapy of Myeloid Leukaemia Using Raman Spectroscopy

P-2 Andrzej Bil
The Bond Evolution in the Course of the Dissociation of Strain-Free and Strained Macrocyclic Disulfide Complexes – Topological Study

P-3 Balázs Brém
Development of Dual Acting Platinum(IV)-Based Anti-Tumour Agents Carrying Anti inflammatori Moieties

P-4 Małgorzata A. Broda
Inclusion Complexes of Selected Antiasthmatic Drugs

P-5 Tomasz Buchwald
Following Evolution's Fingerprint: Raman Spectroscopy Insights into the Secondary Structure of Spongin

P-6 Aneta Buczek
Water Modulated Influence of Intramolecular Hydrogen-Bonding on the Conformational Properties of Cannabidiol (CBD)

P-7 Daria Bumażnik
UV-Induced Photo-Transformations of 2-Aminothiazole-4-carboxylic Acid in Low Temperature Matrices

P-8 Janusz Cukras
Modeling the MChD and Other Dichroic Spectra of Chosen Organic Molecules

P-9 Tomasz Pawel Czaja
Near-Infrared Spectroscopy for Biogas Optimization: A Green Analytical Solution

P-10 Heiner Detert
Studies on the Isomerization of Liquid-Crystalline Tristriazolotriazines

P-11 Galyna Dovbeshko
Quantitative Assessment of Tryptophan Content in the Blood Plasma of Oropharyngeal Cancer Patients After COVID-19

P-12 Galyna Dovbeshko
Multiscale Imaging of Non-Adherent Tumor Cells: From Optical to Electron Microscopy

P-13 Marek Drozd
Macroscopic and Spectroscopic Properties of Bromo-Substituted Benzophenones

P-14 Marek Drozd
Variable-Temperature FT-IR and DSC Studies of Fatty-Acid Eutectic Binary Mixtures

P-15 Lucia Ďuríšková
Insights into Mononucleotide G-Quadruplex Self-Assembly via Raman Spectroscopy and Association Model Fitting

P-16 Jasmine S. Furter
Interactions of Polymers with Efficient Solid SERS Substrates for Sensitive Detection

P-17 Emese Gál
Meso-Substituted Phenothiazinyl-Porphyrins and their Indium and Zinc Complexes: Photophysical Properties, Photosensitisers for Photodynamic Therapy of Ovarian Cancer Cells

P-18 Shivangi Garg
UV-Driven Self-Repair of Uracil Dimers in RNA via Directional Photoinduced Charge Transfer

P-19 Aleksander Gorski
Photostability of Free-Base and Palladium meso-substituted Porphyrins in Organic Solvents and Aqueous Micellar Solutions

P-20 Herbert Michael Heise
Infrared ATR Spectroscopy of Polyethylene Using ZnSe and Ge-ATR Crystals and Comparison of Results from Advanced ATR-Correction

P-21 Herbert Michael Heise
Infrared ATR-Spectroscopy of Proteins, Spectral Variance and Band Distortions Shedding Light on the Available Advanced Correction Algorithm

P-22 Herbert Michael Heise
Development of Reference Materials for NIR Spectrometric Moisture Determination in Harvested Crops Using Reflection Measurement

P-23 Herbert Michael Heise
Investigations on the Permeation of Solvents Through Polymer Materials of Protection Gloves Using ATR IR Spectroscopy with Importance to Occupational Safety

P-24 Sara Helscher
Dielectric Properties of Reverse Micelles Formed by Nonionic Surfactants

P-25 Gulce O. Ildiz
Single-Crystal Polarized Raman Spectra of 6-Bromopyridine-2-carbaldehyde

P-26 Hrittik Karmakar
Infrared Photodissociation Spectroscopy of $Cu_2(OAc)_2(D_2)_n^+$ and its Isotopologues

P-27 Barbara Keresztes
Cosmic-Ray-Driven Chemistry in the CH_3CH_2OH, NH_3, and CH3CH2OH : NH3 Interstellar Ice Analogs

P-28 Matěj Kmetík
Electrochemical SERS Investigation of Thiol-Based Molecular Layers on Plasmonic Substrates

P-29 Monika Kopeć
The Role of Cardiolipin and Cytochrome C in Mitochondrial Metabolism of Cancer Cells Determined by Raman Imaging: in vitro Study on the Brain Glioblastoma U-87 MG Cell Line

P-30 Justyna Krupa
Hydrogen Bonding in Glycolic Acid–Water Complexes: Experimental and Computational Study

P-31 Edyta Kucharska
6-Methyl-3-nitro-2-[2-(5-nitropyridin-2-yl)hydrazinyl]pyridine: Synthesis, Spectroscopic Characterization, Structural Relationships and Potential Biological Activity

P-32 Edyta Kucharska
Synthesis, Structural Characterization, and Spectroscopic Analysis of 6-Methyl-3-nitro-2-[(E)-(5-nitropyridin-2-yl)diazenyl]pyridine: a Potential Azo-Linked Dye

P-33 Maria Rosa Lopez-Ramirez
Characterization of Extraterrestrial Materials Using Spectroscopic Techniques

P-34 Magdalena Malik
Comprehensive Structural and Spectroscopic Study of Transition Metal Complexes Featuring {CoN_2O_4} and {NiN_2O_4} Coordination Cores

P-35 Jacek Michalski
3-Nitro-2-[(E)-phenyldiazenyl]pyridine: Synthesis, Spectroscopic Characterization and DFT Study of a Potential Azo-Ligand for Coordination and Optoelectronic Applications

P-36 Jacek Michalski
DFT-Assisted Study of the Structural, Electronic, and Vibrational Properties of 6-Methyl-2-aminopyridine N-Oxide

P-37 Karolina Mucha
Photochemical and Spectroscopic Characterization of 3-Thio-1,2,4-triazole Complexes with CO_2 and N_2: A Comparative Matrix Isolation Study

P-38 Karolina Musiał
Conformational Dynamics of Lysozyme in the Presence of Model Membranes and Modulatory Compounds: Insights from FTIR and PCA Analyses

P-39 Karol Okła
Spectroscopic Characterization of Series of New Heteroleptic Rhodium(III) Complexes

P-40 Sylwia Olsztyńska-Janus
Insight from ATR-IR and 2D-COS into Structural Changes of Main Animal Plasma Components During Extracorporeal Circulation

P-41 Sylwia Olsztyńska-Janus
Post-Operational Rheological and ATR-IR Evaluation of Lithium and Calcium Sulfonate Greases in Mining Machinery

P-42 Magdalena Pagacz-Kostrzewa
Phototransformations of Indazole-3-carboxylic Acid Isolated in Low Temperature Matrices

P-43 Vlada Pashynska
Interactions between Anticancer Thioderivatives of Nucleobases and Nanosomes Components: Drug Delivery Related Study by FTIR Spectroscopy and Mass Spectrometry

P-44 Dominika Pasik
Unveiling the Role of Acyl Peroxy Radicals in Atmospheric Oxidation of Volatile Organic Compounds

P-45 Iwona Płowaś-Korus
Dielectric Spectroscopy into the Cooperative Dynamics of MPPyrNTf2 - Sulfolane Mixtures

P-46 Michał Pocheć
Machine Learning in Studies of RNA Nucleosides Conformations

P-47 Fariha Binte Rahman
Plasmon Assisted Surface Enhanced Linear and Nonlinear Raman Scattering Spectra of Biomolecules with Gold and Silver Nanostructures

P-48 Septila Renata
Detection of Serum Uric Acid on Gold Nanorods by Surface-enhanced Raman Spectroscopy

P-49 Olga Ryazanova
Spectroscopic Study on Binding of Multi-charged meso-Porphyrins to Synthetic Polynucleotides of Various Base Composition and Spatial Structure

P-50 Magdalena Sałdyka
UV-Induced Photodecomposition of Matrix Isolated Salicylhydroxamic Acid. FTIR and Theoretical Studies

P-51 Jakub M. Surmacki
Modulation of Cytochrome c Redox Status by Retinoids in Human Breast Cancer Cells: Insights from Raman Imaging

P-52 Jakub M. Surmacki
Raman Spectroscopy and Artificial Intelligence as a Novel Approach for HER2 Status Assessment in Breast Cancer

P-53 Marie Svecova
SERS Detection of Organic Films on Cu Substrates Treated by Controlled Corrosion

P-54 Wioleta Śmiszek-Lindert
Theoretical (DFT) and Experimental (FT-IR, FT-Raman) Studies on N-Phenylthioformamide

P-55 Roel van de Ven
Finding a Needle in a Needle Stack: Leveraging Vibrational Spectra and Machine Learning to Guide Conformational Search

P-56 Aleksandra Wesełucha-Birczyńska
The Secret of Tinctures of Selected Glycosides with Cardiac Action

P-57 Jakub Włodarski
Preparation and Thermal Properties of a Phase Change Material Based on Arachidic and Palmitic Acids

P-58 Kamil Wojtkowiak
Weak Hydrogen Bonds in the Binding Pocket of Carbonic Anhydrase II – Quantum Chemical Investigations

P-59 Emilia Wrona
Does Sample Preparation Affect Spectroscopic Results?

P-60 Emilia Wrona
New Glycosides for in vivo Raman Imaging

P-61 Kewin Żmigrodzki
Non-linear Dielectric Effect in Solutions of Menthol

P-62 M. A. Thottappali
Excited State and Charge Transfer Dynamics in Metal-Ligand Coordination Polymers for Synapse-Mimicking Memristors

Investigating Differentiation Therapy of Myeloid Leukaemia Using Raman Spectroscopy

Adriana Adamczyk[a], Anna M. Nowakowska[a], Justyna Jakubowska[b], Małgorzata Barańska[a], Katarzyna Majzner[a]
[a]*Jagiellonian University in Krakow, Faculty of Chemistry, 2 Gronostajowa Str., 30-387, Krakow, Poland*
[b] *Medical University of Lodz, Department of Pediatrics, Oncology and Hematology,4 Czechoslowacka Str., 92-216 Lodz*
adriana.adamczyk@uj.edu.pl

Myeloid leukaemia occurs when myeloid lineage precursors undergo abnormal proliferation and loss of proper function, triggered by a wide range of genetic mutations. The traditional treatment involves highly toxic chemotherapy to both malignant and healthy cells. However, the phenotype and morphology of dysfunctional myeloid precursor cells can be altered to a form without a tumour phenotype by various agents. This approach usually has lower toxicity than the traditional approach[1].
Changes in phenotype are associated with the disruption of subcellular compartments in the biological state. The method that provides good spatial resolution for studying single organelles is Raman microscopy, which allows for non-destructive identification of sample components[2]. The research hypothesis is therefore the presence of unique and sensitive biomarkers (chemical and morphological) detectable by Raman imaging that will allow for the clear indication of the type and phenotype of differentiated cells, as well as early biochemical changes due to the induced differentiation process. The majority of studies examining the influence of pharmaceutical agents on cell maturation, metabolic activity, and other factors are conducted using in vitro cell lines, such as HL-60, U937, and K562[2,3]. These cell lines can provide a stable and easily maintained model system. We studied ATRA-induced differentiation of HL-60 cells into neutrophil-like cells, PMA-induced monocytic differentiation of U937 cells, megakaryocytic differentiation, and doxorubicin-induced erythroid differentiation. Raman microscopy of living cells, combined with chemometric analysis, revealed the characteristic spectral markers of myeloid progenitors, neutrophils, monocytes, megakaryocytes, and erythrocyte-like cells. Nuclear remodelling (790 cm^{-1}), changes in lipid metabolism (1260, 1306, 1440, 1660 cm^{-1}), the synthesis of granular proteins, and haemoproteins (753, 943, 1550 cm^{-1}) were detected. The obtained results can serve as a valuable database for studies on various therapies using new chemical agents.

References
1. H. de Thé, et al., *Nat Rev Cancer*, 18 (2018) 117.
2. A. Adamczyk, et al., *Cell Dev. Biol*., 8 (2020) 592035.
3. A. Adamczyk, et al., *ChemRxiv*, (2025).

Acknowledgements: This work was founded by National Science Centre (Poland), project PRELUDIUM—No. UMO-2021/41/N/ST4/03069.

The Bond Evolution in the Course of the Dissociation of Strain-Free and Strained Macrocyclic Disulfide Complexes – Topological Study

Andrzej Bil, Przemysław Dopieralski
Faculty of Chemistry, University of Wrocław, F. Joliot Curie 14, 50-383 Wrocław, Poland
andrzej.bil@uwr.edu.pl

The mechanism of the cleavage of disulfide bonds is important for many chemical reasons and has been studied in many contexts, eg., [1] with the recent contributions from covalent mechanochemistry.[2] Recently, we have analysed a reaction in a constrained system, where the disulfide is a macrocycle adopting two distinctive conformations, one of which is depicted in the Figure 1 on the left, with some possible strain effects not present in chain disulfides, and the nucleophile is OH anion. The reaction was studied in aqueous solution using DFT metadynamics technique combined with computational mechanochemistry techniques to model an external force acting on the disulfide group. [3]
To extend the project we have been studying the course of the reaction from the point of view of bonding situation and bonds evolution along the reaction path. For some structures extracted from the path we have performed Atoms in Molecules analysis and Electron Localization Indicator study with a special attention on the nature of S-S bond and the emerging new S-O bond.

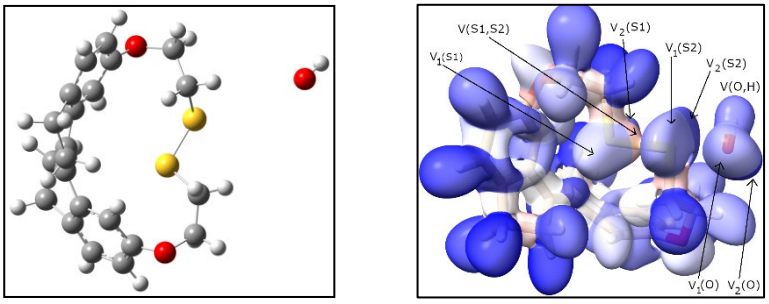


Figure 1 – The macrocycle attacked by the OH nucleophile (on the left); The bonding situation at the transition structure on the basis of ELI-D

In Figure 1, right, there are the ELI-D basins, $V_i(X)$, indicating the layout of the lone pairs at OH^- nucleophile, the sulfur atoms, the OH bond V(O,H) and the S-S bond at the stage of its decomposition, V(S1,S2). No covalent O-S bond at this stage of the reaction was detected.

References
1. A. Bil, K. Grzechnik, K. Mierzwicki, Z. Mielke, *J. Phys. Chem. A*, 117 (2013) 8263.
2. P. Dopieralski, M. E. Zoloff Michoff, D. Marx, *Phys. Chem. Chem. Phys.*, 22 (2020) 25112.
3. P. Dopieralski, A. Bil, *Chemistry-A European Journal*, 30 (2024) e202402982/1.

Acknowledgements: The authors gratefully acknowledge financial support via the National Science Centre of Poland - NCN - (2020/37/B/ST4/00423) as well as additional computational support by Wroclaw Supercomputer Center (WCSS) and the computers of Centre of Informatics Tricity Academic Supercomputer & Network

Development of Dual Acting Platinum(IV)-Based Anti-Tumour Agents Carrying Anti inflammatori Moieties

Balázs Brém, Emese Gál, Bianca Stoean (Vasile), Ioana-Luiza Găină
Research Center on Fundamental and Applied Heterochemistry, Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, 11 Arany Janos str., RO-400028 Cluj-Napoca, România;
balazs.brem@ubbcluj.ro

The development of novel anti-cancer therapies remains a critical area of research, particularly in addressing challenges such as drug resistance and systemic toxicity associated with conventional platinum-based chemotherapy.
Here, we describe the synthesis of new platinum(IV) prodrugs that combine cisplatin with one or two axially coordinated molecules of non-steroidal anti-inflammatory cancer-selective drug. The results suggest that these Pt(IV) complexes exhibit mechanisms of action typical for Pt(II) complex and NSAID, simultaneously. The presence of NSAID ligand(s) in the Pt(IV) complexes promotes the antiproliferative activity and selectivity of cisplatin by inhibiting lactate transporters, resulting in blockage of the glycolytic process and impairment of mitochondrial potential.

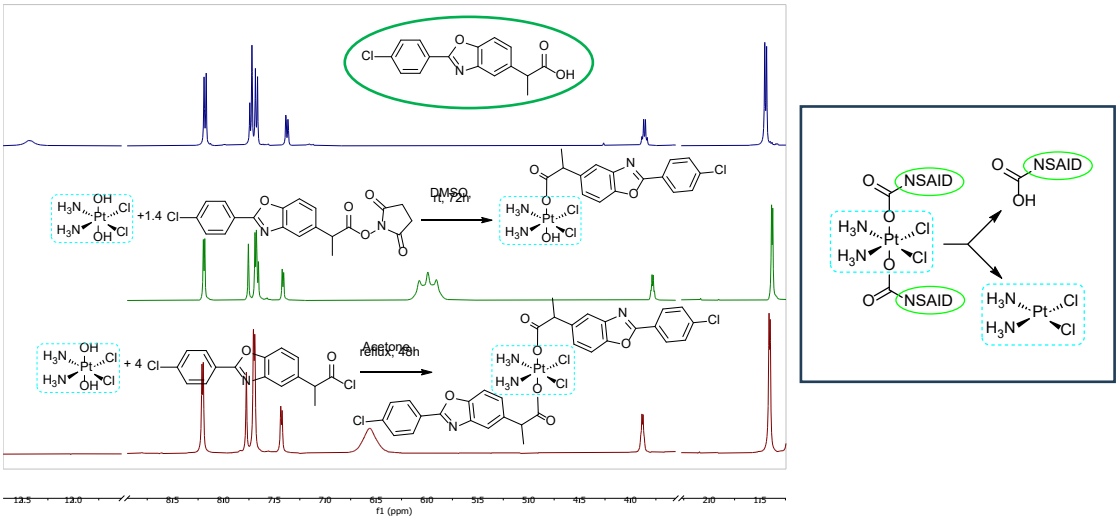


Figure 1 – Synthesis and characterisation of cisplatin complexes

References

1. S. Richter, P. Lönnecke, D. Bovan, N. Andrian, B. Stoean, M. Lehene, R. Silaghi-Dumitrescu, L. Gaina, S. Mijatović, D. Maksimović-Ivanić, G.N. Kaluđerović, E. Hey-Hawkins, *Dalton Trans.*, 54 (2025) 35970.
2. P. Fronik, I. Poetsch, A. Kastner, T. Mendrina, S. Hager, K. Hohenwallner, H. Schueffl, D. Herndler-Brandstetter, G. Koellensperger, E. Rampler, J. Kopecka, Ch. Riganti, W. Berger, B.K. Keppler, P. Heffeter, Ch.R. Kowol, *J. Med. Chem.,* 64 (2021) 12132.

Acknowledgements: This work was supported by the project "Targeted Tumor Therapy with multifunctional platinum(iv)-drug conjugates (T^3-Pt)" funded by European Union – NextGenerationEU and Romanian Government, PNRR, contract no 760240/28.12.2023, cod PNRR-C9-I8-CF 76/31.07.2023, through the Romanian Ministry of Research, Innovation and Digitalization, within Component 9, "Investment I8".

Inclusion Complexes of Selected Antiasthmatic Drugs

Małgorzata A. Broda, Kacper Czaja
Department of Chemistry and Pharmacy, University of Opole, ul. Oleska 48, 45-052 Opole, Poland
broda@uni.opole.pl

Inclusion complexes are widely employed to enhance various pharmaceutical properties of drugs, including solubility, stability, and release profiles [1]. These complexes are stabilized through a range of noncovalent interactions, such as hydrogen bonding, dispersion forces, and halogen bonding [2]. This study explores the formation and characteristics of inclusion complexes between β-cyclodextrin and two selected anti-asthmatic drugs: salbutamol (SAL) [3] and tulobuterol (TUL). Using the M06-2X/6-31+G(d,p) method for both gas phase and aqueous media (via a continuum model), we explored the energetic and structural aspects of complexation. The preferred conformers of SAL and TUL, stabilized primarily by intramolecular hydrogen bonds, were identified, and two orientations of drug molecules within β-cyclodextrin—head-first (aromatic ring inside the cavity) and tail-first (aliphatic chain insertion)—were analyzed. We compared the low-energy inclusion complexes of salbutamol (SAL) and tulobuterol (TUL) with β-cyclodextrin (β-CD) to evaluate their stabilization mechanisms. Our results highlight the critical role of dispersion interactions in stabilizing these complexes, with estimated interaction energies of approximately −28 kcal/mol for SAL and −20 kcal/mol for TUL. Computational analysis indicates a preference for a head-first insertion orientation, yielding stabilization energies of just under −6 kcal/mol for SAL and slightly over −3 kcal/mol for TUL. While TUL/β-CD complexes exhibited fewer hydrogen bonds than their SAL counterparts, they were additionally stabilized by Cl···O halogen interactions (~3 Å). Notably, no stable TUL/β-CD complex was obtained using the B3LYP method without dispersion corrections, underscoring the essential role of dispersion forces in accurately modelling such systems. These findings provide valuable insights into the molecular interactions underlying β-cyclodextrin's ability to enhance the pharmacological properties of anti-asthmatic drugs.

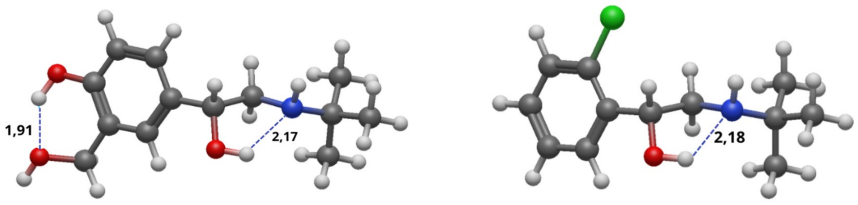


Figure 1 – Lowest-energy conformers of the anti-asthmatic drugs salbutamol and tulobuterol, optimized using the M06-2X/6-31+G(d,p) level of theory

References
1. A. Cid-Samamed, J. Rakmai, J.C. Mejuto, J. Simal-Gandara, G. Astray, *Food Chem.*, 384 (2022) 132467.
2. J. Řezáč, K.E. Riley, P. Hobza, *JCTC*, 8 (2012) 4285.
3. A.B.M. Buanz, M.H. Saunders, A.W. Basit, S. Gaisford, *Pharm. Res.*, 28 (2011) 2386.
4. A. Nakamura, D. Mori, K. Tojo, *Chem. Pharm. Bull.*, 60 (2012) 300.

Acknowledgements: All calculations were performed using the computational facilities and software provided by WCSS. The authors also acknowledge financial support from the University of Opole.

Following Evolution's Fingerprint: Raman Spectroscopy Insights into the Secondary Structure of Spongin

Tomasz Buchwald[a], Mirosław Szybowicz[a], Hermann Ehrlich[b,c]
[a]*Institute of Materials Research and Quantum Engineering, Poznan University of Technology, Poland*
[b]*Center for Advanced Technology, Adam Mickiewicz University, Poznan, Poland.*
[c]*Institute of Chemical Technology and Engineering, Poznan University of Technology, Poland.*
tomasz.buchwald@put.poznan.pl

Spongin, the primary fibrous component of keratosan demosponges, has long been considered a chemically elusive biopolymer. Our study reveals that spongin is predominantly composed of mammalian-like collagens type I and III. Raman spectroscopy played a pivotal role in this discovery: detailed analysis and deconvolution of the amide I band allowed for precise quantification of secondary structural elements, including alpha helices, beta sheets, and beta turns. The spectral profile and secondary structure composition closely matched those of collagen type III. Spatial distribution of these structures was further visualized using Raman mapping (fig. 1). These results, supported by 13C NMR, FTIR, and proteomic data, redefine spongin as an ancient collagen-based composite.

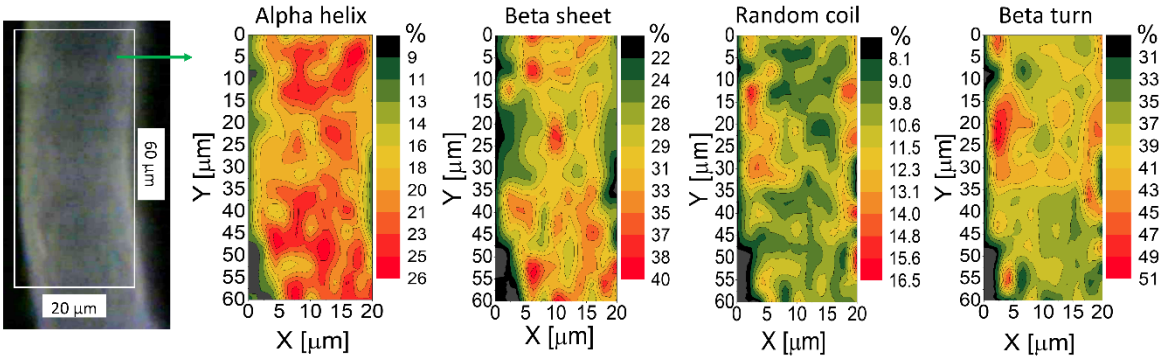


Figure 1 – Raman maps of spongin fiber

References
1. H. Ehrlich, I. Miksik, M.V. Tsurkan, et al., *Nature Communications,* 16 (2025) 2515.
2. M.J. Fiołka, S. Mieszawska, P. Czaplewska, et al., *Scientific Reports,* 10 (2020), 16352.
3. K. Lewtak, M.J. Fiołka, P. Czaplewska, et al., *Scientific reports,* 9 (2019), 12233.

Acknowledgements: This study was financially supported by the Ministry of Science and Higher Education of Poland (Grant No. 0511/SBAD/2551).

Water Modulated Influence of Intramolecular Hydrogen-Bonding on the Conformational Properties of Cannabidiol (CBD)

Aneta Buczek[a], Kacper Rzepiela[a,b], Małgorzata A. Broda[a], Teobald Kupka[a], Birgit Strodel[b,c], Hebah Fatafta[b,d]

[a] *Faculty of Chemistry and Pharmacy, University of Opole, Oleska 48, 45-052 Opole, Poland*

[b] *Institute of Biological Information Processing: Structural Biochemistry, Forschungszentrum Jülich, Jülich, Germany*

[c] *Institute of Theoretical and Computational Chemistry, Heinrich Heine University, Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany*

[d] *Department of Engineering and Communication, Bonn-Rhein-Sieg University of Applied Sciences, Grantham-Allee 20, 53757 Sankt Augustin, Germany*

abuczek@uni.opole.pl

Cannabidiol (CBD, Figure 1), a non-intoxicating compound derived from *Cannabis sativa*, has attracted considerable scientific interest due to its wide-ranging pharmacological effects, including anti-inflammatory, antioxidant, and anxiolytic activities [1,2]. Despite its therapeutic promise, CBD's limited water solubility significantly restricts its systemic bioavailability. We present a comprehensive theoretical analysis aimed at elucidating the conformational characteristics of CBD and their impact on its solubility profile. Density Functional Theory (DFT) methods were employed to investigate the spatial orientation of substituents on the limonene moiety, with particular emphasis on the positioning of hydroxyl groups on the aromatic ring. The conformational energy landscape revealed a pronounced preference for diequatorial substitution patterns, stabilized via intra- and intermolecular -OH···π interactions. Further, all-atom Molecular Dynamics (MD) simulations in aqueous media demonstrated that while individual CBD molecules largely retain their optimized conformations, multiple molecules exhibit a pronounced tendency to aggregate. These molecular-level insights into CBD's behavior in water-rich environments help explain its poor solubility and offer guidance for future formulation strategies aimed at enhancing its pharmacokinetic properties [3].

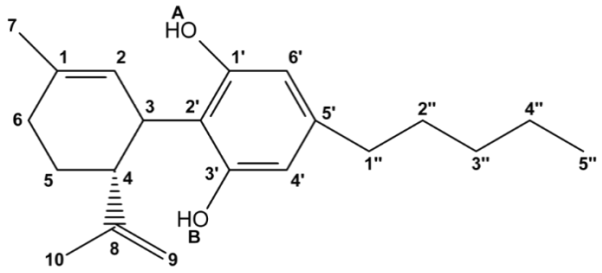


Figure 1 – Chemical formula with atom numbering of cannabidiol (CBD)

References

1. R. Adams, M. Hunt, J.H. Clark, *JACS*, 62 (1940) 196.
2. X. Wang, H. Zhang, Y. Liu, Y. Xu, B. Yang, H. Li, L. Chen, *Bioorg. Chem.*, 140 (2023) 106810.
3. A. Buczek, K. Rzepiela, M.A. Broda, T. Kupka, B. Strodel, H. Fatafta, *J. Mol. Liq.*, 423 (2025) 127033.

Acknowledgements: The authors thank the Wroclaw Centre for Networking and Supercomputing.

UV-Induced Photo-Transformations of 2-Aminothiazole-4-carboxylic Acid in Low Temperature Matrices

Daria Bumażnik, Magdalena Sałdyka
Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383, Wrocław, Poland
daria.bumaznik@uwr.edu.pl

The structure, spectroscopic properties and photo-induced photoisomerization and photodegradation processes of 2-aminothiazole-4-carboxylic acid (ACA), isolated in argon and nitrogen matrices were studied using matrix-isolation FTIR spectroscopy and DFT calculations undertaken at the B3LYPD3/6-311++G(3df,3pd) level of theory.[1,2] The most stable structures, with five-membered ring stabilized by two C=C and C=N double bonds and different arrangement of the carboxyl group, were identified in matrices after deposition. The phototransformations upon irradiation provided by an Optical Parametric Oscillator (OPO) tunable laser system were studied. Following irradiation at 285 or 1456 nm, a rotation of the OH group around the C–O bond in ACA1 leading to increase of ACA2 was detected. The corresponding reverse photo-rotamerization was detected at 296 or 1434 nm, resulting in the recovery of the initial isomer ACA1. Selective UV irradiation of matrices with shorter wavelengths led to photolytic decomposition of ACA. When the ACA/Ar (N_2) matrices were exposed to 270 nm irradiation, the decarboxylation reaction which produced a 2-aminothiazole molecule occurred as the first step of photolysis. Main photoproducts, the carbodiimide derivatives, were produced by a cleavage of the CS–CN bond together with hydrogen atom migration. We have also found that cleavage of the CS–CN bond followed by disruption of the N–C bond produced cyanamide, thiirene, carbodiimide and ethynethiol molecules. The ring-opening photoreaction caused by the cleavage of the CS–CC bond occurred simultaneously, followed by hydrogen atom migration, generated N'-ethynylcarbamimidothioic acid and its derivatives. Cleavage of the CS–CC bond followed by disruption of the N–C bond produced the acetylene and N-thiolcarbodiimide molecules. We also observed several new bands which were tentatively assigned to the isothiocyanic acid and thiofulminic acid complexes with ketenimine. Apart from new photoproduct molecules obtained in the ACA photolysis process, several molecular complexes were also identified as photoproducts.

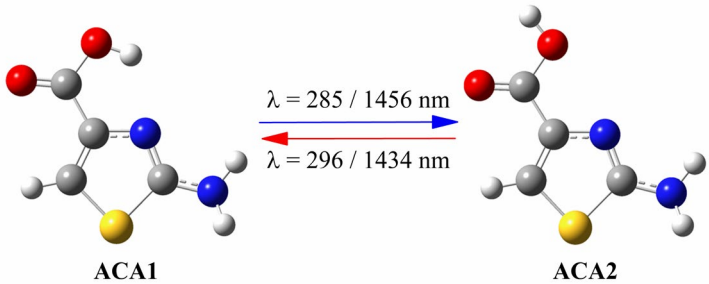


Figure 1 – UV/NIR-induced *cis-trans* isomerization reactions between ACA1 and ACA2

References:
1. D. Bumażnik, M. Sałdyka, *J. Photochem. Photobiol. A*, 455 (2024) 115766.
2. D. Bumażnik, M. Sałdyka, in press.

Acknowledgements: The authors acknowledge the Wroclaw Centre for Networking and Supercomputing (WCSS) for providing computer time and facilities.

Modeling the MChD and Other Dichroic Spectra of Chosen Organic Molecules

Janusz Cukras[a], Grzegorz Skóra[a], Oliwier Misztal[a], Antoni Tarnowski[a], Jakub Szewczyk[a], Sonia Coriani[b]
[1]*Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw*
[2]*DTU Chemistry, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark*
janusz.cukras@uw.edu.pl

Magneto-chiral dichroism (MChD) and magnetic circular dichroism (MCD) are unique chiroptical effects observed for molecules within a magnetic field, offering insights into molecular properties and fundamental light-matter interactions [1,2]. We performed extensive theoretical predictions and methodological studies of MChD spectra, alongside electronic circular dichroism (ECD) and magnetic circular dichroism, for diverse chiral organic molecules [3]. Investigated systems include carbo[*n*]helicenes (from [3]- to [8]helicene), chiral naphthalene diimide (NDI) derivative, and smaller chiral molecules like propylene oxide, substituted cyclopropanones, and 3-(trifluoroacetyl)-camphor.
MChD and MCD properties were computed using complex (damped) quadratic response theory, primarily with the B3LYP functional and aug-cc-pVDZ basis set in the DALTON program suite [4]. A wavelength scaling procedure, benchmarked against available experimental ECD/MCD data, was applied to adjust the modeling procedure and refine MChD predictions. This study delivers the first comprehensive set of MChD spectral predictions for these molecular series. For larger helicenes ([6]-, [7]-, and [8]helicene), MChD dissymmetry factors (g_{MChD}) are predicted around 10^{-6}, suggesting experimental feasibility, with signal strength generally increasing with helicene size. Smaller systems also exhibit distinct predicted MChD features. The agreement with available ECD and MCD experiments is good.
These theoretical benchmarks across varied chiral molecules aim to support experimental MCD spectroscopy and the effort to develop MChD spectroscopy, highlighting molecular features influencing MChD signals and the utility of computational modeling for this complex phenomenon.

References
1. L. D. Barron, J. Vrbancich, *Mol. Phys.*, 51 (1984) 715.
2. G. L. J. A. Rikken, E. Raupach, *Nature*, 390 (1997) 493.
3. S. Coriani, M. Pecul, A. Rizzo, P. Jørgensen, M. Jaszuński, *J. Chem. Phys.*, 117 (2002) 6417.
4. J. Cukras, J. Johansson, P. Norman, A. Rizzo, G. Rikken, S. Coriani, *Phys. Chem. Chem. Phys.*, 18 (2016) 13267.

Acknowledgements: The authors thank the National Science Centre grant OPUS-20 no. 2020/39/B/ST4/01670. Calculations have been carried out using resources provided by Wroclaw Centre for Networking and Supercomputing (https://wcss.pl), grant No. 321.

Near-Infrared Spectroscopy for Biogas Optimization: A Green Analytical Solution

Tomasz Pawel Czaja[a], Bjørn Niels Hansen[b], Morten Rahr Clausen[b], Søren Balling Engelsen[a]
[a]*Department of Food Science, University of Copenhagen, 1958 Frederiksberg C, Denmark*
[b]*BioCirc, Amaliegade 22, 1, 1256 København, Denmark*
tomasz.czaja@food.ku.dk

Minimizing food waste while pursuing sustainable and environmentally friendly energy solutions is becoming increasingly important. Biogas offers a promising renewable energy source by converting organic waste into energy and supporting a circular economy. However, its production remains complex due to variations in feedstock composition, which affect methane yield and overall process efficiency. Additionally, obtaining representative feedstock samples is challenging because of the heterogeneous nature of biogas substrates, which limits the accuracy of conventional analytical methods. Traditional laboratory analyses for feedstock characterization are often time-consuming, labor-intensive, and require specialized equipment—hindering real-time decision-making in biogas plants.

To address these challenges, innovative approaches such as advanced analytical techniques are essential for optimizing biogas production. Near-Infrared Spectroscopy (NIRS) has emerged as a rapid, non-destructive tool for evaluating key feedstock properties. As a green technology, NIRS provides an environmentally friendly alternative to traditional chemical analysis, reducing the use of hazardous reagents and minimizing sample preparation [1].

This study evaluates benchtop and portable NIRS for classifying biogas feedstocks and predicting key parameters such as moisture, volatile solids, and ash content. Using chemometric analysis, NIRS distinguishes feedstock types—like food waste, manure, and agricultural residues—by their spectral signatures. NIRS also addresses sampling challenges by enabling fast and representative analysis of heterogeneous materials, improving process monitoring accuracy. Additionally, low-field nuclear magnetic resonance (LF-NMR) was explored as a complementary method for rapid determination of dry matter content, offering a simple and robust measurement that can support NIRS calibration or serve as a standalone screening tool in specific cases. Integrating NIRS into biogas operations enables real-time, on-site assessment of feedstocks, enhancing process control, improving digestion efficiency, and increasing methane yields—ultimately supporting more stable, cost-effective, and sustainable biogas production.

References

1. T.P. Czaja, S.B. Engelsen, *Spectrochim. Acta A Mol. Biomol. Spectrosc*., 303 (2024) 125028.

Studies on the Isomerization of Liquid-Crystalline Tristriazolotriazines

Matthias Jochem, Daniel Limbach, Heiner Detert
Department Chemie, Johannes Gutenberg-University, D-55099 Mainz, Germany
detert@uni-mainz.de

C3-symmetric Tristriazolotriazines **1** with six to nine alkoxy side chains, prepared according to the Huisgen protocol [1] are a group of discotic liquid crystals with broad hexagonal columnar mesophases.[2,3] These compounds undergo a thermically induced rearrangement that lead to unsymmetrical intermediates, which finally, but much slower, react to a new symmetrical product **2** [4] of identical mass but downfield shifted ^{1}H-NMR signals. This isomerization changes the position of the substitutents from tangential to radial. In the case of liquid crystalline compounds, this can possibly lead to a shift in transition temperatures, the emergence of new mesophases or the loss of mesomorphism. This study focusses on the mechanistics behind this isomerization reactions, initially proposed as a Dimroth-rearrangement. A variety of additives was tested as inhibitors or accelerators of the isomerization. DFT calculations support the proposed pathway.

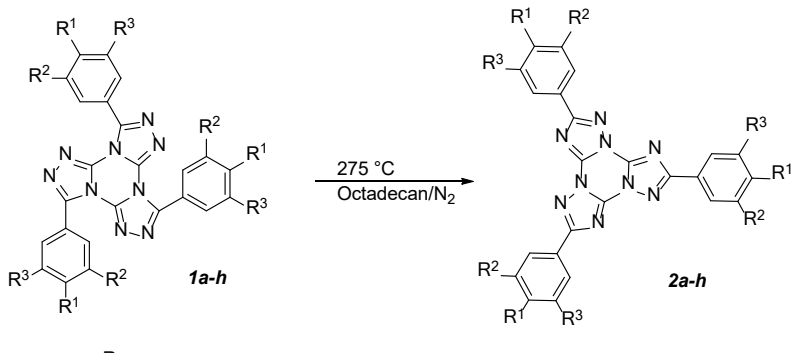


Figure 1 – Thermal isomerisation of tristriazolotriazines

References
1. R. Huisgen, H.J. Sturm, M. Seidel, *Chem. Ber*., 94 (1961) 1555.
2. R. Cristiano, H. Gallardo, A. J. Bortoluzzi, I. H. Bechtold, C.E.M. Campos, R.L. Longo, *Chem. Commun*., (2008) 5134.
3. T. Rieth, T. Marszalek, W. Pisula, H. Detert, *Chemistry,* 20 (2014) 5000.
4. V.A. Tartakovsky, A.E. Frumkin, A.M. Churakov, Yu.A. Strelenko, *Russ. Chem. Bull. Int. Ed.,* 54 (2005) 719.

Quantitative Assessment of Tryptophan Content in the Blood Plasma of Oropharyngeal Cancer Patients After COVID-19

Ivan Gnatyuk[a], Daryna Doni[b], Serhij Verevka[b], Alla Tarasenko[c], Olena Gnatyuk[a], Timur Isokov[a], Galyna Dovbeshko[a]

[a]*Institute of Physics, National Academy of Sciences of Ukraine, Kyiv 03028, Ukraine*
[b]*State Institution "O. S. Kolomiychenko Institute of Otolaryngology, National Academy of Medical Sciences of Ukraine", Kyiv 03057, Ukraine*
[c]*A.V. Palladin Institute of Biochemistry, National Academy of Sciences of Ukraine, Kyiv 02000, Ukraine*
matinelli@gmail.com

☒ I am applying for **Bruker Customer Excellence Award**

Clinical manifestations of various diseases correspond to a number of metabolic disorders. Therefore, the determination of the content of certain metabolites in the blood is one of the traditional methods for assessing the patient's condition, the effectiveness of treatment and the prognosis of possible complications. A comprehensive assessment of the content of free amino acids in blood plasma is informative for the diagnosis of oncological diseases. However, the implementation of this method in wide practice is limited due to the need to use complex laboratory equipment and expensive reagents. Tryptophan has unique luminescent properties, which allows its quantitative determination by the fluorimetric method.

The work examined the blood plasma of 17 patients with oropharyngeal cancer after suffering from COVID-19. Plasma samples were obtained by centrifugation at 4000 rpm for 20 minutes. A mixture of plasmas from three healthy people was used as a control. Precipitation of high-molecular proteins and peptides was carried out by adding an equal volume of 10% perchloric acid and centrifugation. After that, the blood plasma samples were additionally dissolved in phosphate buffer, with the final pH value being 7.5. Fluorescence spectra were measured on an Edinburgh Instruments FS 5 spectrophotometer in the wavelength range from 280 to 550 nm with a maximum under 360 nm, under excitation with a halogen lamp at a wavelength of 280 nm. To quantitatively assess the tryptophan content in blood plasma, a calibration curve was first constructed based on the fluorescence of a tryptophan solution at known concentrations in a system that was similar in composition to that used in the preparation of the samples under study.

The experimental data the content of free tryptophan in the blood plasma of cancer patients show a significant difference compared to control although these data do not have a pronounced correlation and may be either less or more than the control values. This may be a consequence of the different effects of two pathological processes. On the one hand, the intensification of tissue breakdown characteristic of cancer processes leads to changes in the composition of free amino acids in the bloodstream. On the other hand, it has been shown that in patients with COVID-19 and patients with oncopathology, a decrease in the level of tryptophan in the bloodstream is observed. The detected differences between the indicators of individual patients show a different ratio of the manifestation of at least these two processes. The data obtained in this work indicate the feasibility of prolonged determination of the content of free tryptophan in the blood plasma of cancer patients who have suffered COVID-19 or have been exposed to other viral diseases.

Acknowledgements: The authors G.O. and D.G. thank NRFU project "Biophysical characteristics of circulating metastatic cells as potential targets of antimetastatic therapy" 2021.01/0229.

Multiscale Imaging of Non-Adherent Tumor Cells: From Optical to Electron Microscopy

G. Monastyrskyi[a], O. Gnatyuk[a], M. Olenchuk[a], D. Kolesnik[b], A. Boisen[c], Z. Zhang[c], S. Karakhim[d], G. Solyanik[b], G. Dovbeshko[a]

[a]*Institute of Physics, Natl. Acad. of Sci. of Ukraine, Prospect Nauky, 46, UA-03028, Kyiv, Ukraine*
[b]*R.E. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology, Natl. Acad. of Sci. of Ukraine, 45, Vasylkivska str, Kyiv 03022, Ukraine*
[c]*Technical University of Denmark, Ørsteds Plads, Building 345C, DK-2800 Kgs. Lyngby, Denmark*
[d]*O.V. Palladin Institute of Biochemistry, NAS of Ukraine, 9 Leontovicha Str., 01030 Kyiv, Ukraine*
matinelli@gmail.com

Understanding cancer cells' morphological and structural adaptations under different environmental conditions is crucial for elucidating metastatic behaviour and resistance mechanisms. A comprehensive microscopy-based characterization of Lewis lung carcinoma (LLC) cells was performed, focusing on adhesive versus suspension culture conditions. We applied advanced imaging techniques, including scanning electron microscopy (SEM), confocal laser scanning microscopy, and Coherent Anti-Stokes Raman Scattering (CARS), providing an integrated view of cellular morphology, membrane topology, cytoskeletal dynamics, and intracellular lipid distribution. LLC cells were cultured under different conditions: on standard culture substrates promoting adhesion, and during deadhesive growth encountered by circulating tumor cells (CTCs).

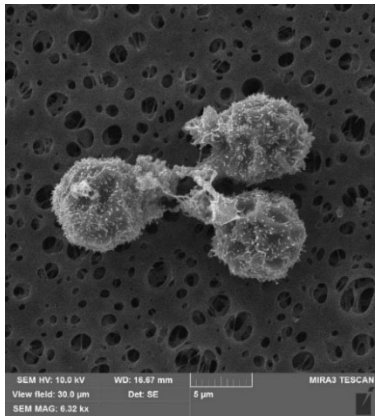


Figure 1 – SEM image in secondary electron (SE) mode of non-adherent LLC cells

SEM analysis revealed differences in cellular morphology between the adhesive and suspension-grown cells. Adherent LLC cells exhibited flat, spread morphologies with extensive lamellipodia and filopodia, facilitating substrate interaction and migration. In contrast, suspension-grown cells retained a near-spherical morphology, with rough surfaces marked by microvilli, membrane blebs, and vesicular protrusions. Confocal microscopy highlighted cytoskeletal adaptation to detachment stress, while CARS and SHG enabled non-invasive, chemically selective imaging of lipid and protein domains. These investigations simulate the biophysical state of CTCs and can thus inform on metastasis-specific morphology and stress responses

Acknowledgements: Authors acknowledge NRFU project No. 2021.01/0229 “Biophysical characteristics of circulating metastatic cells as potential targets of antimetastatic therapy”.

Macroscopic and Spectroscopic Properties of Bromo-Substituted Benzophenones

M. Drozd[a], J. Baran[a], N.A. Davydova[b]
[a] *Institute of Low temperature and Structure Research, PAS, 50-950, Wroclaw, Poland*
[b] *Institute of Physics, NANU, 46 pr. Nauki, 03028 Kyiv, Ukraine*
m.drozd@intibs.pl

It is the nonlinear properties of bromine-benzophenones that have attracted the attention of researchers and made the study of these compounds relevant [1].
The influence of the bromine position in the phenyl ring on the macroscopic and vibrational properties of bromo-substituted benzophenones was studied using spectroscopic and differential scanning calorimetry methods. Specifically, we investigated FT-IR, FT-Raman, low-frequency Raman spectra, and melting temperatures of the bromo-substituted benzophenones differing in the position of the Br atom in one of the phenyl rings (Fig. 1). This study allowed us to elucidate the effect of bromine position on the properties of three isomers of bromo-substituted benzophenones: 2-, 3-, and 4-bromobenzophenone (2-BrBP, 3-BrBP, and 4-BrBP, respectively).

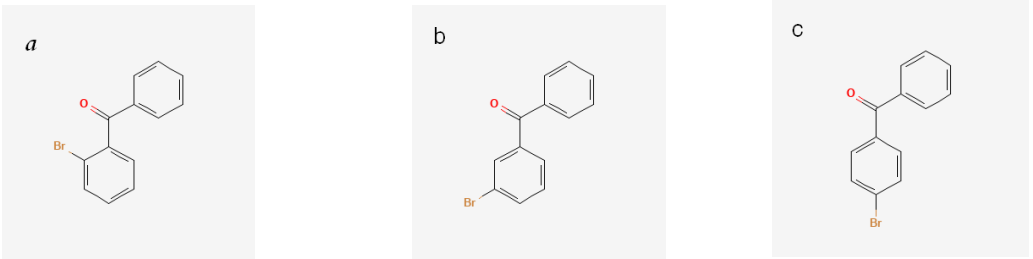


Figure 1 – The molecule structure for 2-BrBP (a); 3-BrBP (b), and 4-BrBP (c)

It was found, that an increase in the distance of the bromine atom relative to the carbonyl group C=O in the phenyl ring leads: to an increase in the melting point from 318.0 K in 2-BrBP to 358.0 K in 4-BrBP. The melting point of pure benzophenone at 326.8 K is located between the melting points in 2-BrBP and 3-BrBP; to a decrease in the stretching vibrations wavenumber Q(C=O) from 1659.4 cm^{-1} in 2-BrBP to 1648.5 cm^{-1} in 4-BrBP in the FT-IR spectra. The same change in the wavenumber of Q(C=O) vibration is also observed in the FT-Raman spectra. In pure benzophenone, the position of the C=O band in both spectra is located between the positions in 2-BrBP and 3-BrBP; to a low-frequency shift of lattice vibrations in bromo-substituted benzophenones relative to the corresponding vibration in pure benzophenone. In this respect, the closer the bromine atom is to the carbonyl group, the larger the shift.
It is important to note that the only difference between the three isomers is structure; thus, any differences in properties are directly related to structure.

References

1. B. Zhao, W.-Q. Lu, Z.-H. Zhou, Y. Wu, *J. Mater. Sci.*, 10 (2000) 1513.

Variable-Temperature FT-IR and DSC Studies of Fatty-Acid Eutectic Binary Mixtures

Tetiana Gavrilko[a,c], Ivan Gnatyuk[a], Viktor Styopkin[a], Natalia Shcherban[b], Jan Baran[c], Marek Drozd[c]

[a]*Institute of Physics, NAS of Ukraine, 46, Nauky Ave., 03028 Kyiv, Ukraine*
[b]*Institute of Physical Chemistry NAS of Ukraine, 31, Nauky Ave., 03028 Kyiv, Ukraine*
[c]*Institute of Low Temperature and Structure Research, PAS, 2, Okolna Str., 50-950 Wroclaw, Poland*
m.drozd@intibs.pl

A wide variety of organic eutectic mixture recently found application in pharmaceutical and pharmacological fields for the purposes of drug delivery systems due to improved physicochemical properties, such as solubility, dissolution rate and melting point. However, engineering of crystalline organic eutectic mixtures is still underdeveloped due to a lack of empirical or theoretical routes for eutectic structure formation. Earlier [1-2], we reported the results obtained on binary systems of long-chain aliphatic compounds containing $C_nH_{2n}O_2$ fatty-acid homologs with n=12, 18 or 22 carbon atoms (the latter called hereafter C_{18} and C_{22}). With precise XRD, DSC and Raman spectroscopy measurements, it was found in the previous study that a key element for C_{18}/C_{22} eutectic mixture microstructure was the presence of asymmetric hydrogen-bonded acid dimers formed by different acid molecules. The resulting multilayer crystal structure of C_{18}/C_{22} binary mixtures causes significant changes in the balance of hydrophobic and electrostatic molecular interactions, which is responsible for unique thermal properties of the mixtures, as compared to traditional behaviour of single acids, such as low melting temperature and unusual phase sequence behaviour. However, due to extremely complicated nature of such systems, molecular interactions and phase change mechanisms in eutectic mixtures are poorly studied so far.
As an extension of our previous work, here we investigated the molecular mechanism underlying phase behaviour of three C_{18}/C_{22} fatty-acid binary mixtures with near-eutectic C_{18}/C_{22} molar ratio using DSC measurements (Perkin-Elmer Model 8000) and temperature-variable FTIR spectroscopy (Bruker IFS-88, SPECAC variable temperature cell P/N 21.500 with Eurotherm controller 847) in 25-100°C temperature range. From the analysis of the FTIR spectral markers, it was shown that the phase transformations revealed by DSC in eutectic mixtures under study are initiated with onset of conformational disorder and orientational motions of methylene chains in asymmetric hydrogen-bonded acid dimers followed by induced overall crystal layer instability. The obtained results would be useful for better understanding of structure-properties relationship of other organic eutectic mixtures with application potential in medicine and pharmacy, food and construction industries.

References

1. T. Gavrilko, I. Gnatuyk, V. Styopkin, N. Shcherban, J. Baran, M. Drozd, *J. Mol. Struct.,* 1284 (2023) 135436.
2. T. Gavrilko, I. Gnatyuk, V. Styopkin, N. Shcherban, J. Baran, M. Drozd, *J. Mol. Struct.,* (2025, submitted).

Acknowledgements: TG greatly acknowledges Polish Academy of Sciences for PAN-NASU fellowship provided under the Long-term Program of Support of the Ukrainian researchers at the Polish Academy of Sciences in collaboration with the U.S. National Academy of Sciences.

Insights into Mononucleotide G-Quadruplex Self-Assembly via Raman Spectroscopy and Association Model Fitting

Lucia Ďuríšková, Štěpán Jílek, Václav Profant
Institute of Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Prague 2, Czech Republic
lucia.duriskova722@student.cuni.cz

Mononucleotide G-quadruplexes (mG4), intricate supramolecular structures formed by self-assembly of guanine mononucleotides, have attracted considerable attention due to their relevance in genomics, prebiotic chemistry, and bionanotechnology.[1] Despite extensive interest, fundamental questions remain regarding their formation mechanisms, cation-dependent topologies, and the nature of intermolecular interactions involved in their stabilization.

In this work, we investigate the self-assembly of guanosine-5'-monophosphate (5'rGMP) into mG4 structures[2] in the presence of sodium and potassium ions, using concentration- and temperature-dependent Raman spectroscopy as the primary analytical tool. By applying an association model that incorporates the stepwise formation of stacked monomers, G-quartets, and their further aggregation within an indefinite isodesmic framework, we extract quantitative insights into the assembly pathway. Deconvolution of the spectral series enables us to assign distinct Raman signatures to individual species: free monomer, stacked 5'rGMP aggregates, and fully formed mG4 structures.

Fitting of the experimental data yields thermodynamic parameters (ΔH, ΔS, K_{assoc}) characterizing each step of the association process, with notable differences observed between Na^+- and K^+-stabilized systems. These findings are corroborated by complementary UV absorption and electronic circular dichroism (ECD) spectroscopy. Our results offer a detailed spectroscopic and thermodynamic characterization of mG4 formation and highlight the utility of Raman spectroscopy combined with association modeling in unraveling complex supramolecular equilibria.

References
1. J.T. Davis, *Angew. Chem. Int. Ed.,* 43 (2004) 668.
2. M.S.P. Kkadan, Š. Jílek, V. Profant, J. Kapitán, J. Kessler, P. Bouř, *Chem. Eur. J.,* 30 (2024) e202403245.

Acknowledgements: This research was supported by the Charles University Grant Agency (GA UK) project no. 298123.

Interactions of Polymers with Efficient Solid SERS Substrates for Sensitive Detection

Jasmine S. Furter, Janina Kneipp
Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany
jasmine.furter@hu-berlin.de

Raman spectroscopy has proven to be useful for the identification, classification and quality control of synthetic polymers and their blends. The short sample preparation procedures, non-destructive nature, fast acquisition and high sensitivity towards non-polar functional groups make Raman spectroscopy an attractive characterisation technique. However, fluorescence arising from plastic additives and the polymers themselves strongly affect the weak Raman signals. One way to address this problem is an enhancement of the Raman signals by surface enhanced Raman scattering (SERS). The use of metal nanostructures that are needed for SERS in close vicinity to the analytes, moreover, helps to reduce sample fluorescence. By using metal nanoparticles in colloidal suspensions, however, the SERS enhancement varies due to their distribution within the focal volume, and altered stability and plasmonic properties due to interaction with the analyte. The immobilisation of SERS substrates in a bottom-up approach by immobilisation of gold nanoparticles on a glass surface [1-2] or the roughening of a metal surface by electrochemical methods [3] leads to a better-defined distribution of the nanostructures, a high (microscopic) homogeneity of the SERS enhancement, and more stable experimental set-up, thereby improving the reproducibility of the SERS signals [2]. We present the characteristics of such solid substrates in terms of surface morphology, plasmonic properties and SERS performance. SERS spectra of different polymer types in solid state, aqueous solution or suspension will be shown and the interaction of the macromolecules with the surface of functionalised and non-functionalised solid SERS substrates will be discussed.

References

1. V. Joseph, M. Gensler, S. Seifert, U. Gernert, J. P. Rabe, J. Kneipp, *J. Phys. Chem. C*, 116 (2012) 6859.
2. Z. Zhang, U. Gernert, R. F. Gerhardt, E.-M. Höhn, D. Belder, J. Kneipp, *ACS Catal.*, 8 (2018) 2443.
3. S. Kruszewski, *Surface & Interface Analysis,* 21 (1994) 830.

Acknowledgements: The authors thank the Swiss National Science Foundation (SNSF) for funding this project.

Meso-Substituted Phenothiazinyl-Porphyrins and their Indium and Zinc Complexes: Photophysical Properties, Photosensitisers for Photodynamic Therapy of Ovarian Cancer Cells

Emese Gál[a], Balázs Brém[a], Bianca Stoean (Vasile)[a], Eva Fischer-Fodor[b], Monica Focsan[c,d], Luiza Găină[a]

[a]*Research Center on Fundamental and Applied Heterochemistry, Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, 11 Arany Janos str., RO-400028 Cluj-Napoca, România;*
[b]*Institute of Oncology "Prof. Dr. Ion Chiricuta", RO-400015 Cluj-Napoca, România*
[c]*Nanobiophotonics and Laser Microspectroscopy Centre, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, 42 Treboniu Laurian Street, 400271, Cluj-Napoca, Romania.*
[d]*Biomolecular Physics Department, Faculty of Physics, Babes-Bolyai University,1 M. Kogalniceanu Street, 400084, Cluj-Napoca, Romania*
emese.gal@ubbcluj.ro

New phenothiazinyl porphyrins and their In(III)/Zn(II) complexes were synthesised and investigated for their fluorescent imaging and photodynamic therapy (PDT) capabilities. All compounds display red fluorescence, even within A2780 ovarian cancer cells. Notably, indium(III) ferrocenylvinyl phenothiazinyl porphyrin (**4a**) demonstrated superior performance as a photosensitizer, exhibiting a 29% fluorescence quantum yield, a 60% singlet oxygen quantum yield, and significant photo-induced cytotoxicity (IC_{50} = 36.38 µM) against A2780 cells, alongside pronounced oxidative stress and Nrf-2 activation.

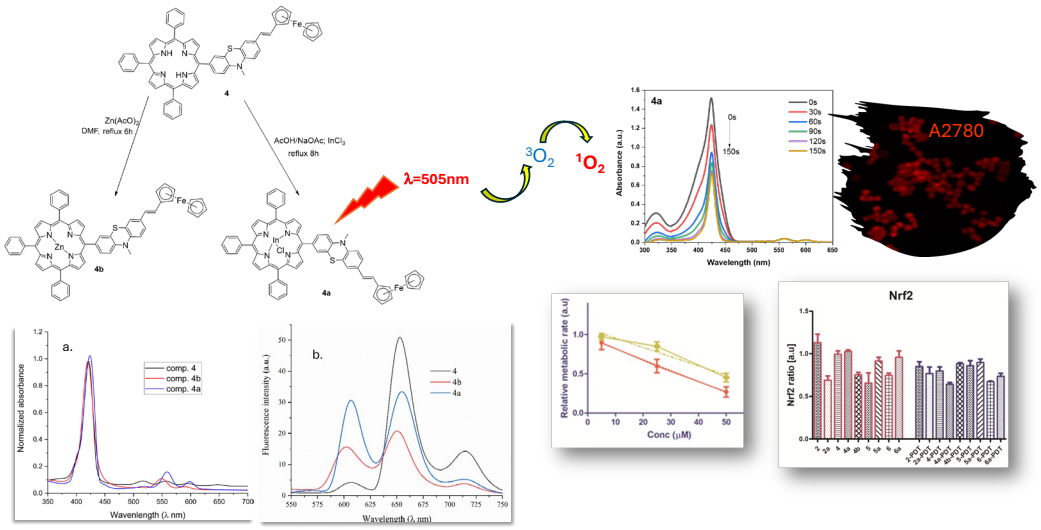


Figure 1 – Synthesis, photophysical characterisation and singlet oxygen generation of ferrocenylvinyl phenothiazinyl porphyrin complexes

References

1. B. Brem, B. Stoean, E. Molnar, E. Fischer-Fodor, O. Balacescu, R. Borlan, M. Focsan, A. Grozav. P. Achimas-Cadariu, E. Gal, L. Gaiana, *RSC Med. Chem.*, 16 (2025) 747.
2. E. Molnar, E. Gál, L. Găină, C. Cristea, L. Silaghi-Dumitrescu, *Molecules, 25*(19) (2020) 4546.
3. E. Molnar, E. Gal, L. Gaina, C. Cristea, E. Fischer-Fodor, M. Perde-Schrepler, P. Achimas-Cadariu, M. Focsan, L. Silaghi-Dumitrescu, *Int. J. Mol. Sci.*, 21 (2020) 3178.

Acknowledgements: This work was supported by the project "Targeted Tumor Therapy with multifunctional platinum(iv)-drug conjugates (T^3-Pt)" funded by European Union – NextGenerationEU and Romanian Government, PNRR, contract no 760240/28.12.2023, cod PNRR-C9-I8-CF 76/31.07.2023, through the Romanian Ministry of Research, Innovation and Digitalization, within Component 9, "Investment I8".

UV-Driven Self-Repair of Uracil Dimers in RNA via Directional Photoinduced Charge Transfer

Shivangi Garg, Barbara K. Lech, Rafał Szabla
Institute of Advanced Materials, Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspianskiego 27, Wrocław, 50-370, Poland
shivangi.garg@pwr.edu.pl

☒ I am applying for **Bruker Customer Excellence Award**

Cyclobutane pyrimidine dimers (CPDs), a common form of ultraviolet (UV)-induced nucleic acid damage, pose serious challenges to genomic integrity. While DNA repair mechanisms have been widely investigated[1-4], RNA self-repair, particularly via intrinsic photochemical pathways, remains largely unexplored. In this study, we demonstrate that RNA can undergo UV-induced self-repair of CPD lesions through a mechanism different from that of DNA. We employ molecular dynamics (MD) and quantum mechanics/molecular mechanics (QM/MM) simulations to study the excited-state dynamics underlying CPD self-repair in RNA tetranucleotides. Focusing on three representative conformers of GAU=U and U=UAG sequences, selected based on their population and stacking interactions, we explore various minima on the first excited-state (S_1) potential energy surface. Our simulations reveal conformer-dependent reactivity; while GAU=U/KM_0 and U=UAG/KM_1 conformers do not show favorable repair pathways, the GAU=U/KM_2 conformer exhibits a shallow S_1 minimum followed by an S_1/ground-state (S_0) conical intersection, indicating an efficient photochemical repair route. Notably, unlike in DNA, where negative charge facilitates thymine dimer repair[1,2], the positive charge on the uracil dimer appears critical for CPD repair in RNA. Frontier molecular orbital and natural transition orbital analyses further highlight the role of charge transfer and π-stacked excitations in modulating repair efficiency. These findings emphasize the importance of sequence context and conformational dynamics in RNA self-repair and suggest that non-enzymatic, excited-state repair pathways may have contributed to the early molecular evolution of life under UV-rich prebiotic conditions.

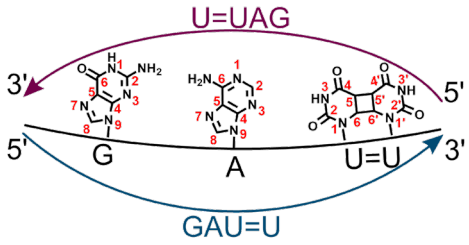


Figure 1 – Molecular structures and 5′→3′ directionality of GAU=U and U=UAG tetranucleotides

References

1. C.L. Kufner, S. Crucilla, D. Ding, P. Stadlbauer, J. Šponer, J.W. Szostak, D.D. Sasselov, R. Szabla, *Chem. Sci.*, 15 (2024) 2158.
2. R. Szabla, H. Kruse, P. Stadlbauer, J. Šponer, A.L. Sobolewski, *Chem. Sci.*, 9 (2018) 3131.
3. Z. Pan, J. Chen, W.J. Schreier, B. Kohler, F.D. Lewis, *J. Phys. Chem. B*, 116 (2012) 698.
4. W. Lee, S. Matsika, *J. Phys. Chem. B,* 127 (2022) 18.

Acknowledgements: The authors thank the National Science Centre Poland (2020/37/B/ST4/04092 to R. S.) for the support.

Photostability of Free-Base and Palladium *meso*-substituted Porphyrins in Organic Solvents and Aqueous Micellar Solutions

Natalia Dutkiewicz[a], Barbara Golec[b], Jarosław Kowalski[b], Jacek Waluk[a,b], Aleksander Gorski[a]
[a] *Institute of Physical Chemistry, Polish Academy of Sciences, 01-224 Warsaw, Poland*
[b] *Faculty of Mathematics and Science, Cardinal Stefan Wyszyński University, 01-815 Warsaw, Poland*
agorski@ichf.edu.pl

Photostability is a crucial parameter in applications involving light–matter interactions. In this work, we revealed that photodegradation efficiency can be significantly reduced by modifying the thermodynamic and kinetic characteristics of a chromophore. Photobleaching quantum yields were determined for a series of free-base octaethylporphyrins and their palladium metallocomplexes (Figure 1), gradually substituted with phenyl groups at the *meso* positions.[1] A comparison of photodegradation efficiencies in oxygenated and deoxygenated toluene samples shows a hundred-fold decrease in photobleaching quantum yields for nonplanar palladium porphyrins, reaching extremely low values of less than 10^{-9}.

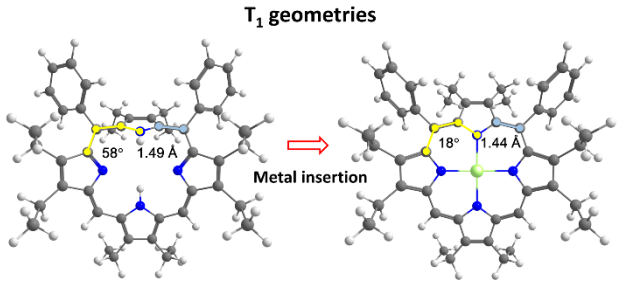


Figure 3 – Structural changes in the triplet state induced by metallation of a porphyrin derivative

We further demonstrate that, in aqueous micellar solutions, the efficiency of singlet oxygen generation and the photostability by different *meso*-aryl-porphyrins is clearly correlated with the experimentally determined microviscosity within Pluronic F127 micelles. Furthermore, we propose a simple and effective method for determining microviscosity based on the viscosity-dependent lifetime of the triplet state of a *meso*-phenyl-substituted octaethylporphyrin.

References

1. M. Banaszek, B. Golec, R. Rybakiewicz-Sekita, J. Kowalski, P. Szczodry. N. Dutkiewicz, J. Waluk, A. Gorski, *J. Phys. Chem. B* (2025), 10.1021/acs.jpcb.5c02423.

Acknowledgements: This work was supported by the Polish National Science Center grant no OPUS 2020/39/B/ST4/01956.

Infrared ATR Spectroscopy of Polyethylene Using ZnSe and Ge-ATR Crystals and Comparison of Results from Advanced ATR-Correction

P.R. Janissek[a], H.M. Heise[b]
[a] *Instituto Federal de Educação, Ciência e Tecnologia do Rio Grande do Sul (IFRS), Rua Avelino Antônio de Souza, 1730, Bairro Nossa Senhora de Fátima, CEP: 95043-700, Brazil*
[b] *Interdisciplinary Center for Life Sciences, South-Westphalia University of Applied Sciences, Frauenstuhlweg 31, D-58644 Iserlohn, Germany*
heise.h@fh-swf.de

Polyethylen (PE) is one of the most commonly used plastics in the world. It can be found in packaging, household goods, cable insulation, pipes and many other applications. There are different types, such as LDPE and HDPE, which can be mouldable, rigid or flexible depending on requirements. Its chemical resistance to many chemicals is particularly noteworthy. Due to its durability, it contributes to global plastic pollution if not disposed of correctly, causing drastic environmental problems.[1] Given its wide application and related environmental problems, its analysis is extremely relevant, and infrared spectroscopy is often used for characterization and quantitative analysis, especially with biodegradation.[2,3]

For routine measurements, transmission spectra, e.g. of thin films, have been recorded, which may have problems due to the strong material absorption bands, and the occurrence of disturbing interference fringes due to multi-beam interferometry must be mentioned. Attenuated total reflection (ATR) spectroscopy is an alternative measurement technique, by which the whole spectrum can be advantageously displayed owing to the wavelength dependent radiation penetration depth. However, dispersion effects, especially for strong absorption bands can have some drastic changes in band shapes and wavenumber shifts of the band maxima.[4] Therefore, a correction software package has been provided by several instrument manufacturers; for an overview on the opportunities, see a recent publication.[5] Here, spectra of polyethylene, recorded by multi-reflection ATR accessories from ZnSe and Ge, are presented for different reflection angles, and their ATR-effect corrected spectra obtained by Bruker OPUS software, minimizing the distortions observed in the ATR spectra, are shown with comparison to film transmission spectra and PE-powder, embedded in KBr and prepared as disk. Refractive index spectra of the same LDPE material obtained from ellipsometry measurements are also presented.

References

1. Z. Yao, H.J. Seong, Y.-S. Jang, *Ecotoxicol. Environ. Saf.*, 242 (2022) 113933.
2. S. Phan, J.L. Padilla-Gamiño, C.K. Luscombe, *Polym. Test.,* 116 (2022).
3. J.V. Gulmine, P.R. Janissek, H.M. Heise, L. Akcelrud, *Polym. Test.* 21 (2002) 557.
4. E.V. Miseo, P.J. Larkin, *Appl. Spectrosc. Pract.*, 3 (2025) 1.
5. T.G. Mayerhöfer, J. Popp, *Appl. Spectrosc.,* 79 (2025) 298.

Acknowledgements: Support from the Instituto de Tecnologia para o Desenvolvimento LACTEC, Curitiba, Brazil is gratefully acknowledged. Spectra from ellipsometry measurements were provided by Dr. Karsten Hinrichs, when he was with the Leibniz-Institut für Analytische Wissenschaften ISAS, Berlin

Infrared ATR-Spectroscopy of Proteins, Spectral Variance and Band Distortions Shedding Light on the Available Advanced Correction Algorithm

H.M. Heise, S. Paramasivam
Interdisciplinary Center for Life Sciences, South-Westphalia University of Applied Sciences, Frauenstuhlweg 31, D-58644 Iserlohn, Germany
heise.h@fh-swf.de

Infrared biospectroscopy has been applied to various fields of clinical chemistry for the analysis of biofluids and for medical diagnostics studying cells and tissues with the advantages of being non-destructive and label free.[1] Attenuated total reflection (ATR) spectroscopy is nowadays a routine measurement technique, by which the whole spectrum can be advantageously displayed owing to the wavelength dependent radiation penetration depth, which allows – dependent on the used accessory - adjusted effective pathlengths into the sample medium. However, dispersion effects, especially for strong absorption bands can have some drastic changes in band shapes and wavenumber shifts of the band maxima.[2] Therefore, a correction software package has been provided by several instrument manufacturers, conditions of which have recently been discussed.[3]
Dry film spectra of bovine serum albumin prepared from aqueous solutions were recorded by employing as ATR elements either a diamond prism with single reflection or a fiber-optic coupled Ge cone with two reflections, all under 45° as reflection angle. Different albumin layer thicknesses were prepared, and the recorded spectra were also undertaken for the advanced correction algorithm, provided by the Bruker OPUS software. For comparison, dry-film spectra were also recorded in transmission on a rough PTFE foil or prepared by the KBr pellet technique with albumin embedded in a refractive index constant matrix for avoiding dispersion effects. Further focus was on the application of the ATR measurement technique to investigate inhomogeneous samples such as monocytes with different ATR layer thicknesses and to analyze spectral band shift effects and how these could be "repaired" by the correction software. This is very important for secondary structure analysis of proteins, where the amide I band can be used for monitoring, e.g., of protein misfolding or a change in effective layer composition due to intra-cellular processes such as the cell membrane fusion of glucose transporter (GLUT4) molecules - with main α-helix secondary structure elements - from inner-cell storage vesicles after insulin stimulation. Especially, near cell membrane changes were to be time-dependently analyzed. Cellular depth dependent studies had been carried out, for example, for the identification of multiresistant leukemia cells, an important problem in cancer chemotherapy.[4]

References
1. M.J. Baker, J. Trevisan, P. Bassan et al., *Nat. Protoc.,* 9 (2014) 1771.
2. E.V. Miseo, P.J. Larkin, *Appl. Spectrosc. Pract.*, 3 (2025) 1.
3. T.G. Mayerhöfer, J. Popp, *Appl. Spectrosc.,* 79 (2025) 298.
4. A. Gaigneaux, E. Goormaghtigh, *Analyst,* 138 (2013) 4070.

Development of Reference Materials for NIR Spectrometric Moisture Determination in Harvested Crops Using Reflection Measurement

O. Tyshkovets, R. Schulenburg, H.M. Heise
Interdisciplinary Center for Life Sciences, South-Westphalia University of Applied Sciences, Frauenstuhlweg 31, D-58644 Iserlohn, Germany
heise.h@fh-swf.de

For many decades now, NIR spectroscopy has been used for rapid and non-destructive quantitative multicomponent analyses of organic materials and especially of forages. A powerful measurement technique is diffuse reflection spectroscopy, which can be applied to powders, requiring little or even no sample preparation.[1] Especially in the field of agricultural products, the determination of moisture content, constituents such as crude protein, fiber content and other parameters plays an important role using calibrations with NIR reflectance spectra. Here, chemometric aspects and the use of reference materials are fundamentally important, especially when it comes to quality assurance and especially the performance testing of NIR spectrometers. The main focus was on long-term stable reference materials with defined water content without decomposition of the organic material or evaporation of the water leading to changes in the spectrum of the reference materials.
In the past, enormous spectral differences between previously suggested substitute materials as reference standards and forage samples, problems from the volatility of moisture present in harvested material, and the decomposition of moist biomass by bacterial processes if complete sterility cannot be guaranteed, must be noted. The complications could either completely eliminated or greatly attenuated by an innovative combination of mixing water-binding silica gel and dry feed. Preliminary tests were carried out with precisely water-loaded silica gel in combination with whole-plant chaff preserved by drying. It was found that blends of water-loaded silica gel of different types (with maximum water holding capacity of about 40 %) and dried forage powders showed tremendous spectral similarity compared to wet chaff with defined moisture. The silica content in the blended samples could be easily increased without causing any significant spectral deviations especially in the intervals of 5500 to 4500 cm^{-1} as well as of 7700 to 6000 cm^{-1} when compared to the spectra, e.g., of wet forage specimens showing significant water absorption bands. To verify the suitability of such mixtures as standard reference materials, as well as the possibility of setting defined moisture contents, standards were prepared and analyzed for their water concentration using a pre-developed PLS method based on reflectance spectra of whole-plant chaff with defined moisture content. It was found that the prediction results of silica blends differed only minimally from the actual moisture values from gravimetry. In addition, the prepared reflectance standards could be sealed in an appropriate housing with a sapphire disk to achieve long-term stability.

Reference
1. H.M. Heise, R. Schulenburg, Near-infrared spectroscopy for medical, food and forage applications, in: *Molecular and Laser Spectroscopy: Advances and Applications*, V.P. Gupta (ed.), Vol. III, Elsevier, Singapore, 2022, chapter 6.

Investigations on the Permeation of Solvents Through Polymer Materials of Protection Gloves Using ATR IR Spectroscopy with Importance to Occupational Safety

Y. Fu, H.M. Heise
Interdisciplinary Center for Life Sciences, South-Westphalia University of Applied Sciences, Frauenstuhlweg 31, D-58644 Iserlohn, Germany
heise.h@fh-swf.de

In the last decades, occupational skin exposure to hazardous chemicals increased significantly. Various strategies have been implemented to reduce dermal exposure at the workplace, comprising also the substitution of chemicals used with less toxic options or the isolation of the contamination source, but the use of personal protective equipment (PPE) is still the implemented solution to create a barrier for isolating the skin of the worker from possible contact with hazardous substances. Chemical resistant protective gloves are fundamental to protect against dermal exposure, whereas the chemical permeation through gloves is normally assessed using a standardized diffusion cell.[1] In the past, infrared spectroscopy using the attenuated total reflection technique (ATR) has been successfully used to study permeation of chemicals through polymer materials.[2,3]
This study also focused on the ATR technique to evaluate the suitability of different types of protective gloves, such as polyethylene (PE), latex and nitrile, all of different thicknesses, as personal protective equipment (PPE) against different chemical solvents. Real-time data collection and analysis of the time dependent solvent absorbances by suitable exponential functions was used to investigate how these materials resist solvents such as n-hexane, toluene and methanol in order to provide practical recommendations for the selection of suitable protective gloves. The experimental results show that the permeation resistance of the gloves is highly dependent on the material and thickness. Nitrile gloves offer the best protection against organic solvents, especially thicker variants show excellent resistance to n-hexane and toluene. For PE gloves, on the other hand, the fastest permeation for all chemicals tested was experienced, and this polymer also exhibited unconventional permeation dynamics, possibly related to material swelling. Latex gloves provided a medium barrier, but proved to be less than ideal for long-term protection against organic solvents.
Despite the comprehensive analysis, there are some limitations of this study, as the experiments were carried out under controlled laboratory conditions. However, factors such as temperature, pressure and mechanical stress on the gloves could significantly influence the actual permeation rate in practical applications. These limitations should be taken into account when interpreting the results.

References

1. M. Creta, L.D. Savory, R.C. Duca, W.K. Chu, K. Poels et al., *J. Hazard. Mater.*, 411 (2021) 1.
2. P. Heinrich, R. Wyzgol, B. Schrader, A. Hatzilazaru, D.W. Lübbers, *Appl. Spectrosc.*, 44 (1990) 1641.
3. K. O'Callaghan, P.M. Fredericks, D. Bromwich, *Appl. Spectrosc.*, 55 (2001) 555.

Dielectric Properties of Reverse Micelles Formed by Nonionic Surfactants

Sara Helscher, Kazimierz Orzechowski
Faculty of Chemistry, University of Wrocław, Fryderyka Joliot-Curie 14, 50-383 Wrocław, Poland
333205@uwr.edu.pl

Reverse micelles formed by nonionic surfactants in nonpolar solvents offer a useful model for studying confined water and aggregation phenomena at the nanoscale. This work investigates such systems composed of polyoxyethylene-based surfactant Tween 20 and cyclohexane, with varying water content, focusing on their dielectric properties and aggregation behavior.

Measurements of the nonlinear dielectric effect (NDE), consisting of a comparison of the electric permittivity measured at strong and weak electric fields [1], revealed a negative effect in these systems, reflected in a slight decrease of dielectric permittivity under strong electric fields (Figure 1). In contrast, in reverse micelles formed by ionic surfactant, an exceptionally large positive NDE effect was observed [3,4]. The present finding confirms the former interpretation of the positive NDE effect, assumed to be a result of ion movement in micro-inhomogeneous environments. In the system with nonionic surfactants, the positive NDE effect was observed only in samples suspected of exhibiting liquid crystalline ordering.

Complementary analyses included the construction of phase diagram and measurements of viscosity, density, and refractive index, enabling a broader interpretation of structural trends. The dielectric behavior and NDE response were found to depend sensitively on both hydration level and surfactant concentration, underscoring the value of these methods in probing microstructural organization in soft matter systems.

These findings demonstrate that dielectric spectroscopy, and especially NDE, can serve as an effective and noninvasive tool for characterizing reverse micellar systems based on nonionic surfactants.

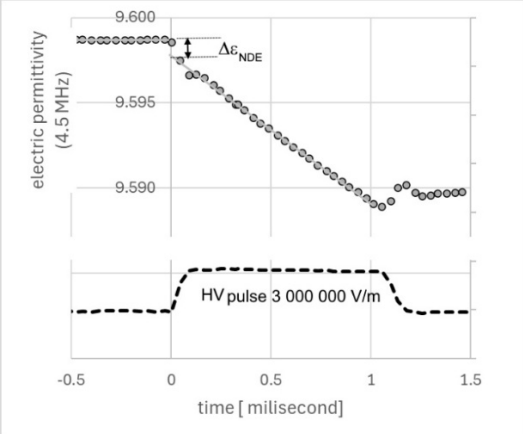


Figure 4 – Exemplary NDE response for a reverse micellar solution composed of Tween 20, water and cyclohexane at fixed composition (92.5 wt% Tween 20, 2.5 wt% water, 5 wt% cyclohexane). The dashed line represents the high-field polarizing pulse

References

1. A. Chełkowski, A. *Dielectric Physics* (Vol. 9). Elsevier Scientific Publishing Company / PWN – Polish Scientific Publishers, 1980.
2. K. Małycha, M. Pocheć, K. Orzechowski, *J. Mol. Liq*., 291 (2019) 111344.
3. K. Małycha, K. Orzechowski, A. Burakowski, *J. Mol. Struct*., 1318 (2024) 139370.

Single-Crystal Polarized Raman Spectra of 6-Bromopyridine-2-carbaldehyde

Gulce O. Ildiz[a,b], Anna Luiza B. Brito[b], Bernardo A. Nogueira[b,c], Matteo Tommasini[d], Rui Fausto[a,b]

[a]*Spectroscopy@IKU, Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Ataköy Campus, Bakırköy, Istanbul, Türkiye*

[b]*CQC-IMS, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal*

[c]*International Iberian Nanotechnology Laboratory (INL), 4715-330 Braga, Portugal*

[d]*Dipartimento di Chimica, Materiali e Ingegneria Chimica 'Giulio Natta', Politecnico di Milano, Piazza Leonardo da Vinci 32, Milano, I-20133, Italy*

g.ogruc@iku.edu.tr

The room temperature (RT) single-crystal polarized Raman spectra of 6-bromopyridine-2-carbaldehyde (BPCA) have been obtained and interpreted based on fully periodic DFT calculations for the $P2_{1/a}$ (No. 14; monoclinic) crystal of the compound. The calculations, performed with the CRYSTAL software employing the Becke three parameters Lee, Yang and Parr (B3LYP) functional and the polarization-consistent triple-zeta valence plus polarization basis set (pob-TZVP), were able to reproduce very well the experimental data, thus allowing detailed assignment of the Raman active A_g and B_g modes to individual bands. The isotropic non-polarized Raman spectrum of BPCA was also calculated and also shown to agree very well with the corresponding experimental Raman spectrum. Finally, the RT infrared spectrum of BPCA was also revisited at light of the performed periodic calculations, improving on previously reported interpretation based on extrapolation of the interpretation of the spectra obtained for the isolated molecule of the compound to the crystalline phase. In this crystalline system, intermolecular interactions exert only a minor influence on the intramolecular vibrational potential. As such, this study also serves as a benchmark for the employed computational approach, demonstrating its ability to capture the effects of both crystallographic periodicity and symmetry on the polarization features of vibrational spectra.

References

1. R. Fausto, G.O. Ildiz, C.M. Nunes, *Chem. Soc. Rev.*, 51 (2022) 2853.

Acknowledgements: The author thanks the Horizon-Widera-2023-Talents-01 ERA-Chair 1011848998 Spectroscopy@IKU "Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals", which is Funded by the European Union. The IMS-CQC is funded by the Portuguese Science Foundation, projects UIDB/00313/2025 (https://doi.org/10.54499/UIDB/00313/2025), UIDP/00313/2025 (https://doi.org/10.54499/UIDP/00313/2025) and IMS-LA/P/0056/2020 (https://doi.org/ 10. 54499/ LA/P/ 0056/ 2020).

Infrared Photodissociation Spectroscopy of $Cu_2(OAc)_2(D_2)_n^+$ and its Isotopologues

Hrittik Karmakar, Shabnam Haque, Jiaye Jin, Knut R. Asmis
Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Linnéstraße 2, 04103 Leipzig, Germany.
hrittik.karmakar@uni-leipzig.de

☒ I am applying for **Bruker Customer Excellence Award**

Dihydrogen complexation by metal cations has been extensively investigated in the context of H_2 activation.[1] More recently, dihydrogen adsorption at metal sites particularly Cu(I) within metal organic framework materials has gained attention for potential applications in H_2/D_2 separation.[2] To better understand the binding interaction that govern such isotope separation, we investigate the interaction of H_2 and D_2 with a Cu(I) paddlewheel motif under isolated gas-phase conditions, free from the influences of condensed phase environments.
In this study, we report the infrared photodissociation (IRPD) spectra of mass-selected $Cu_2(OAc)_2(H_2)_n^+$ and $Cu_2(OAc)_2(D_2)_n^+$ complexes (n = 1–2), recorded in a cryogenic ion trap at 10 K and 12 K, respectively. These measurements are complemented by anharmonic vibrational analysis at the VPT2/MP2/def2-TZVPP level of theory, enabling structural assignments and interpretation of vibrational features. The spectra show distinct vibrational signatures of dihydrogen isotopes, including fundamental H–H and D–D stretching bands as well as combination modes involving Cu^+–(H_2/D_2). Frequency shifts and intensity patterns reveal isotope dependent effects, which are discussed in comparison to previously studied systems such as $Cu(H_2)_4^+$ and $Cu(H_2O)(H_2)_2^+$.[3,4] The results highlight the role of the acetate-based paddlewheel scaffold in tuning the strength and dynamics of H_2/D_2 binding at Cu(I) centres under isolated gas-phase conditions. These findings will be helpful to understand the role of Cu(I) sites for the separation of hydrogen isotope.

References
1. V. Dryza, B.L.J. Poadw, E.J. Bieske, *Phys. Chem. Chem. Phys.*, 14 (2012) 14954.
2. I. Weinrauch, I. Savchenko, D. Denysenko, S.M. Souliou, H.H. Kim, M. Le Tacon, L.L. Daemen, Y. Cheng, A. Mavrandonakis, A.J. Ramirez-Cuesta, D. Volkmer, G. Schütz, M. Hirscher, T. Heine, *Nat. Commun.*, 8 (2017) 1.
3. J. Jin, T. Wulf, M. Jorewitz, T. Heine, K. R. Asmis, *Phys. Chem. Chem. Phys.*, 25 (2023) 5262.
4. E. G. Dongmo, S. Haque, F. Kreuter, T. Wulf, J. Jin, R. Tonner-Zech, T. Heine, K. R. Asmis, *Chem. Sci.*, 15 (2024) 14635.

Acknowledgements: This work was funded by the Deutsche Forschungsgemeinschaft (DFG) Project ID 443871192 – GRK 2721: "Hydrogen Isotopes, ^{1,2,3}H".

Cosmic-Ray-Driven Chemistry in the CH_3CH_2OH, NH_3, and CH_3CH_2OH : NH_3 Interstellar Ice Analogs

Barbara Keresztes[a,b], Sándor Góbi[a], Anita Schneiker[a,b], György Tarczay[a,c]
[a]*Laboratory of Molecular Spectroscopy, Institute of Chemistry, ELTE H-1518 Budapest, Hungary*
[b]*Hevesy György PhD School of Chemistry, Institute of Chemistry, ELTE H-1518 Budapest, Hungary*
[c]*Centre for Astrophysics and Space Science, ELTE H-1518 Budapest, Hungary*
barbi1226@gmail.com

☒ I am applying for **Bruker Customer Excellence Award**

The icy surface of interstellar grains could be a source of chemical complexity in the interstellar medium (ISM). In these icy mantles, gas-phase species of the ISM can freeze out, and then chemical reactions can be triggered by ultraviolet (UV) irradiation, cosmic ray (CR) radiation, or various radicals.[1] Afterward, the reaction products can sublime, modifying the chemical composition of the gas-phase ISM.[1,2]
In our experiments, we modeled the chemistry of these icy cover under laboratory conditions, focusing on the reactions of ethanol (CH_3CH_2OH) ice, ammonia (NH_3) ice, and CH_3CH_2OH : NH_3 ice mixtures. CH_3CH_2OH and NH_3 are two astrochemically important molecules, as both have already been identified in the ISM.[3,4] To simulate CR irradiation, the ice samples were bombarded with 5 keV electrons. Subsequently, to mimic the desorption of the reaction products from the ice phase, temperature-programmed desorption (TPD) was applied, in which the ice samples were heated up from 3 K to 300 K. During this process, different methods were used in separate experiments. In the first set of experiments, the chemical composition of the ice was monitored throughout the entire TPD phase. In another set of experiments, the sublimating molecules were captured and isolated in an Ar matrix, enabling their more sensitive identification. Fourier-transform infrared (FTIR) spectroscopy was utilized during all the experimental steps to follow chemical changes.
Upon the analysis of the IR spectra the following reaction products of CH_3CH_2OH were identified: CH_4, CH_3CH_3, CH_2CH_2, $CH_3CH_2CH_3$, CH_2CHOH, CH_2O, CH_3CHO, CH_2CO, $CH_3C(O)CH_3$, CH_3COOH, CO, CO_2, $H\dot{C}O$, $H_2\dot{C}OH$, CH_3OH, CH_2CHCHO, and HCOOH. For pure NH_3 ice, the experimental results were consistent with previous studies.[5] In the case of the CH_3CH_2OH : NH_3 ice mixture, in addition to the products detected in the one-component experiments, several N- and O-containing organic molecules were formed. These molecules, which are crucial for the possible formation of biomolecules, included acetamide ($CH_3C(O)NH_2$), formamide (NH_2CHO), and isocyanic acid (HNCO). The results of these experiments enhance our understanding of the chemistry of the ISM, particularly the origin of interstellar complex organic molecules and indirectly the origin of life.

References

1. E.F. van Dishoeck, G.A. Blake, *Annu. Rev. Astron. Astrophys.,* 36 (1998) 317.
2. W.D. Watson, E.E. Salpeter, *Astrophys. J.,* 174 (1972) 321.
3. B. Zuckerman, et al., *Astrophys. J.,* 196 (1975) L99.
4. A.C. Cheung, et al., *Phys. Rev. Lett.,* 21 (1968) 1701.
5. W. Zheng, D. Jewitt, Y. Osamura, R.I. Kaiser, *Astrophys. J.,* 674 (2008) 1242.

Acknowledgements: The authors thank for the Hungarian Scientific Research Fund (OTKA K143196) and the NKFIH excellence grant (TKP2021-NKTA-64) for funding the research work. The authors were also supported by the "DKOP-23 Doctoral Excellence Program" (B.K.), and "EKOP-24 University Excellence Scholarship Program" (A.S.) of the KIM from the source of the NKFIH, and by the "Bolyai Scholarship" (S.G.) of MTA.

Electrochemical SERS Investigation of Thiol-Based Molecular Layers on Plasmonic Substrates

Matěj Kmetík[a], Jakub Havránek[a], Ivan Kopal[a,b], Marcela Dendisová[a]
[a]*Department of Physical Chemistry, University of Chemistry and Technology Prague, Technická 5, Prague 6, 166 28, Czech Republic*
[b]*Institute of Photonics and Electronics, Czech Academic of Sciences, Chaberská 1014/57, Prague 8, 182 00, Czech Republic*
kmetikm@vscht.cz

Electrochemical surface-enhanced Raman scattering (EC-SERS) is a technique with a history of more than 50 years and offers numerous advantages. However, the precise interpretation of SERS spectra under applied potential remains a significant challenge. This difficulty arises from the interplay of various enhancement mechanisms and the possible electrochemical transformation of the probed molecule. On the other hand, the applied potential eliminates the necessity to wait for the molecule to adsorb onto the plasmonic substrate spontaneously. It also enables a deeper investigation into the chemical enhancement mechanism, which, although not yet fully understood, is an integral and particularly intriguing part of the Raman enhancement on metallic substrates. Despite the numerous SERS-related publications documenting chemical transformations of molecules on surfaces, EC-SERS provides an additional and more detailed perspective, thanks to the applied potential even for well-studied model analytes such as thiols. [1,2]

In this study, we present our observations on the behavior of aromatic thiols (4-aminobenzenethiol and *p*-xylene-*α*-thiol) on a gold substrate. Thanks to a newly custom-designed electrochemical cell tailored for our inVia Renishaw Raman microscope, it was possible to monitor not only the reaction kinetics of molecular adsorption on the substrate without an applied potential but also under electrochemical control. SERS, adsorption kinetic, and EC-SERS measurements were conducted using a 785 nm laser. Based on the collected data, we were able to determine the adsorption mechanism and the course of molecular transformations on plasmonic substrates.

Thanks to the broader insight provided by our custom-built spectroelectrochemical cell, we believe that our findings make a significant contribution to the clarification of the chemical enhancement mechanism and the possible modes of molecular interaction with the substrate.

References
1. I. Kopal, M. Švecová, V. Jeřábek, D. Palounek, A. Michalcová, et al., *ACS Omega*, 9 (2024) 6005.
2. R. Moldovan, E. Vereshchagina, K. Milenko, et al., *Anal. Chim. Acta*, 1209 (2022), 339250.

Acknowledgements: The authors acknowledge support from the grant Specific university research – No. A1_FCHI_2025_001.

The Role of Cardiolipin and Cytochrome *C* in Mitochondrial Metabolism of Cancer Cells Determined by Raman Imaging: *in vitro* Study on the Brain Glioblastoma U-87 MG Cell Line

Monika Kopec[a,b], Aleksandra Borek-Dorosz[b], Karolina Jarczewska[a], Malgorzata Baranska[b], Halina Abramczyk[a]

[a]*Lodz University of Technology, Faculty of Chemistry, Institute of Applied Radiation Chemistry, Laboratory of Laser Molecular Spectroscopy, Wroblewskiego 15, 93-590 Lodz, Poland*

[b]*Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387 Krakow, Poland*

monika.kopec@p.lodz.pl

Within the central nervous system (CNS), cardiolipin is found to be an essential player within both neuronal and non-neuronal glial cells, where it regulates metabolic processes, supports mitochondrial functions, and promotes brain cell viability. The cardiolipin–cytochrome *c* interactions can affect the cell's ability to regulate mitochondrial activity. [1] It is now widely accepted that cardiolipin plays a central role in mitochondrial metabolism by maintaining the proper flexibility and morphology of the mitochondrial membranes and by regulating the activity of a variety of enzymes and proteins, including cytochrome *c* involved in mitochondrial function. [2] However, the mechanisms are still not well understood. Understanding the underlying regulatory mechanisms requires pathway-targeted, informative experimental data. However, practical experimental design approaches are still in their infancy.

An experimental framework by Raman imaging and a model for the identification of regulatory mechanisms in cancers induced by cardiolipin has been proposed. It has been provided that cardiolipin–cytochrome *c* interactions are key to mitochondrial energy homeostasis by controlling the redox status of cytochrome *c* in the electron transport chain, switching on/off Fe^{2+}/Fe^{3+} of cytochrome *c* in the electron transport chain and turning on the peroxidase activity. The decrease of the Raman signals of the oxidized Fe^{3+} cytochrome *c* in mitochondria in a cancer cell upon interactions with cardiolipin suggests the transformation into iron-oxo (ferryl) intermediates called compound I and compound II, which are (unprotonated) Fe^{IV}=O or (protonated) Fe^{IV}-OH. These species are formed when the binding of cytochrome *c* to cardiolipin converts it from an electron shuttle carrier in the electron transport chain into a peroxidase complex that catalyzes cardiolipin oxidation; this process plays a pivotal role in the mitochondrial stage of oxidative phosphorylation (respiration) and the execution of the cell death program via apoptosis. [3]

The newly discovered role of cytochrome *c* in the electron transport chain, apoptosis and ROS activity will allow the exploitation of this knowledge for drug discovery purposes based on their ability to manipulate cardiolipin peroxidation in cytochrome *c*/cardiolipin complexes.

References

1. V. E. Kagan, H. A. Bayir, N. A. Belikova, O. Kapralov, Y. Y. Tyurina, V. A. Tyurin, J. Jiang, D. A. Stoyanovsky, P. Wipf, P. M. Kochanek, J. S. Greenberger, B. Pitt, A. A. Shvedova, G. Borisenko, *Free Radicals Biol. Med*., 46 (2009) 1439.
2. A. J. Chicco, G. C. Sparagna, *Am. J. Physiol.: Cell Physiol.*, 292 (2007) 33.
3. M. Kopec, A. Borek-Dorosz, K. Jarczewska, M. Barańska, H. Abramczyk, *Analyst*, 149 (2024) 2697.

Acknowledgments: This work was supported by the National Science Centre of Poland (Narodowe Centrum Nauki, OPUS, UMO-2021/43/B/ST4/01547)

Hydrogen Bonding in Glycolic Acid–Water Complexes: Experimental and Computational Study

Justyna Krupa[a], Iwona Kosendiak[a], Maria Wierzejewska[a], Jan Lundell[b]
[a]*Faculty of Chemistry, University of Wrocław, Joliot-Curie 14, 50-383 Wrocław, Poland;*
[b]*Department of Chemistry, University of Helsinki, P.O.Box 55 (A.I.Virtasen aukio 1), 00014 University of Helsinki, Finland*
justyna.krupa@uwr.edu.pl

Glycolic acid (GA), the smallest α-hydroxycarboxylic acid, contains two OH groups capable of forming intra- and intermolecular hydrogen bonds. While the most stable conformer is known to dominate under various conditions [1,2], molecular complexes of GA have received less attention. This work investigates the 1:1 hydrogen-bonded GA–H_2O complexes using matrix isolation FTIR spectroscopy supported by MP2 and B3LYPD3 calculations [3].

Five low-energy GA···H_2O complexes were characterized computationally (Figure 1). The most stable structure, C1, features a six-member ring formed by two intermolecular O–H···O hydrogen bonds, where water acts both as a proton donor and acceptor. This structure retains the intramolecular hydrogen bond in GA and was unambiguously identified in solid argon matrices. Two other forms, C2a and C2b, tentatively present based on weak IR bands, result from water insertion into the internal GA hydrogen bond, forming seven-membered rings. The experimental IR spectra agree best with MP2-predicted vibrational shifts, confirming C1 as the dominant complex. The observed C1 geometry corresponds to the glycine–water complex reported in jet spectroscopy [4], suggesting a recurring hydrogen-bonding pattern among small carboxylic acids.

This work highlights the subtle balance of intra- and intermolecular interactions in aqueous environments and provides experimental insight into the conformational preferences of GA–water complexes, with implications for atmospheric and biological chemistry.

Figure 1 – The MP2 optimized structures of the 1:1 complexes of GA with water

References
1. C.M. Nunes, I. Reva, R. Fausto, *Phys. Chem. Chem. Phys.,* 21 (2019) 24993.
2. I. Reva, S. Jarmelo, L. Lapinski, R. Fausto, *Chem. Phys. Lett.*, 389 (2004) 68.
3. J. Krupa, I. Kosendiak, M. Wierzejewska, J. Lundell, *Spectrochim. Acta A,* 325 (2025) 125081.
4. J.L. Alonso, E.J. Cocinero, A. Lesarri, M.E. Sanz, J.C. Lopez, *Angew. Chem. Int. Ed.,* 45 (2006) 3471.

Acknowledgements: Allocation of computer time from the Wrocław Centre for Networking and Supercomputing (Wrocław, Poland) is gratefully acknowledged. The support of the COST Action CA21101 (COSY) is highly appreciated. Funding: This research was funded by the Academy of Finland [grant number 332023], for the work performed at the University of Jyväskylä.

6-Methyl-3-nitro-2-[2-(5-nitropyridin-2-yl)hydrazinyl]pyridine: Synthesis, Spectroscopic Characterization, Structural Relationships and Potential Biological Activity

E. Kucharska[a], J. Michalski[a], I. Bryndal[b], L. Dymińska[a], A. Pyra[c], W. Sąsiadek[a], M. Ptak[d], J. Hanuza[d]

[a]*Wroclaw University of Economics and Business, 53-345 Wrocław, Poland*
[b]*Faculty of Pharmacy, Wroclaw Medical University, 50-556 Wrocław, Poland*
[c]*Faculty of Chemistry, University of Wroclaw, 50-383 Wrocław, Poland*
[d]*Institute of Low Temperature and Structure Research, PAN, 50-422 Wrocław, Poland*
edyta.kucharska@ue.wroc.pl

☒ I am applying for **Bruker Customer Excellence Award**

Hydrazo aromatic derivatives are an important group of organic compounds used as ingredients of drugs and metal complexes [1,2] or nonlinear optical materials [3,4].
The structure of newly obtained 6-methyl-3-nitro-2-[2-(5-nitropyridin-2-yl)hydrazinyl] pyridine (MNHP) was established by spectroscopic NMR, IR, Raman and UV-Vis studies. MNHP crystallizes in the orthorhombic Pbca space group with one crystallographically independent molecule in the asymmetric unit. Experimental single-crystal X-ray studies were performed and the results were compared with the molecular structure (Figure 1) obtained from DFT calculations (B3LYP/6-311G(2d,2p)) with particular attention to the conformation of the C-NH-NH-C hydrazo bridge and intra- and intermolecular hydrogen bonds.

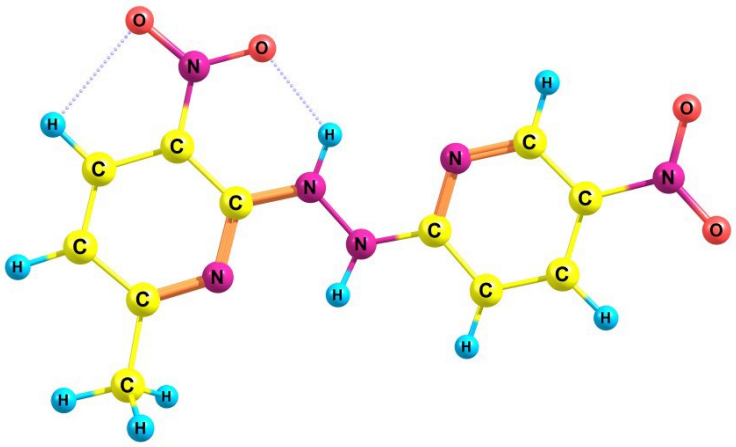


Figure 1 – Molecular structure of 6-methyl-3-nitro-2-[2-(5-nitropyridin-2-yl)hydrazinyl]pyridine

References
1. D.A. Tafere, M. Gebrezgiabher, F. Elemo, T. Sani, T.B. Atisme, T.G. Ashebr, I.N. Ahmed, *RSC Adv.*, 15 (2025) 6191.
2. M. Moreira, S. dos Santos Félix Vieira, G. de Deus Correia, L. Nascimento de Almeida, S. Finoto, C.A. Brandl, A.A. Msumange, F. Galvão, K.M.P. de Oliveira, G.C. Paveglio, M.M. da Silva, B. Tirloni, C.T. de Carvalho, D. Roman, *ACS Omega*, 10 (2025) 7428.
3. P. Justin, K. Anitha, *J. Mol. Struct.*, 1245 (2021) 131199.
4. D. Hannachi, N. Khelfaoui, M. Zaidi, D. Yahiaoui, S. Lakehal, C. Morell, H. Chermette, *New J. Chem.*, 47 (2023) 18359.

Synthesis, Structural Characterization, and Spectroscopic Analysis of 6-Methyl-3-nitro-2-[(*E*)-(5-nitropyridin-2-yl)diazenyl]pyridine: a Potential Azo-Linked Dye

E. Kucharska[a], J. Michalski[a], I. Bryndal[b], L. Dymińska[a], A. Pyra[c], W. Sąsiadek[a], M. Ptak[d], J. Hanuza[d]

[a]*Wroclaw University of Economics and Business, 53-345 Wrocław, Poland*
[b]*Faculty of Pharmacy, Wroclaw Medical University, 50-556 Wrocław, Poland*
[c]*Faculty of Chemistry, University of Wroclaw, 50-383 Wrocław, Poland*
[d]*Institute of Low Temperature and Structure Research, PAN, 50-422 Wrocław, Poland*
edyta.kucharska@ue.wroc.pl

☒ I am applying for **Bruker Customer Excellence Award**

Azo aromatic derivatives are widely used as dyes [1,2]. This study is a continuation of our earlier work on azo derivatives of pyridine [3].

New compound 6-methyl-3-nitro-2-[(*E*)-(5-nitropyridin-2-yl)diazenyl]pyridine (MNAP) was synthesized and its structural and optical properties were described. The MNAP molecule consists of two pyridine subunits, each bearing different substituents, linked by an azo bond. The IR, Raman, NMR, electron UV-VIS and emission spectra measurements were carried out and the experimental data were analyzed in terms of theoretical data obtained by quantum chemical DFT calculations. The 6-311G(2d,2p) basis set with the B3LYP functional was used to discuss their optimized structures and vibrational dynamics. The molecular structure of MNAP (Figure 1) was further studied by single-crystal X-ray diffraction. MNAP crystallizes in the non-centrosymmetric space group *Cc* of the monoclinic system with four symmetry-independent molecules in the asymmetric unit.

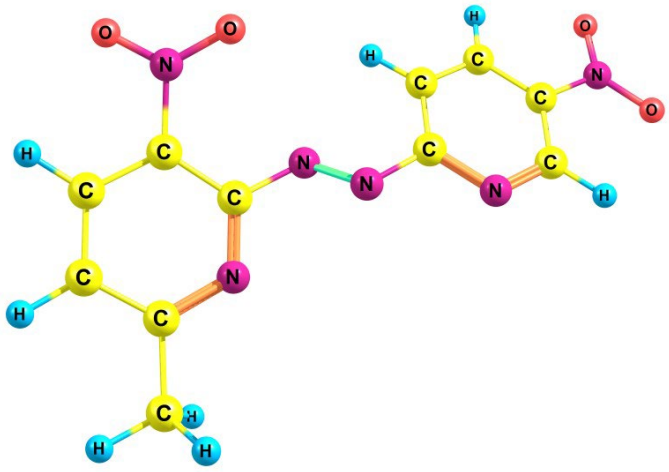


Figure 1 – Molecular structure of 6-methyl-3-nitro-2-[(E)-(5-nitropyridin-2-yl)diazenyl]pyridine

References
1. P.O. Gupta, N. Sekar, *J. Mol. Struct.*, 1321 (2025) 140035.
2. C.W. Ghanavatkar, V.R. Mishra, N. Sekar, *Dyes Pigm.*, 191 (2021) 109367.
3. E. Kucharska, J. Hanuza, J. Lorenc, *Spectrochim. Acta Part A*, 127 (2014) 370.

Characterization of Extraterrestrial Materials Using Spectroscopic Techniques

Maria Rosa Lopez-Ramirez[a], Jon Larsen[b], María Gritsevich[c]
[a]*Department. of Physical Chemistry, Faculty of Science, University of Málaga, 29071 Málaga, Spain*
[b]*Department of Geosciences, University of Oslo (Norway)*
[c]*University of Helsinki, Faculty of Science, Gustaf Hällsrömin katu 2, FI-00014 Helsinki, Finland*
mrlopez@uma.es

Micrometeorites (MMs) are extraterrestrial dust particles that survive atmospheric entry and accumulate on planetary surfaces. They represent a significant portion of the extraterrestrial material deposited on Earth [1]. The mineralogical and textural features of MMs—such as phase relationships and crystal morphologies—offer insights into their thermal and chemical alterations during atmospheric entry.

Since 2010, Jon Larsen has systematically collected and analyzed dust samples from populated areas worldwide. His extensive collection, built over more than a decade, spans approximately 50 countries and over 1,000 field searches across all continents [2].

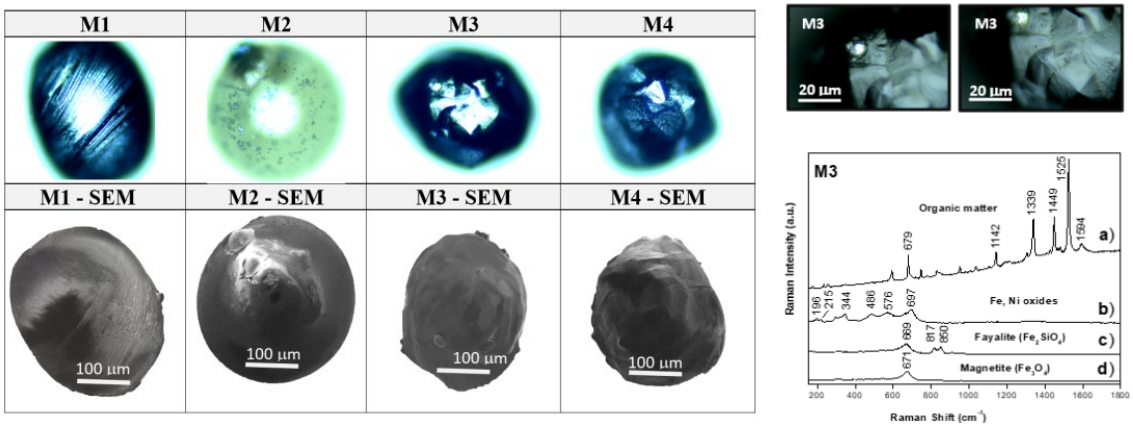


Figure 1 – Optical and SEM images of the MM samples studied in this work and their Raman spectra

In this study, MMs from Larsen's collection, each smaller than ~2 mm in diameter, were analyzed for their chemical composition using an Invia Qontor Renishaw micro-Raman spectrometer with laser excitation wavelengths of 532 and 785 nm. Raman spectroscopy, a powerful, non-destructive technique previously applied to meteorite studies, enables rapid, semi-quantitative mineralogical characterization at a microscopic scale.

References

1. J. Moilanen, M. Gritsevich, E. Lyytinen, *MNRAS*, 503 (2021) 3337.
2. J. Larsen, *In Search of Stardust: Amazing Micrometeorites and Their Terrestrial Imposters*. Ed. Voyageur Press (2017). ISBN-13: 978-0760352649.

Acknowledgements: This work was supported by the Academy of Finland project no. 325806 "Planetary spectrometry".

Comprehensive Structural and Spectroscopic Study of Transition Metal Complexes Featuring $\{CoN_2O_4\}$ and $\{NiN_2O_4\}$ Coordination Cores

Magdalena Malik[a], Tomasz Mazur[a], Anna Świtlicka[b], Alina Bieńko[c], Marta Gordel-Wójcik[c], Andrew Ozarowski[d], Dariusz C. Bieńko[a]

[a]*Faculty of Chemistry, Wroclaw University of Science Technology, Wybrzeze Wyspiańskiego 27, Wroclaw 50-370, Poland*

[b] *Department of Crystallography, Institute of Chemistry, University of Silesia, Szkolna 9, 40-006 Katowice, Poland*

[c] *Faculty of Chemistry, University of Wroclaw, Joliot–Curie 14, 50–383 Wroclaw, Poland*

[d] *National High Magnetic Field Laboratory, Florida State University, 1800 East Paul Dirac, Tallahassee, Florida 32310, United States*

magdalena.malik@pwr.edu.pl

The structural characterization, and spectroscopic investigation of two distinct series of transition metal complexes based on cobalt(II) and nickel(II) centers coordinated by bioactive ligands was made. The cobalt complexes feature mononuclear Co(II) centers with *trans*- and *cis*-$\{Co^{II}N_2O_4\}$ coordination environments, as confirmed by single-crystal X-ray diffraction. Advanced *ab initio* CASSCF and NEVPT2 calculations elucidate their electronic structures, revealing quasi-degenerate ground states in some cases and orbitally non-degenerate states in others. High-field electron paramagnetic resonance (HFEPR) spectra provide zero-field splitting parameters that correlate well with magnetic susceptibility and magnetization data, demonstrating slow magnetic relaxation behavior characterized by multiple relaxation channels under applied magnetic fields.

Parallel investigations on nickel(II) complexes bearing bidentate pyridyl alcohol ligands and mixed-ligand systems with memantine and acetylacetone reveal distorted octahedral geometries with a $\{Ni^{II}N_2O_4\}$ core. These complexes exhibit variation in ligand orientation, molecular symmetry, and supramolecular packing motifs, as evidenced by single-crystal X-ray diffraction and complementary FT-IR, Raman, and UV-Vis spectroscopies. Photophysical studies indicate comparable emission lifetimes among the complexes, while thermal and solution stability tests highlight differences in complex robustness linked to ligand composition.

The integration of experimental structural data with computational insights provides a comprehensive understanding of how subtle variations in metal-ligand arrangements modulate magnetic and spectroscopic behaviors, paving the way for the rational design of multifunctional transition metal complexes with tailored properties.

Acknowledgements: The authors acknowledge the financial support provided by the Faculty of Chemistry internal grants (No 2/2023 and No 8/2025), Wroclaw University of Science and Technology. Slovak grant agency is acknowledged for the financial support (VEGA 1/0191/22). HFEPR and FIRMS performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-2128556, DMR-1644779 and the State of Florida.

3-Nitro-2-[(*E*)-phenyldiazenyl]pyridine: Synthesis, Spectroscopic Characterization and DFT Study of a Potential Azo-Ligand for Coordination and Optoelectronic Applications

J. Michalski[a], E. Kucharska[a], L. Dymińska[a], W. Sąsiadek[a], P. Ropuszyńska-Robak[a], M. Ptak[b], J. Hanuza[b]
[a]*Wroclaw University of Economics and Business, 53-345 Wrocław, Poland*
[b]*Institute of Low Temperature and Structure Research, PAN, 50-422 Wrocław, Poland*
jacek.michalski@ue.wroc.pl

☒ I am applying for **Bruker Customer Excellence Award**

Azo aromatic derivatives are an important group of organic compounds used as dyes [1,2], transition metal complexes, optoelectronic materials [3] and as synthetic intermediates [4]. New compound 6-methyl-3-nitro-2-[(*E*)-(5-nitropyridin-2-yl)diazenyl]pyridine (PMNAB) was synthesized (Fig. 1) and its structural and optical properties were described.
The FTIR, Raman, NMR, electronic UV-VIS and emission spectra assessments were performed and the experimental findings regarding theoretical data acquired *via* quantum chemical DFT and NBO computations were analyzed. The 6-311G(2d,2p) basis set with the B3LYP functional was utilized to discuss their optimized structures and vibrational dynamics. The role and influence of the azo and nitro groups on vibrational and electronic properties of the compound have been studied.

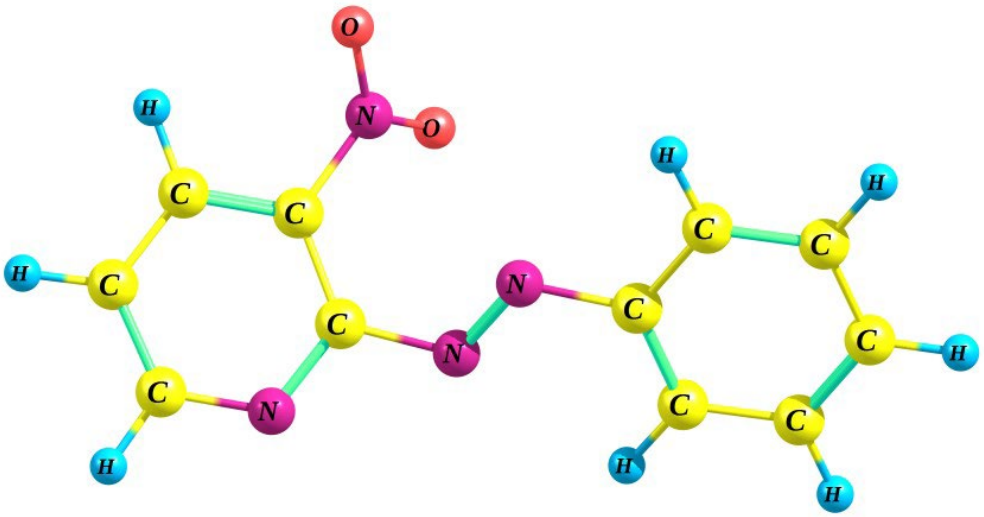


Figure 1 – Molecular structure of 3-nitro-2-[(E)-phenyldiazenyl]pyridine

References
1. M.A. Cardona, D. Makuc, K. Szaciłowski J. Plavec, D.C. Magri, *ACS Omega,* 2 (2017) 6159.
2. G. Féraud, C. Dedonder-Lardeux, C. Jouvet, E. Marceca, *J. Phys. Chem. A*, 120 (2016) 3897.
3. J. Michalski, I. Bryndal, J. Lorenc, K. Hermanowicz, J. Janczak, J. Hanuza, *Spectrochim. Acta A*, 191 (2018) 521.
4. P. Godlewska, J. Hanuza, J. Janczak, R. Lisiecki, M. Basiak, A. Zając, L. Dymińska, *Int. J. Mol. Sci., 26* (2025) 2874.

DFT-Assisted Study of the Structural, Electronic, and Vibrational Properties of 6-Methyl-2-aminopyridine *N*-Oxide

J. Michalski[a], E. Kucharska[a], L. Dymińska[a], W. Sąsiadek[a], P. Godlewska[a], M. Ptak[b] , J. Hanuza[b]
[a]*Wroclaw University of Economics and Business, 53-345 Wrocław, Poland*
[b]*Institute of Low Temperature and Structure Research, PAN, 50-422 Wrocław, Poland*
jacek.michalski@ue.wroc.pl

☒ I am applying for **Bruker Customer Excellence Award**

N-oxide aromatic methyl derivatives constitute an important group of organic compounds used as substrates in subsequent synthesis [1,2] and nonlinear optical materials [3]. Due to the presence of *N*-oxide and amine groups, they can potentially form complexes with metals such as Eu and Tb, which are employed in biological and medical probes [4,5].
The compound 6-methyl-2-aminopyridine *N*-oxide (MAPNO) was synthesized (Fig. 1) and its structural, electronic and vibrational properties were characterized. Its IR, Raman, electron absorption and emission spectra were measured and analyzed using DFT quantum chemical methods and NBO calculations, employing the B3LYP/6-311G(2d,2p) approach. The vibrational characteristics of the methyl, amino and *N*-oxide groups were reported in relation to the molecule's conformation. The role of the interactions e.g. hydrogen bonding in this material is discussed.

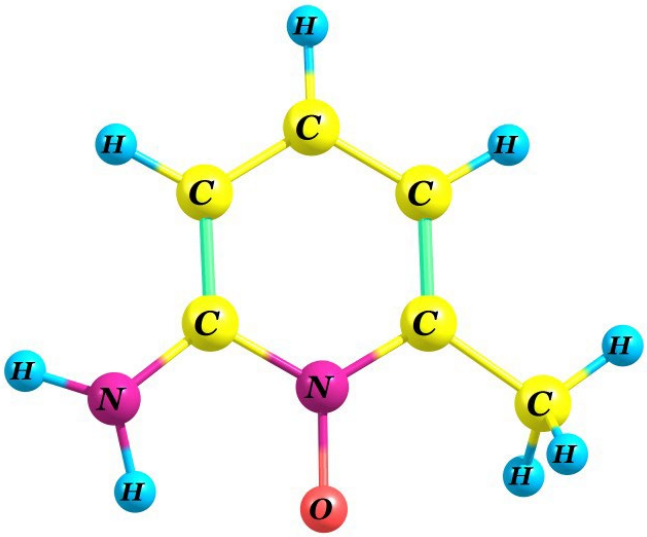


Figure 1 – Molecular structure of 6-methyl-2-aminopyridine N-Oxide

References

1. R. Kaliammal, G. Parvathya, G. Maheshwarana, V. Kousalya Devi, M. Krishna Kumar, K. Sankaranarayanana, S. Sudhahar, *J. Mol. Struct.*, 1254 (2022) 132330.
2. H. Soscu´n, O. Castellano, Y. Bermu´dez, C. Toro-Mendoza, A. Marcano, Y. Alvarado, *J. Mol. Struct.*, 592 (2002) 19.
3. S. Madrahimov, A. Mostafa, V. Yempally, J. Fadlallah, S.Y. AlQaradawi, *J. Mol. Struct.*, 1199 (2020) 127021.
4. M. Kobus, T. Friedrich, E. Zorn, N. Burmeister, W. Maison, *J. Med. Chem.*, 67 (2024) 5168.

Photochemical and Spectroscopic Characterization of 3-Thio-1,2,4-triazole Complexes with CO_2 and N_2: A Comparative Matrix Isolation Study

Karolina Mucha, Magdalena Pagacz-Kostrzewa, Maria Wierzejewska
Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 53-383 Wrocław, Poland
karolina.mucha@uwr.edu.pl

Heterocyclic compounds capable of reversible photochemical transformations and selective intermolecular interactions are increasingly explored for applications in molecular recognition, gas capture, and photoresponsive materials. Among these, 3-thio-1,2,4-triazole (ST) stands out due to its ability to undergo UV-induced thione–thiol tautomerization and to form non-covalent complexes via hydrogen bonding and van der Waals interactions.
In this study, we examine the spectroscopic and structural behavior of ST complexed with carbon dioxide (CO_2) and dinitrogen (N_2) under cryogenic conditions using matrix isolation Fourier-transform infrared (FTIR) spectroscopy and density functional theory (DFT) calculations at the B3LYP-D3/6-311++G(d,p) level. Both 1:1 and 1:2 complexes were successfully characterized in argon matrices, revealing distinct spectroscopic signatures and optimized geometries.
UV irradiation at λ = 270 nm promoted tautomerization from the thione to thiol form and induced the formation of new thiol···gas complexes. Notably, this work presents the first experimental observation of thiol···N_2 complexes, expanding the scope of photogenerated molecular assemblies. While CO_2 interactions were found to be stronger and more directional—owing to its higher polarizability—the impact of N_2 complexation on the phototautomerization process was more pronounced, effectively slowing the reaction rate.
These findings underscore the dual role of the matrix and interacting gas in modulating both structure and photoreactivity. This comparative study provides a deeper understanding of gas–heterocycle interactions at the molecular level and highlights the potential of ST derivatives for environmentally responsive molecular design.

References
1. K. Mucha, M. Pagacz-Kostrzewa, M. Wierzejewska, *RSC Advances,* 15 (2025) 17379.
2. K. Mucha, M. Pagacz-Kostrzewa, M. Wierzejewska, *J. Photochem. Photobiol. A,* 443 (2023) 114873.

Acknowledgements: Allocation of computer time from the Wrocław Centre for Networking and Supercomputing (Wrocław, Poland) is gratefully acknowledged. The authors thank Prof. Dr. Małgorzata Biczysko and Prof. Jarosław Panek for fruitful discussions concerning the theoretical part of this work.

Conformational Dynamics of Lysozyme in the Presence of Model Membranes and Modulatory Compounds: Insights from FTIR and PCA Analyses

Karolina Musiał, Katarzyna Cieślik-Boczula.
Faculty of Chemistry, University of Wrocław, Fryderyka Joliot-Curie 14, 50-383 Wrocław, Poland
karolina.musial@uwr.edu.pl

Protein–membrane interactions are fundamental to numerous biological processes, including membrane trafficking, cellular signaling, and protein misfolding diseases. A growing body of evidence highlights the pivotal role of membrane composition in modulating protein structure, stability, and aggregation. In this study, we explore the structural response of lysozyme (LSZ) to lipid environments using well-defined model systems composed of zwitterionic DPPC and negatively charged DPPC/DPPG membranes. Particular attention is given to the influence of physiological salts (NaCl, KCl, $MgCl_2$) and their modulation by bioactive small molecules—polyphenols (quercetin, resveratrol) and selected antibiotics (rifampicin, D-cycloserine).

Using Fourier-transform infrared spectroscopy (FTIR) combined with principal component analysis (PCA), we show that in the absence of salts, DPPC membranes subtly alter the secondary structure of LSZ without inducing aggregation. In contrast, the presence of DPPG lipids promotes β-sheet-rich structures indicative of early aggregation. Upon addition of physiological salts, especially NaCl and KCl, the system undergoes marked destabilization. We observe membrane fusion, lipid extraction, and the formation of fibrous LSZ–lipid aggregates resembling amyloid intermediates. These transitions are accompanied by a distinctive $\beta \rightarrow \alpha \rightarrow \beta$ rearrangement in LSZ, particularly pronounced in thermal cycling experiments.

The application of PCA to temperature-resolved FTIR spectra allowed us to deconvolute overlapping processes and pinpoint conformational switches at specific temperature ranges. Importantly, small molecules such as polyphenols and antibiotics reduced the extent of membrane destabilization and protein aggregation, although not entirely preventing the structural transitions.

Our results underline the dual role of membranes as both stabilizers and triggers of protein misfolding and demonstrate how molecular components of the environment—especially ionic and small-molecule modulators—can influence this delicate balance. This work establishes a mechanistic framework for understanding membrane-associated protein aggregation and offers a spectroscopic strategy to evaluate modulatory compounds with potential biomedical relevance.

References
1. T. Al Kayal, S. Nappini, E. Russo, D. Berti, M. Bucciantini, M. Stefani, P. Baglioni, *Soft Matter*, 8 (2012) 4524.
2. J.-J. Luo, F.-G. Wu, S.-S. Qin, Z.-W. Yu. *J. Phys. Chem. B*, 116 (2012) 12381.
3. S. Strazdaite, E. Navakauskas, J. Kirschner, T. Sneideris, G. Niaura. *Langmuir*, 36 (2020) 4766.

Acknowledgements: This work was supported by National Science Centre, Poland, project OPUS 22 with decision number UMO-2021/43/B/NZ9/00345.

Spectroscopic Characterization of Series of New Heteroleptic Rhodium(III) Complexes

Karol Okła[a], Joanna Masternak[a], Anna Kamecka[b], Jerzy Sitkowski[c], Katarzyna Kazimierczuk[d], Barbara Barszcz[a]
[a]*Institute of Chemistry, Jan Kochanowski University in Kielce, Uniwersytecka 7, 25-406 Kielce*
[b]*Faculty of Sciences, University of Siedlce, 3-Maja 54, 08-110 Siedlce*
[c]*Institute of Organic Chemistry, Polish Academy of Sciences, Marcina Kasprzaka 44/52, 01-224 Warsaw*
[d]*Faculty of Chemistry, Gdańsk University of Technology, Gabriela Narutowicza 11/12, 80-233 Gdańsk*
karol.okla@onet.pl

Organometallic transition metal complexes that contain at least one direct bond between a metal ion and an aromatic carbon atom exhibit a range of intriguing properties, including promising antiproliferative activity [1]. Heteroleptic complexes composed of cyclometalating C^N-donor ligands and chelating auxiliary ligands have attracted growing interest over the past decades due to their unique luminescent behaviour. Cyclometalated complexes of d^6-electron rhodium(III) and iridium(III) ions have found applications in organic light-emitting diodes (OLEDs), cellular imaging, and as potential cytostatic agents [2,3].
In the present study, we describe novel Rh(III) coordination compounds incorporating a cyclometalating pyrazole-derived ligand (Hdmppz – 3,5-dimethyl-1-phenyl-1H-pyrazole) along with auxiliary N^N-donor heterocyclic aromatic ligands: 2-(2-pyridyl)benzimidazole (PyBIm, 1), 2,2'-biimidazole (H_2biim, 2), and di(2-pyridyl)ketone (Py_2CO, 3).
The synthesized complexes were characterized using FT-IR, UV-Vis, fluorescence, NMR, and mass spectrometry.

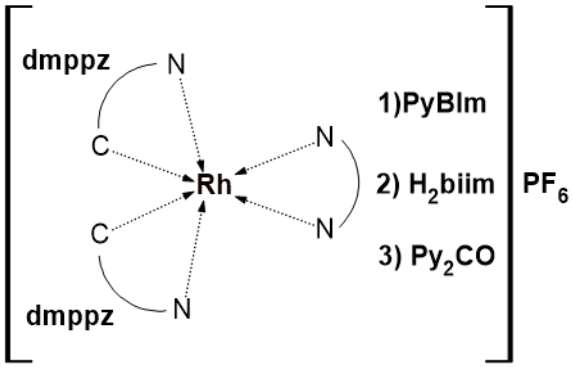


Figure 1 - Structural representation of novel heteroleptic Rh(III) complexes

References
1. Y.Y. Lam, N.S. Lee, S.F. Lee, C.Y.S. Chung, *J. Organomet. Chem.,* 1005 (2024).
2. G. Li, D. Zhu, X. Wang, Z. Su, M.R. Bryce, *Chem. Soc. Rev.,* 49 (2020) 765.
3. M. Sohrabi, M. Saeedi, B. Larijani, M. Mahdavi, *Eur. J. Med. Chem.,* 216 (2021).

Acknowledgements: The authors thank JKU SUPD.RN.25.021 grant for financial support for participation in EUCMOS 2025.

Insight from ATR-IR and 2D-COS into Structural Changes of Main Animal Plasma Components During Extracorporeal Circulation

Sylwia Olsztyńska-Janus[a], Mirosław A. Czarnecki[b]
[a]*Department of Biomedical Engineering, Wrocław University of Science and Technology, pl. Grunwaldzki 13, 50-370 Wrocław, Poland.*
[b]*Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland.*
sylwia.olsztynska-janus@pwr.edu.pl

An increasing number of patients with severe cardiac and/or respiratory problems require connection to extracorporeal circulation (ECC). Despite its life-saving role, using ECC is associated with serious complications arising from structural changes in the plasma components. As a result, in the body occurs a systemic inflammatory response [1], and the side effects of this response may lead to serious health problems [2, 3]. To date, the molecular mechanism of these transformations has not been fully elucidated, encouraging us to undertake a pioneering spectroscopic study on structural changes in plasma during ECC. For this purpose, we applied vibrational spectroscopy in combination with two-dimensional correlation spectroscopy (2D-COS). The spectra of animal plasma were recorded using the attenuated total reflection infrared (ATR-IR) technique, which enables the non-destructive measurement of strongly absorbing samples in their native state. An application of 2D-COS and moving-window approach allows for detailed insight into the correlation between spectral features and functional groups.

Our results reveal that after connection to ECC, the most pronounced changes are observed for the ν(OH) bands from water. This means that the changes in the state of water precede the structural changes for the other plasma components. Moving-window analysis shows that during ECC the hydrogen bonding between water and protein polar groups is weakened or even completely disrupted. As a result, in the 2D-COS and moving-window spectra appear new bands from weakly bonded water (3607 cm^{-1}) and dangling OH group (3726 cm^{-1}). Since water is an essential component of biological processes, changes in its state strongly affect the structure of plasma proteins and their physiological functions. The disruption of hydrogen bonds stabilizing the structure of proteins alters the hydration shell and may contribute to protein unfolding. Moreover, we have observed other processes such as oxidative stress and inflammation influence ATR-IR spectra after ECC connection.

References
1. A. Oleszko, S. Olsztyńska-Janus, T. Walski, K. Grzeszczuk-Kuć, J. Bujok, K. Gałecka, A. Czerski, W. Witkiewicz, M. Komorowska, *Biomed. Res. Int.*, 2015 (2015) 245607.
2. A.S. Thiara, V.Y. Andersen, V. Videm, T.E. Mollnes, K. Svennevig, T.N. Hoel, A.E. Fiane, *Perfusion*, 25 (2010) 9.
3. I. Karu, G. Taal, K. Zilmer, C. Pruunsild, J. Starkopf, M. Zilmer, *Scand. Cardiovasc. J.*, 44 (2010) 119.

Acknowledgements: The list of people to whom the authors would like to express their gratitude is very long and will be presented on the poster. This work was supported by statutory funds of the Department of Biomedical Engineering, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, Poland.

Post-Operational Rheological and ATR-IR Evaluation of Lithium and Calcium Sulfonate Greases in Mining Machinery

M. Paszkowski[a], S. Olsztyńska-Janus[b], P.A. Stelmaszek[c]
[a]*Department of Fundamentals of Machine Design and Mechatronic Systems, Wroclaw University of Science and Technology, Ignacego Łukasiewicza 7/9, 50-371 Wroclaw, Poland.*
[b]*Department of Biomedical Engineering, Wrocław University of Science and Technology, pl. Grunwaldzki 13, 50-370 Wrocław, Poland.*
[c]*KGHM Polska Miedź S.A., Marii Skłodowskiej-Curie 48, 59-301 Lubin, Poland.*
sylwia.olsztynska-janus@pwr.edu.pl

Greases for application in the deep mining industry must possess optimal properties to effectively lubricate the tribological components of specialized self-propelled wheeled machinery. The selection of lubricating greases is influenced by challenging operational conditions such as elevated temperature, high humidity, and the presence of contaminants, all of which can adversely affect the greases' structure and performance. Two widely recommended greases for such applications are 12-hydroxystearate lithium and calcium sulfonate grease [1].

For this work, rheological tests and ATR-IR spectroscopy were used. Samples of the two commercial greases were collected from one of the pin joints of the LKP-0903 bucket loader (KGHM Zanam, Poland). This study aims to analyze and compare the structural and performance characteristics of greases before and after 3,000 hours of operation in the friction node of the mining machine.

Shear stress and mine contaminants reduced the intensity of CH_2 bands in lithium grease. In sulfonate grease, the H-bonded OH band intensity decreased and blue-shifted, while the intensity of the CH_3 bands diminished due to altered hydrogen bonding and thickener-oil interactions. These changes likely stem from the lubricants' initial structures: lithium grease's hydrophobic chains are organized into fibrils by capillary and van der Waals forces [2], whereas calcium sulfonate grease forms more stable reverse micelle structures [3]. Operational stress may disrupt lithium grease's thickener fibrils, while in sulfonate grease, only the outer CH_3 groups are affected. Such structural alterations can influence the rheological properties of the greases.

Rheological studies using a three-interval thixotropic test (3ITT) have shown that the mining environment affects the viscoelastic properties of both greases. After operation, lithium grease exhibited lower viscosity, while sulfonate grease showed the opposite effect, an increase in viscosity and consistency. Additionally, the resolidification process following the shearing of greases in the second interval of the thixotropic test revealed distinct differences: post-operation, the thickener microstructure in lithium grease rebuilt itself by almost 40% during the third interval, whereas sulfonate grease showed a significantly slower return to its pre-shearing viscoelastic properties.

References
1. PM. Lugt, *Grease lubrication in rolling bearings,* Wiley, Chichester, United Kingdom (2013).
2. F. Cyriac, PM. Lugt, R. Bosman, *Trib. Lett.,* 59 (2016) 679.
3. R. Bosman, PM. Lugt, *Trib. Trans.,* 61(5) (2018) 842.

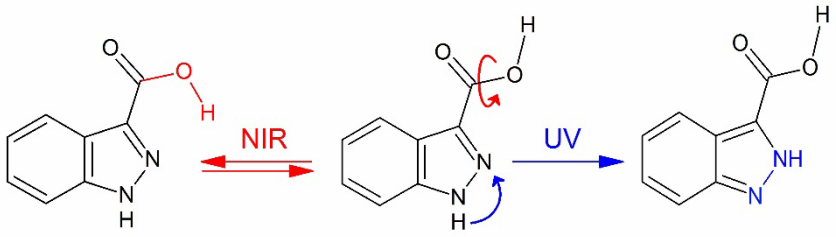
Acknowledgements: This work was supported by statutory funds of the Department of Fundamentals of Machine Design and Mechatronic Systems of the Faculty of Mechanical Engineering and the Department of Biomedical Engineering, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, Poland.

Phototransformations of Indazole-3-carboxylic Acid Isolated in Low Temperature Matrices

Magdalena Pagacz-Kostrzewa, Maria Wierzejewska
Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland
magdalena.pagacz-kostrzewa@uwr.edu.pl

Substances containing azole rings represent one of the most biologically active classes of compounds and receive many applications in the synthesis of compounds with diverse pharmacological activities. In order to understand the biological activity of these species the knowledge of their conformational preferences becomes really important. In turn, the obtained information on conformational equilibria and tautomerization processes of selected azoles can be used to explain the conformation/tautomerism effect on photochemical preferences in these species. [1-3]

In this contribution, the molecular structure and photochemistry of indazole-3-carboxylic acid (IC) were studied in argon and nitrogen matrices by infrared spectroscopy and B3LYP/6-311++G(2d,2p) calculations.[4] IC exists in two tautomeric forms: 1*H* and 2*H*. The infrared spectra of IC/Ar and IC/N_2 show that only the three most stable conformers of the 1*H* tautomer are present in both matrices after deposition (1HIC1, 1HIC2 and 1HIC3). Upon NIR irradiation a dominant process was rotamerization within the carboxylic group leading to changes in the population of the *trans* 1HIC1 and *cis* 1HIC2 forms. In turn, at UV irradiation at λ = 260 nm two new tautomers (2HIC2 and 2HIC3) were generated indicating that the hydrogen atom transfer in pyrazole ring took place. Based on the obtained kinetic curves, differences in the phototransformation rates in different matrices were indicated.



1HIC1 1HIC2 2HIC2

References
1. M. Pagacz-Kostrzewa, M. Sałdyka, A. Bil, W. Gul, M. Wierzejewska, D.M. Khomenko, R.O. Doroschuk, *J. Phys. Chem. A*, 123 (2019) 841.
2. M. Pagacz-Kostrzewa, M. Sałdyka, A. Bil, W. Gul, M. Wierzejewska, D.M. Khomenko, R.O. Doroschuk, *J. Photochem. Photobiol. A*, 371 (2019) 292.
3. M. Pagacz-Kostrzewa, A. Bil, M. Wierzejewska, *J. Photochem. Photobiol. A*, 335 (2017) 124.
4. M. Pagacz-Kostrzewa, W. Szaniawska, M. Wierzejewska, *Spectrochim. Acta A*, 290 (2023) 122283.

Acknowledgements: The authors acknowledge the Wroclaw Centre for Networking and Supercomputing (WCSS) for providing computer time and facilities.

Interactions between Anticancer Thioderivatives of Nucleobases and Nanosomes Components: Drug Delivery Related Study by FTIR Spectroscopy and Mass Spectrometry

V. Pashynska[a], O. Gnatyuk[b], A. Gomory[c], L. Drahos[c], M. Kosevich[a], G. Dovbeshko[b]
[a]*B. Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, 47 Nauky Ave., Kharkiv, 61103, Ukraine*
[b]*Institute of Physics of the NAS of Ukraine, 46 Nauky Ave., 03028, Kyiv, Ukraine*
[c]*Institute of Organic Chemistry of the HUN-REN Research Center for Natural Sciences, Budapest, Hungary*
vlada.pashynska@gmail.com

Molecular interactions of biologically significant molecules are in the focus of the modern spectroscopic and mass spectrometric studies because of their importance for biomedical practice. The data about intermolecular interactions of drugs with the components of drug delivery nanosomes (liposomes and other structures) may input significantly into revealing of the drug delivery molecular mechanisms. Providing effective drug transportation by drug delivery structures is extremely important for poorly soluble and toxic anticancer agents. The aim of the current study was to examine the molecular interactions of anticancer thioderivatives of nucleobases – 6-thiopurine (TP) and 2-thioadenine (TA) with selected lipid molecules which can be used to create liposomes for targeted delivery of these toxic drugs.

Using FTIR spectroscopy method we probed the pair systems containing TP (or TA) and liposomal phospholipids (1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) or sphingomyelin (SM)) organized in the model membrane structures. The comparative analysis of the spectra of the pair systems and spectra of the individual components revealed the nonadditive changes in some characteristic spectral bands, particularly, in the spectral ranges of H-bonded of -PO_2 vibration and -C-H groups. The results obtained indicate the existence of molecular interactions of the liposomal components with the antitumor drugs, the structure of the latter determines the features of the interactions.

To go inside the nature of the molecular interactions of the anticancer drugs with liposomal phospholipids we used the electrospray ionization mass spectrometry (ESI MS) technique to examine the noncovalent complexes formation between the components of pair model systems (TP+DPPC) and (TA+DPPC) dissolved in polar solvent methanol in molar ratio 1:5. In the mass spectra obtained the peaks of noncovalent complexes of $[TP \cdot DPPC \cdot H]^+$ and $[TA \cdot DPPC \cdot H]^+$ were observed, but the peaks intensity was not abundant. Basing on the previous results as for the ESI MS study of the biologically active component of nanosomes - ascorbyl palmitate (AP) [1] we probed the model systems (TP +AP) and (TA+AP) in methanol. The abundant peaks of the stable noncovalent complexes TA and TP with AP were recorded in the ESI spectra. Following the MS results obtained we propose to include AP in the liposomes for the transportation of TA and TP as an anchor for these anticancer drugs noncovalent binding with the nanosomes components. The data obtained are useful for the development of the nanosomal structures for the anticancer thioderivatives of nucleobases targeted delivery.

References

1. V. Pashynska, M. Koseich, A. Gomory, L. Dragos, *Funct. Mater.*, 29 (2022) 100.

Acknowledgements: The authors O. Gnatyuk and G. Dovbeshko thank NRFU project No 2021.01/0229, V. Pashynska and M. Kosevich thank NASU grant N0123U100628.

Unveiling the Role of Acyl Peroxy Radicals in Atmospheric Oxidation of Volatile Organic Compounds

Dominika Pasik[a,b], Benjamin N. Frandsen[c], Emelda Ahongshangbam[a,b], Siddharth Iyer[c], Nanna Myllys[a,b]
[a]*Department of Chemistry, University of Helsinki, Helsinki, Finland, 00014*
[b]*Institute for Atmospheric and Earth System Research (INAR), Helsinki, Finland, 00014*
[c]*Aerosol Physics Laboratory, Tampere University, 33100*
dominika.pasik@helsinki.fi

Air quality influences climate change and human health and remains a pressing global challenge with particle formation processes playing a critical yet poorly understood role. To mitigate their negative impacts, better understanding of reactions occurring within the atmosphere is needed. Of particular interest are reactions that produce low-volatility oxygenated products, as they are known to be important contributors in aerosol formation and growth. However, how they are formed in the atmosphere remains largely unknown.
Volatile organic compounds (VOCs) are considered as essential reactive species in the atmosphere, driving complex oxidation pathways. In this study, we investigate oxidation reactions of atmospherically significant VOCs with novel oxidants - acyl peroxy radicals (APRs) - aiming to find new mechanisms that would explain missing gaps in the formation of low-volatility products in the atmosphere.
This research utilizes state-of-the-art computational chemistry tools to study oxidation reactions between VOCs and APRs. APRs are known to be more reactive compared to non-functionalized peroxy radicals. Our calculations show that indeed reactions between VOCs and APRs exhibit low energy barriers and can occur under atmospheric conditions. Experimental results support this reaction mechanism. Moreover, we study subsequent oxidation steps to determine the fate of oxidation products initiated by APRs. These novel findings open up completely new mechanisms that may lead to highly oxygenated, more functionalized products capable of partitioning in aerosol processes.

References
1. D. Pasik, B. N. Frandsen, M. Meder, S. Iyer, T. Kurtén, N. Myllys, *J. Am. Chem. Soc.*, 146 (2024) 13427.
2. D. Pasik, T. Golin Almeida, E. Ahongshangbam, S. Iyer, N. Myllys, *Atmos. Chem. Phys.*, 25 (2025) 4313.

Acknowledgements: The authors thank CSC-IT Center for Science in Espoo, Finland, for computational resources. Dominika thanks the Doctoral Programme in Atmospheric Sciences (ATM-DP) at the University of Helsinki for provided funding.

Dielectric Spectroscopy into the Cooperative Dynamics of MPPyrNTf2 - Sulfolane Mixtures

Iwona Płowaś-Korus[a], Agnieszka Świderska-Mocek[b], Agnieszka Gabryelczyk[b], Richard Buchner[c]
[a]*Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznan, Poland*
[b]*Faculty of Chemical Technology, Poznan University of Technology, 60-965 Poznan, Poland*
[c]*Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040 Regensburg, Germany*
iwplowas@ifmpan.poznan.pl

During the last three decades research on room temperature ionic liquids (RTILs; generally organic salts with T_m < 100 °C) has grown into a mature field with many promises. This arises from the seemingly infinite variety of possible cation-anion combinations, which allows to finetune RTIL properties as desired. Even further variability comes by mixing RTILs with molecular solvents, allowing the design of task-specific reaction media [1-3].
In this contribution we report preliminary results on the cooperative dynamics of mixtures of the molecular liquid tetramethylene sulfone (TMS, sulfolane) with the RTIL 1-methyl-1-propylpyrrolidinium bis(trifluoromethylsulfonyl)imide (MPPyrNTf$_2$), obtained with broadband dielectric relaxation spectroscopy (DRS [4]) in the frequency range of 0.05 ≤ ν/GHz ≤ 50 at 30 °C. The obtained spectra of relative permittivity, ε'(ν), and dielectric loss, ε''(ν) (corrected for dc conductivity), of the neat RTIL are best described by a superposition of four Debye modes (the D+D+D+D model) centred at ~0.2, ~1.3, ~8 and ~40-90 GHz, whereas neat TMS exhibits a dominant mode at ~5 GHz and a weak high-frequency contribution (~40 GHz). Mixture spectra are also best fitted by the D+D+D+D model. The relaxation times and amplitudes (relaxation strengths) of the two fastest components (modes 3 & 4) vary smoothly from the values of neat TMS to those of MPPyrNTf$_2$, indicating that both components contribute. On the other hand, the lower-frequency modes 1 & 2 are clearly RTIL-related, although the observed maxima of their amplitudes at w_{IL} ≈ 0.5 suggest a contribution from dynamically retarded TMS dipoles.

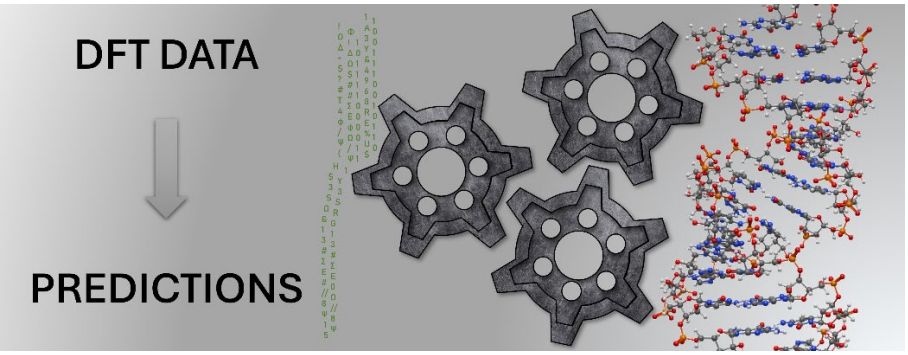
References

1. Y.-L. Wang, B. Li, S. Sarman, F. Mocci, Z.-Y. Lu, J. Yuan, A. Laaksonen, M. D. Fayer, *Chem. Rev.*, 120 (2020) 5798.
2. T. Zhou, C. Gui, L. Sun, Y. Hu, H. Lyu, Z. Wang, Z. Song, G. Yu, *Chem. Rev.*, 123 (2023) 12170.
3. Z. Lei, C. Dai, J. Hallett, M. Shiflett, *Chem. Rev.*, 124 (2024) 7533.
4. T. Sonnleitner, D. A. Turton, S.Waselikowski, J. Hunger, A. Stoppa, M. Walther, K. Wynne, R. Buchner, *J. Mol. Liq.,* 192 (2014) 19.

Machine Learning in Studies of RNA Nucleosides Conformations

Michał Pocheć, Rafał Szabla
Institute of Advanced Materials, Wrocław University of Science and Technology,
Wybrzeże Stanisława Wyspiańskiego 27, 50-370 Wrocław
michal.pochec@pwr.edu.pl

Machine learning has gained significant attention within the scientific community as both the subject of studies, as well as a potentially powerful tool of scientific inquiry. From simple kernel machines to powerful deep neural networks, the ML solutions have a significant advantage when compared to the quantum chemical calculations - they are usually at least an order of magnitude faster, comparable even to classical force fields. The main drawback is the fact that the accuracy of results heavily depends on the quality (and sometimes quantity) of data used in training.



This work presents the preliminary results of studies of nucleosides conformations using machine learning tools. The necessary component of any ML procedure is the construction of the training set. AQML [1] has been used to generate amons - smaller pieces of input molecules. Then, dimers of the amons containing up to 3 heavy atoms have been prepared using CREST [2] to ensure reproduction of non-covalent interactions. Special dimers have also been constructed from methanol or ethanol with heterocycles found in nucleosides. Molecular dynamics simulations have been performed for all system in XTB suite [3] and for each of the steps single point calculations have been performed using ωB97M-V functional and def2-TZVP basis set. This resulted in the dataset consisting of 353839 unique entries. ML training and evaluation were performed using the SpookyNet [4]. Results include prediction error metrics for conformers of RNA nucleosides and describe the predictive power of different setups for the learning process. Viability of different iterations of the training set and varying sets of hyperparameters have been evaluated.

References
1. B. Huang, O.A. von Lilienfeld, *Nat. Chem.*, 12 (2020) 945.
2. P. Pracht, F. Bohle, S. Grimme, *Phys. Chem. Chem. Phys*., 22 (2020) 7169.
3. C. Bannwarth, S. Ehlert, S. Grimme, *J. Chem. Theory Comput*., 15 (2019) 1652.
4. O. Unke, et al., *Nat. Commun.*, 12 (2021) 7273.

Acknowledgements: This work has been supported by a grant from NCN, Poland (2022/46/E/ST4/00377). Authors would like to gratefully acknowledge Wrocław Center for Networking and Supercomputing for providing the computational resources.

Plasmon Assisted Surface Enhanced Linear and Nonlinear Raman Scattering Spectra of Biomolecules with Gold and Silver Nanostructures

Fariha Binte Rahman, Lars Dannenberg, Cecilia Spedalieri, Janina Kneipp
Department of Chemistry, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany
fariha.binte.rahman@hu-berlin.de

Hyper Raman scattering (HRS) is the two-photon analogue of spontaneous Raman scattering (RS), where the scattered light is shifted relative to the second harmonic of the excitation wavelength. Due to different selection rules, HRS can provide additional information that is inaccessible by Raman scattering. Similar to RS in surface enhanced Raman scattering (SERS), HRS can also be significantly enhanced by exploiting the highly localized optical fields around plasmonic substrates. While it can be more challenging to find a metal nanostructure substrate for surface enhanced hyper Raman scattering (SEHRS) because of the large gap in excitation and scattering wavelengths [1], the enhancement is also more sensitive to molecule orientation on the metal nanostructures, making it a great approach to study plasmon-molecule systems [2].
Here, we present SEHRS spectra of resonant and non-resonant molecules excited at 1064 nm, obtained with spherical gold nanoparticles of different sizes as substrate. As a model molecule that shows two-photon electronic resonance, we test our substrates using the dye crystal violet [3], while the non-resonant molecules studied include amino acids and polypeptides. We compare them to their SERS spectra with 785 nm excitation and examine the spectral differences arising from the different selection rules. We also report SEHRS from silver substrates and discuss the metal molecule interactions that might be responsible for the enhancement.

References
1. A. Dusa, F. Madzharova, J. Kneipp, *Front. Chem.*, 9 (2021) 680905.
2. F. Madzharova, Z. Heiner, J. Kneipp, *Chem. Soc. Rev.*, 46 (2017) 3980.
3. M. Gühlke, Z. Heiner, J. Kneipp, *Phys. Chem. Chem. Phys.*, 18 (2016) 14228.

Acknowledgements: L.D. acknowledges funding by a short-term research grant of the School of Analytical Sciences Adlershof (SALSA STF23-04). C.S. acknowledges funding by DFG EXC 2008 UniSysCat.

Detection of Serum Uric Acid on Gold Nanorods by Surface-enhanced Raman Spectroscopy

Septila Renata[a], Dragos Olariu[a], Ciprian-Paul Măirean[a], Vanda-Gianina Moraru[a], Magdalena Aflori[b], Brindusa Dragoi[a,c], Rares-Ionut Stiufiuc[a,d]
[a]*Nanotechnology Laboratory, TRANSCEND Department, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot, 700483 Iași, Romania*
[b]*Department of Physics of Polymers and Polymeric Materials, "Petru Poni" Institute of Macromolecular Chemistry, 700487 Iasi, Romania*
[c]*Faculty of Chemistry, Alexandru Ioan Cuza University of Iași, 11 Bd. Carol I, 700506 Iași, Romania*
[d]*Department of NanoSciences, Institute for Biomedical Research- MedFUTURE, "Iuliu Hatieganu" University of Medicine and Pharmacy, 4-6 Pasteur Street, 400349 Cluj-Napoca, Romania*
septila01@gmail.com

Uric acid is an end product of endogenous and dietary purine metabolism. It is considered as an important biomarker in blood and urine as its elevated level, known as hyperuricemia, is associated with gout, kidney disease, hypertension, cardiovascular diseases, and certain types of cancer. [1,2] The normal concentration of serum uric acid in men and post-menopausal women is 3.5 – 7.2 mg/dL while in pre-menopausal women it varies between 2.6 – 6.0 mg/dL.[3] Hence, the routine serum uric acid analysis is highly necessary to prevent and monitor diseases linked to hyperuricemia.
Surface-enhanced Raman Spectroscopy (SERS) is an attractive tool for analysis and quantification of biologically relevant molecules as it provides highly sensitive fingerprint molecular information.[4] In this work, label-free detection of serum uric acid has been performed by means of SERS. Gold nanorods (AuNRs) have been designed and synthesized in order to be used as SERS substrate. The optimization of uric acid analysis has also been performed. AuNRs were choosen since their L_{SPR} value can be tuned in accordance with the excitation laser used for SERS analysis. Four classes of AuNRs with diferent L_{SPR} and aspect ratio were synthesized, and characterized using UV-vis, TEM and zeta potential, to get the highest enhancement of Raman signal for uric acid mesurement. Gold nanospheres has also been synthesized and used as plasmonic substrates and the results have been compared.

References

1. L. A.B. Joosten, T. O. Crisan, P. Bjornstad, R. J. Johnson, *Nat. Rev. Rheumatol.*, 16 (2020) 75.
2. A. Yiu, M. V. Hemelrijck, H. Garmo, L. Holmberg, H. Malmström, M. Lambe, N. Hammar, G. Walldius, I. Jungner, W. Wulaningsih, *Oncotarget*, 8 (2017) 42332.
3. G. Desideri, G. Castaldo, A. Lombardi, M. Mussap, A. Testa, R. Pontremoli, L. Punzi, C. Borghi, *Eur. Rev. Med. Pharmacol. Sci.*, 18 (2014) 1295.
4. S. Renata, N. Verma, R. K. Peddinti, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, 329 (2025) 125631.

Acknowledgements: This work was supported by a H2020 grant – ERA-Chair, no 952390

Spectroscopic Study on Binding of Multi-charged *meso*-Porphyrins to Synthetic Polynucleotides of Various Base Composition and Spatial Structure

Olga Ryazanova
Department of Molecular Biophysics, B. Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, 47 Nauky ave, 61103 Kharkiv, Ukraine
ryazanova@ilt.kharkov.ua

The porphyrins are macrocyclic compounds with unique spectroscopic and photophysical properties and a high biological activity. They are widely used as probes for the structure and dynamics of nucleic acids, as photosensitizers in anticancer photodynamic therapy, antiviral and antimicrobial agents, as a carrier of antisense oligonucleotides for their delivery, stabilizers of G-quadruplexes. Dependence of the spectroscopic changes in the absorption and fluorescence spectra of multi-charged $TMPyP^{4+}$ and $TMPyP^{3+}$ porphyrins (Figure 1) resulting from their binding to double-stranded DNA (B-form) and RNA (A-form) polynucleotides, as well as to DNA·RNA hybrids (A-form) on the biopolymer base composition and spatial structure are analyzed by comparing our [1,2] and literature data and summarized.

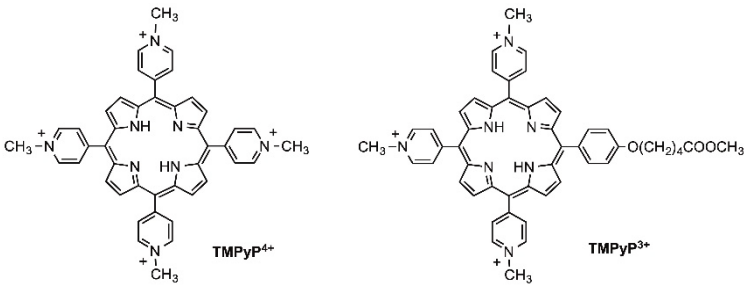


Figure 1 – Molecular structures of tetracationic $TMPyP^{4+}$ and tricationic $TMPyP^{3+}$ porphyrins

The porphyrins bind effectively to the biopolymers via two binding modes, which manifest themselves at low and high *P/D* ratios correspondingly. It was established that $TMPyP^{4+}$ and $TMPyP^{3+}$ discriminate between polynucleotide duplexes containing A·U (A·T) and G·C base pairs at low *P/D* ratios resulting in the porphyrin emission enhancement in the first case, and its quenching in the last case. It was shown that in contrast to $TMPyP^{4+}$, large bathochromic shift of the $TMPyP^{3+}$ Soret band at high *P/D* is observed for all these polynucleotides regardless of their base composition and type of the helical structure. The features of the porphyrin aggregation at a near-stoichiometric in charge phosphate-to-dye ratio were analyzed.

References

1. O. Ryazanova, V. Zozulya et al., *Methods Appl. Fluoresc.*, 4(3) (2016) 034005.
2. O. Ryazanova, V. Zozulya et al., *J. Fluoresc.*, (2024) https://doi.org/10.1007/s10895-024-04000-4.

Acknowledgements: The author acknowledges the National Academy of Sciences of Ukraine for the financial support (Grant No. 0123U100628) and Wolfgang Pauli Institute (Vienna, Austria) for Pauli Postdoc research training scholarships “Data analysis in molecular biophysics” 2021/22.

UV-Induced Photodecomposition of Matrix Isolated Salicylhydroxamic Acid. FTIR and Theoretical Studies

Magdalena Sałdyka, Zofia Mielke
Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland
magdalena.saldyka@uwr.edu.pl

Laser photolysis of salicylhydroxamic acid (SHA), compound important from the point of view of biology and medicine, in two low temperature matrices was performed for the first time. After irradiation with 340 nm laser line, the formation of new isocyanate complexes was observed: $C_6H_4(OH)NCO\cdots H_2O$ (1), $C_6H_4(OH)C(O)N\cdots H_2O$ (2), $C_6H_4(OH)_2\cdots HNCO$ (3), for which spectroscopic characteristics in the infrared range were obtained. The N-*o*-hydroxyphenylhydroxylamine molecule was identified for the first time, as the co-product of SHA photodissociation reaction: $C_6H_4(OH)CONHOH \rightarrow C_6H_4(OH)NHOH + CO$ (4). UV-induced photodecomposition channels were determined for SHA. It was demonstrated that one of the two reaction channels is the scission of the N-O bond (creating the complexes (1), (2) and (3)), while the second path leads to the C-N bond breaking (creating the complex (4)). In both studied matrices, photochemical reactions occurred according to the same mechanism, but a clear influence of the nitrogen matrix on the formation of specific structures of the isocyanic acid-1,2-dihydroxybenzene complex was observed: two structures were identified in the Ar matrix and one structure in the N_2 matrix. The B3LYPD3/6-311++G(2d,2p) method was used to optimize the structures of the four complexes produced throughout SHA photolysis. Four stable structures have been obtained for the $C_6H_4(OH)NCO\cdots H_2O$ and $C_6H_4(OH)_2\cdots HNCO$ complexes, and three configurations for the $C_6H_4(OH)C(O)N\cdots H_2O$ and $C_6H_4(OH)NHOH\cdots CO$ pairs. The spectra evidenced that during SHA photodissociation the structures corresponding to the global minimum as well as those due to the local minima are formed [1].

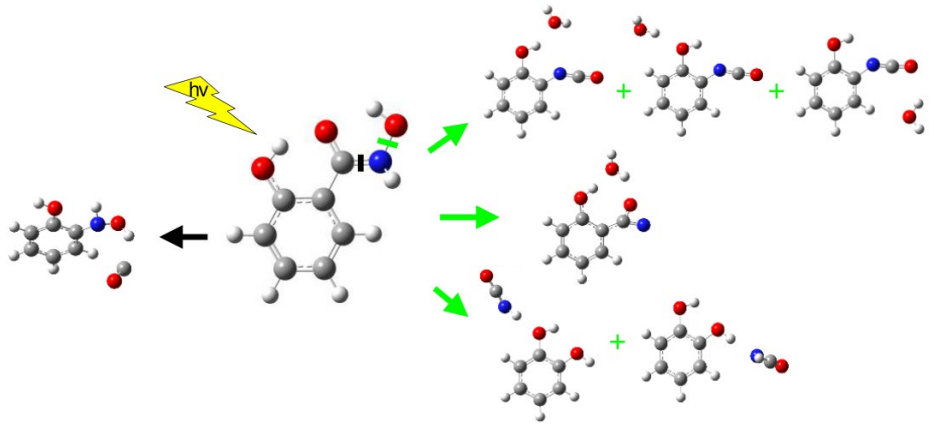


Figure 1 – Photolysis of salicylhydroxamic acid

References
1. M. Sałdyka, Z. Mielke, *Molecules*, 29 (2024) 862.

Acknowledgements: The authors thank the Wroclaw Centre for Networking and Supercomputing (WCSS) for providing computer time and facilities.

Modulation of Cytochrome C Redox Status by Retinoids in Human Breast Cancer Cells: Insights from Raman Imaging

Jakub M. Surmacki, Halina Abramczyk
Laboratory of Laser Molecular Spectroscopy, Institute of Applied Radiation Chemistry, Faculty of Chemistry, Lodz University of Technology, Wróblewskiego 15, 93-590 Łódź, Poland
jakub.surmacki@p.lodz.pl

We investigated the influence of the redox status of the central iron ion within the heme group of cytochrome c in human breast cancer cells. Using Raman imaging, we determined the redox state of cytochrome c in various subcellular compartments, including mitochondria, cytoplasm, lipid droplets, and the endoplasmic reticulum. Human breast adenocarcinoma cells (SK-BR-3) were incubated with 50 µM of retinoic acid, retinol, or retinyl palmitate for 24 hours. Raman spectra and corresponding images were acquired to assess the redox modulation induced by these retinoids.
Our results demonstrate that retinoic acid and retinol play a crucial role in maintaining mitochondrial energy homeostasis by modulating the redox status of cytochrome c in the electron transport chain, thereby influencing oxidative phosphorylation and apoptotic pathways. We further discuss the implications of retinoid-induced redox changes in cancer cell metabolism and signaling. Additionally, we provide experimental support for the theoretical hypothesis that retinoic acid and retinol catalyze resonance energy transfer processes and regulate the activation/inactivation cycle of protein kinase C delta (PKCδ), thereby contributing to oncogenic signaling regulation.

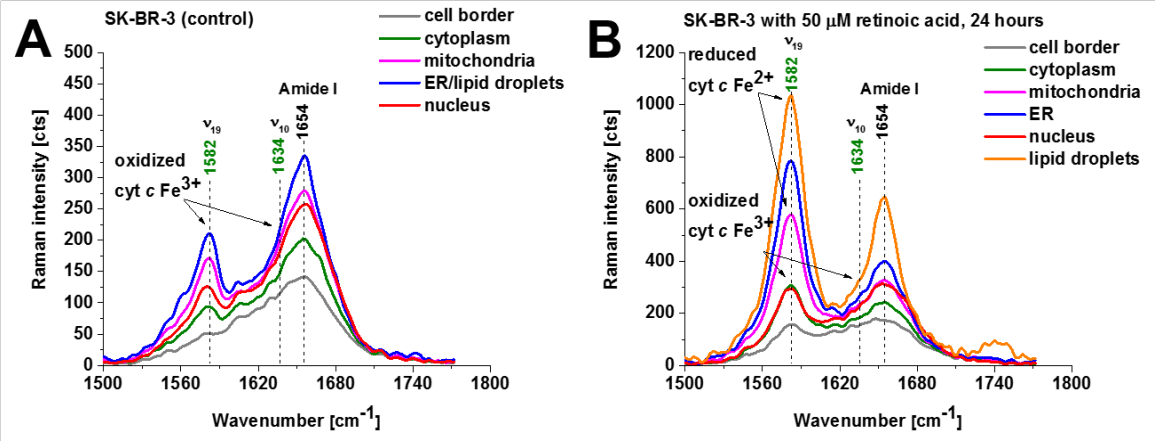


Figure 1 – Average Raman spectra of SK-BR-3 breast cancer cells acquired using 532 nm excitation: (A) control cells and (B) cells incubated with retinoic acid (50 µM) for 24 hours. Spectral contributions from different subcellular components are color-coded as follows: nucleus (red), lipid droplets (orange), endoplasmic reticulum (blue), cytoplasm (green), mitochondria (magenta), and cell border (light grey)

References

1. J. M. Surmacki, H. Abramczyk, *Sci. Rep.*, 13 (2023) 15049.

Acknowledgements: The authors thank the National Science Centre of Poland for financial support of this work (Grant: UMO-2021/43/B/ST4/01547).

Raman Spectroscopy and Artificial Intelligence as a Novel Approach for HER2 Status Assessment in Breast Cancer

Jakub M. Surmacki, Monika Kopeć, Halina Abramczyk
Laboratory of Laser Molecular Spectroscopy, Institute of Applied Radiation Chemistry, Faculty of Chemistry, Lodz University of Technology, Wróblewskiego 15, 93-590 Łódź, Poland
jakub.surmacki@p.lodz.pl

Conventional diagnostic methods such as immunohistochemistry (IHC) and in situ hybridization (ISH), routinely employed to determine the human epidermal growth factor receptor 2 (HER2) status in breast cancer, present several limitations, including subjectivity, semi-quantitative nature, and inter-observer variability. In this study, we investigated a novel immunodetection approach based on Raman spectroscopy and Raman imaging, integrated with artificial intelligence models, to assess HER2 expression across a spectrum of breast cancer phenotypes.

We evaluated the correlation between Raman-based analysis and standard HER2 testing methodologies (IHC and ISH). Raman spectral measurements exhibited a strong linear correlation with IHC results ($p = 0.05$, $R^2 = 0.9816$) across a panel of breast cell lines, including MCF-10A (non-tumorigenic epithelial), MCF-7 (luminal A), MDA-MB-231 (triple-negative), HTB-30/SK-BR-3, and AU-565 (HER2-positive). These results suggest that Raman spectroscopy and imaging offer a robust, label-free, and potentially more objective alternative for assessing HER2 status.

Our findings highlight the potential of Raman-based techniques, particularly when combined with AI-driven data analysis, to enhance diagnostic precision and support more personalized therapeutic strategies in breast cancer management.

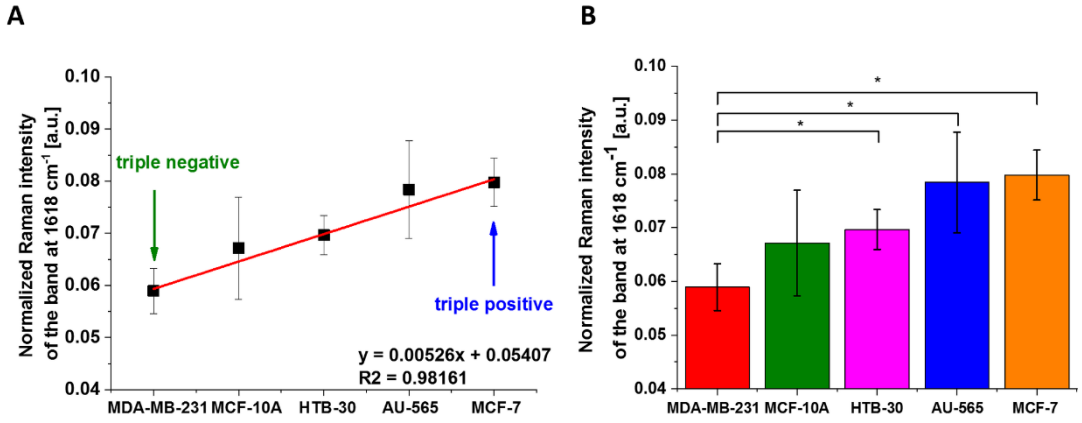


Figure 1 – Normalized Raman intensity of the band at 1618 cm^{-1} of breast cancer cells membranes for triple-positive (MCF-7), overexpressing HER2 (HTB-30 and AU-565), the normal cells (MCF-10A) (HER2 at the normal level), and triple-negative aggressive breast cancer (MDA-MB-231).
(A) Linear fitting R2 = 0.98161. (B) Normalized Raman band intensity (1618 cm^{-1}) as a function of breast cancer (mean ± SD); the statistically significant results have been marked with an asterisk ($p < 0.05$)

References

1. J. M. Surmacki, M. Kopeć, H. Abramczyk, *J. Med. Chem.*, 67 (2024) 19.

Acknowledgements: The authors thank the National Science Centre of Poland for financial support of this work (Grant: UMO-2021/43/B/ST4/01547).

SERS Detection of Organic Films on Cu Substrates Treated by Controlled Corrosion

Marie Svecova[a,b], Magnus Johnson[a]
[a]*Division of Surface and Corrosion Science, KTH Royal Institute of Technology, Stockholm, 100 44*
[b]*Department of Analytical Chemistry, University of Chemistry and Technology Prague, Prague, 166 28*
svecovam@vscht.cz; svecova@kth.se

Copper structures are commonly employed as enhancing substrates in the field of Surface-Enhanced Raman Scattering (SERS). Cu structures excel over other metallic substrates in their lower price of preparation and better interactions with organic compounds with lower affinity to the metallic surfaces [1]. Unfortunately, there is a challenge to store these substrates properly since Cu is prone to atmospheric corrosion in several environments.
Cu structures exposed to a corrosive environment result in the formation of a layer of copper oxides/hydroxides on the surface, also in the presence of humid air [2]. Such conditions lead to the changes on the Cu surface in terms of morphology, chemical composition, dielectric properties, and affect the final enhancing properties of the prepared substrate (Figure 1).

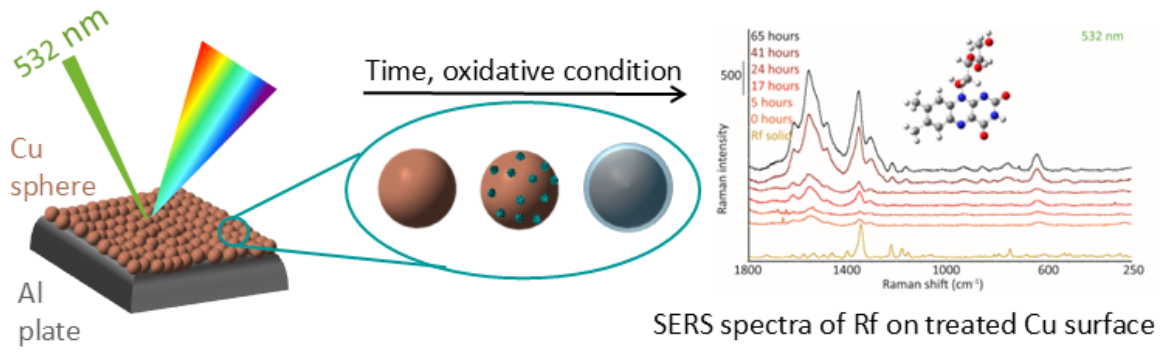


Figure 1 – Schematic illustration of the study

In this study, we aim at an improved understanding of the corrosive processes of Cu enhancing substrates and to assess their influence on the final SERS enhancement. The structures are characterized using scanning electron microscopy coupled with energy dispersive spectroscopy and atomic force microscopy. The SERS effect is primarily monitored by the detection of riboflavin (Rf) films excited by 785 nm, 532 nm, and 405 nm lasers. The application possibilities of Cu substrates treated by controlled corrosion are additionally demonstrated on other samples such as flavonoids, organic phosphonic acids, and organic pigments.

References

1. O. Volochanskyi, M. Svecova, V. Bartunek, V. Prokopec, *Colloids Surf. A.*, 616 (2021) 126310.
2. W.Zhao, R.P. Babu, T. Chnag, I. Odnevall, P. Hedström, C.M. Johnson, C. Leygraf, *Corros. Sci.*, 195. (2022) 109995.

Acknowledgements: This work was financially supported by the Czech Science Foundation (Project No. 23-07610O).

Theoretical (DFT) and Experimental (FT-IR, FT-Raman) Studies on N-Phenylthioformamide

Wioleta Śmiszek-Lindert, Leszek Marynowski
Faculty of Natural Sciences, University of Silesia, 60 Będzińska Street, 41-200 Sosnowiec, Poland
wioleta.smiszek-lindert@us.edu.pl

In this study, a new N-phenylthioformamide compound was synthesized and characterized using FT-IR, FT-Raman and single-crystal X-ray diffraction method. The optimized geometric parameters, normal mode frequencies and corresponding vibrational assignments of the molecules have been examined by means of the density functional theory (DFT/B3LYP) methods with 6-311++G(d,p) and 6-311++G(3df,2pd) basis sets. All quantum-mechanical calculations were performed using the GAUSSIAN 09 software program.
For analysis of the intermolecular interactions in the crystal lattice of N-phenylthioformamide the Hirshfeld Surface method has been used.
It has been shown that the observed and calculated frequencies are found to be in good agreement, as well as the analysis of the Hirshfeld surface has been well correlated to the spectroscopic studies. Additionally, the highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), the energy gap between E_{HOMO} and E_{LUMO} ($\Delta E_{HOMO–LUMO}$), molecular electrostatic potential and global reactivity descriptors viz. chemical potential, global hardness and electrophilicity have been calculated.

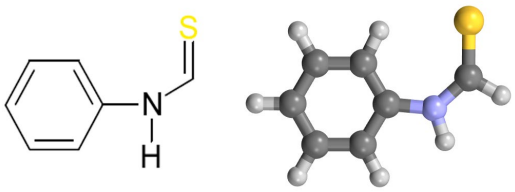


Figure 1 – The chemical structure of N-phenylthioformamide molecule

Acknowledgements: Calculations have been carried out using resources provided by Wroclaw Centre for Networking and Supercomputing (http://wcss.pl).

Finding a Needle in a Needle Stack: Leveraging Vibrational Spectra and Machine Learning to Guide Conformational Search

Roel van de Ven, Daria Ruth Galimberti
Institute for Molecules and Material, Radboud University, Nijmegen, The Netherlands
Roel.vandeven@ru.nl

The standard approach for identifying the conformer corresponding to an experimental infrared (IR) spectrum involves exploring the potential energy surface (PES), locating the minima and calculating the spectra of each conformation until a match is found. This sampling approach is highly inefficient because it requires numerous frequency calculations on structures that, in the end, are discarded. It becomes unfeasible for larger molecules since the number of minima on the PES will increase exponentially.
I will present a new methodology to cleverly direct the conformational search using molecular dynamics (MD) simulations informed by an on-the-fly machine learning (ML) model based on generated vibrational spectra. Our program starts from a random position on the PES and the machine learning model learns how to modify the molecular conformation to optimize the spectral similarity until the correct conformation is found. The ML model uses the generated vibrational spectra to predict biases that are applied in a MD simulation to push the molecule to the desired conformer.
Here I will discuss the possible compromises between accuracy and computational cost for MD simulations, geometry optimizations, and frequency calculations. I will show that Density Functional Tight Binding (DFTB) with the 3-ob-3-1 parameterization shows good accuracy at a low cost for MD simulations. While for geometry optimizations and frequency calculations need DFT calculations with polarized basis sets and preferably hybrid functionals.

The Secret of Tinctures of Selected Glycosides with Cardiac Action

Timofey Punko[a], Paulina Moskal[a], Elżbieta Kwasnowska[b],
Aleksandra Wesełucha-Birczyńska[a]
[a]*Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, Kraków 30-387, Poland*
[b]*Department of Medical Biochemistry, Jagiellonian University, Medical College, Mikołaja Kopernika 7C, 31-034 Kraków, Poland*
birczyns@chemia.uj.edu.pl

Cardiac glycosides are naturally derived compounds utilized in the treatment of cardiac-origin heart failure, a condition characterized by impaired myocardial contractility. This condition represents a critical pathological state, given that cardiovascular diseases currently constitute the leading cause of mortality in industrialized nations [1].
Glycosides act directly on the cardiac muscle, resulting in increased sensitivity to stimuli, enhanced contractile strength, and improved energy utilization by the myocardium. They do not increase blood pressure; instead, their pharmacological effects involve augmenting the force and amplitude of cardiac contractions, shortening the duration of systole while concurrently prolonging the duration and increasing the depth of diastole [2].
Due to advancements in pharmacology, particularly the introduction of angiotensin-converting enzyme (ACE) inhibitors such as captopril and enalapril, cardiac glycosides are no longer the first-line treatment for various types of cardiovascular failure, and some have been withdrawn from use. However, several compounds from this class remain effective and continue to attract considerable interest, especially in combination therapy [3].
The aim of the study was to assess the quantitative composition of a tincture containing strophanthin G/ouabain, originating from the herbal medicine market, as well as spectroscopic studies of three selected cardiac glycosides. The quantitative analysis used in the study was based on Raman spectra [4].

References

1. A. Zejc, M. Gorczyca, *Drug Chemistry (in Polish)*, PZWL, 3rd Ed., Warszawa, 2008, pp. 341-342.
2. G. Rajtar-Cynke, *Pharmacology (in Polish)*, Czelej, 3rd Ed., Lublin, 2015, pp. 264-270.
3. A. Kołodziejczyk, *Natural Organic Compounds (in Polish)*, PWN, 3rd Ed. 3, Warszawa, 2013, pp. 521-526.
4. H. Barańska, A. Łabuzińska, J. Terpiński, *Laser Raman Spectroscopy (in Polish),* PWN, Warszawa, 1981; pp. 13, 121-125.

Acknowledgements: The study was carried out using research infrastructure funded by the European Union, Poland, in the framework of the Smart Growth Operational Programme, Measure 4.2; Grant No. POIR.04.02.00-00- D001/20, "ATOMIN 2.0 – Center for materials research on ATOMic scale for the INnovative economy". This study was supported by the subsidiary research part of Jagiellonian University Faculty of Chemistry, Krakow, Poland from the Ministry of Science and Higher Education, Poland.

Preparation and Thermal Properties of a Phase Change Material Based on Arachidic and Palmitic Acids

Jakub Włodarski, Marcin Sobczyk
Faculty of Chemistry, University of Wrocław, ul. F. Joliot-Curie 14, 50-383 Wrocław, Poland.
jakub.wlodarski@uwr.edu.pl

Phase change materials are the main component of active heat storage systems which help increase energy efficiency of temperature control in both commercial and private sectors. For practical use phase change materials must exhibit specific qualities. Most importantly, a well-defined melting point, high enthalpy of fusion, good thermal conductivity and stability over many work cycles. These characteristics have been studied for an eutectic mixture of arachidic and palmitic acids [1]. The eutectic is formed with the molar fraction of arachidic acid equal to 0.3, it shows the melting point of 51.8°C and the latent heat of fusion of 161.3 $J \times g^{-1}$, determined with differential scanning calorimetry. The specific heat capacity of the mixture was determined across the temperature range of 20-45°C giving values between 1.75 and 2.81 $J \times g^{-1} \times °C^{-1}$, using a method described by Cabeza et al. [2] modified for better compatibility with the samples. Additionally the thermal conductivity coefficient was determined to be 0.291 $W \times m^{-1} \times °C^{-1}$ using a custom-built Poensgen apparatus. The mixture also maintained a good stability over 500 work cycles as evidenced by the lack of significant changes in its properties.

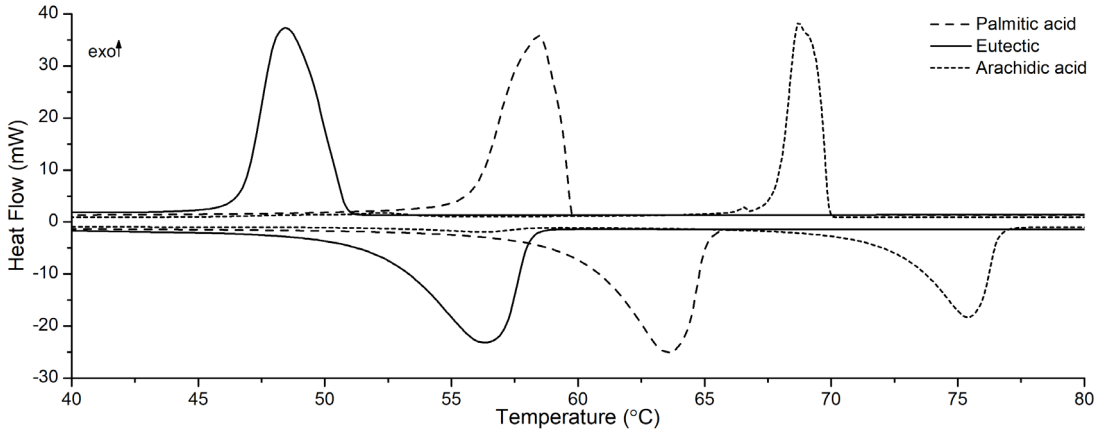


Figure 1 – DSC curves of palmitic acid, arachidic acid, and the eutectic mixture

References

1. J. Włodarski, M. Sobczyk, *in press*.
2. G. Ferrer, C. Barreneche, A. Sole, I. Martorell, L. F. Cabeza*, J. Energy Storage*, 11 (2017) 1.

Weak Hydrogen Bonds in the Binding Pocket of Carbonic Anhydrase II – Quantum Chemical Investigations

Kamil Wojtkowiak, Aneta Jezierska
Faculty of Chemistry, University of Wrocław, Fryderyka Joliot-Curie 14, 50-383 Wrocław, Poland
kamil.wojtkowiak2@uwr.edu.pl

Carbonic Anhydrase (CA II) enzyme family is mainly known for its pivotal role in the maintaining plasma acid-base equilibrium. Nonetheless, more and more studies link overexpression of CA II with obesity, cancer progression or drug resistance [1]. Therefore, it is of utmost importance to understand and analyze the interactions in which Carbonic Anhydrase inhibitors (CAIs) can be involved in. For this purpose, static as well as dynamical methods of computational chemistry were applied to the model systems in the continuum solvation model, crystalline phase as well as native protein environment. Furthermore, the theoretical frameworks such as Quantum Theory of Atoms in Molecules, Reduced Density Gradient analysis and Natural Bond Orbitals were employed to pinpoint the characteristics of the observed hydrogen bonds in the examined systems [2,3,4]. The obtained results indicate the weak nature of studied interactions and provide its comprehensive characterization.

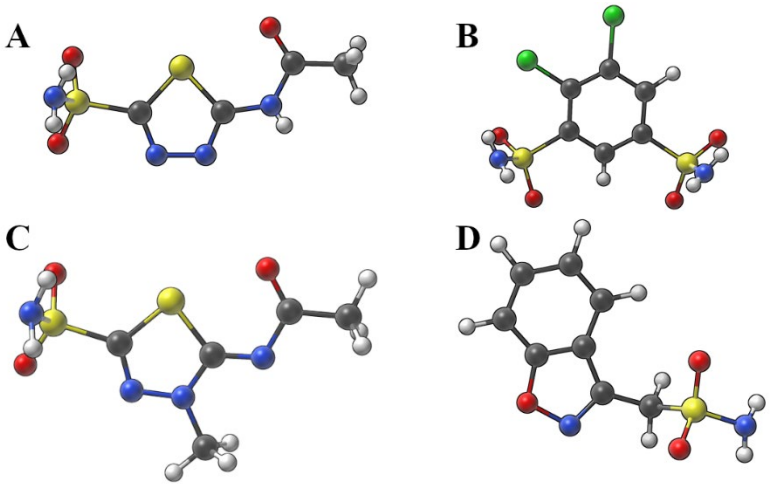


Figure 1 – CPK visualization of examined Carbonic Anhydrase inhibitors structures. A – acetazolamide, B – diclofenamide, C – methazolamide, D – zonisamide

References
1. C.T. Supuran, *Nat. Rev. Drug Discov.*, 7 (2008) 168.
2. R. Bader, *Atoms in Molecules: A Quantum Theory*, Clarendon Press: Oxford, 1994.
3. E.R. Johnson, S. Keinan, et al., *J. Am. Chem. Soc.*, 132 (2010) 6498.
4. F. Weinhold, R.A. Klein, *Chem. Educ. Res. Pract.* 15 (2014) 276.

Acknowledgements: The author thanks to the PL-Grid intrastructure in the Academic Cyfronet Center (Ares), Wrocław Centre for Networking and Supercomputing as well as Poznan Supercomputing and Networking Center (PSNC) for providing computer facilities.

Does Sample Preparation Affect Spectroscopic Results?

Emilia Wrona[a,b], Anna Błasiak[c], Gabriela Stopka[b,c], Aleksandra Nogaj[b,c], Aleksandra Kurek[a], Aleksandra Wesełucha-Birczyńska[a]
[a]*Faculty of Chemistry, Jagiellonian University, 30-387 Kraków, Poland*
[b]*Doctoral School of Exact and Natural Sciences, Jagiellonian University, 30-348 Kraków, Poland*
[c]*Department of Neurophysiology and Chronobiology, Institute of Zoology and Biomedical Research, Jagiellonian University, 30-387 Kraków, Poland*
emilia.wrona@doctoral.uj.edu.pl

Raman spectroscopy makes it possible to observe healthy brain tissue and its changes associated with the development of diseases such as brain tumours, as well as neurodegenerative diseases - epilepsy or Alzhaimer's disease[1-3]. The composition and concentration of lipids in brain tissue can change significantly in diseased tissues, making it a useful diagnostic parameter for determining the type and severity of a brain tumour or neurodegenerative disorder[4].
To obtain the highest quality Raman spectrum, the measurement parameters and sample preparation must be properly selected[4]. No fixation method was applied to prepare the samples. Based on a literature review, three different temperature ranges were selected for which measurements were carried out[1,5-8]. The influence of the solution on the quality of the measurement was also checked. Brain tissue for methods I-IV was stored in artificial cerebrospinal fluid (ACSF), which was carbogenated. Method I: the tissue was stored at room temperature and kept in ACSF solution during the measurement. Method II: the tissue was stored at room temperature, 0.9% NaCl solution was used for the measurement. Method III: before measurement, the tissue was stored in a container placed on a cooling pad, ACSF solution was used for measurement. Method IV: before measurement, the tissue was stored in a container placed on a cooling pad, 0.9% NaCl solution was used for measurement. Method V: the tissue was frozen in liquid nitrogen. Then the tissue was heated and immersed in 0.9% NaCl solution and the measurement was performed. During the measurement temperature was maintained at about 32°C.
The recorded spectra, were processed and averaged. Then the resulting spectra, were subjected to statistical analysis. The analysis of the results indicates differences in the range of vibrations characteristic for lipids and proteins, which are discussed.

References

1. P. Chen, et al., *Appl Opt,* 48 (2009) 4743.
2. J. Desroches, et al., *Sci Rep*, 8 (2018) 2380.
3. J. Sacharz, et al., *Spectrochim Acta A*, 188 (2018) 581.
4. J. Sacharz, et al., *Analytical Methods*, 12 (2020) 4334.
5. R. Pinto Aguiar, et al., *Lasers Med Sci*, 37 (2020) 121.
6. A. Wesełucha-Birczyńska, et al., *Vib Spectrosc*, 85 (2016) 48.
7. J. Zięba-Palus, et al., *J. Mol. Struct*, 1147 (2017) 310.
8. L. Chrobok, et al., *Neuroscience*, 329 (2016) 306.

Acknowledgements: The study was carried out using research infrastructure funded by the European Union, Poland, in the framework of the Smart Growth Operational Programme, Measure 4.2; Grant No. POIR.04.02.00-00- D001/20, "ATOMIN 2.0 – Center for materials research on ATOMic scale for the INnovative economy". This study was supported by the subsidiary research part of Jagiellonian University Faculty of Chemistry, Krakow, Poland from the Ministry of Science and Higher Education, Poland.

New Glycosides for *in vivo* Raman Imaging

Emilia Wrona[a,b], Pierre Lafite[c], Martyna Kucharska[a], Aleksandra Wesełucha-Birczyńska[a]
[a]*Faculty of Chemistry, Jagiellonian University, 30-387 Kraków, Poland*
[b]*Doctoral School of Exact and Natural Sciences, Jagiellonian University, 30-348 Kraków, Poland*
[c]*Institute of Organic and Analytical Chemistry, University of Orleans, 45067 Orléans Cedex 2, France*
emilia.wrona@doctoral.uj.edu.pl

As a highly sensitive and non-invasive technique, Raman spectroscopy is finding its place in biological research and diagnostics[1]. Many diseases result from underlying biochemical changes in cells, which Raman spectroscopy is able to detect, sometimes with high sensitivity[2]. The technique allows the analysis of biochemical markers of cancer cells, i.e. specific proteins, hormones and enzymes[1]. It is now known that glycosides are part of several important classes of compounds, including hormones[3].
The aim of the study was to synthesise a series of model glycosidic compounds using an enzymatic reaction to obtain O- or S- glycoside analogues (Fig.1). Another series of compounds consisted of deuterated glycosides. The purified glycosides were then investigated spectroscopically using a Raman spectroscopy method.

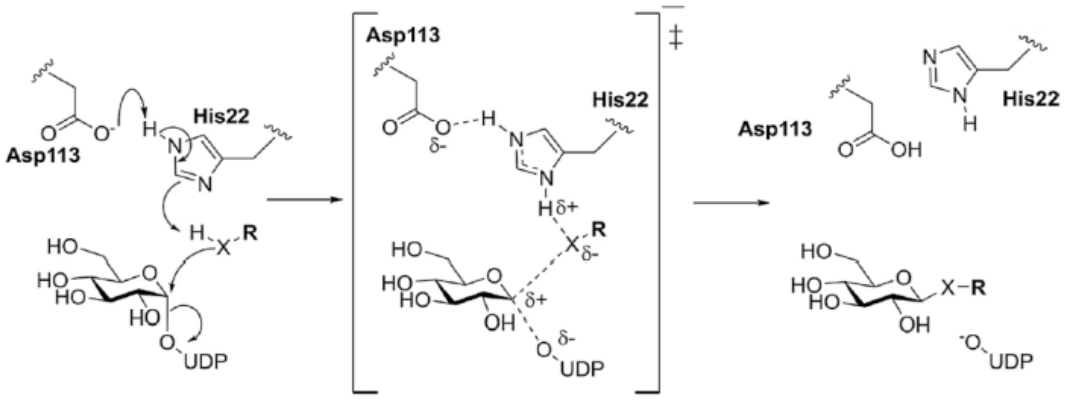


Figure 1 – Mechanism of the glycosylation reaction catalyzed by the enzyme UGT74B1 (X = S or O)[4]

The resulting glycosides were checked for the presence of marker bands that could be used as spectral signatures for future applications such as imaging. For S-glycosides, a strong vibration at about 500-600 cm^{-1} is visible, which is not present in O-glycosides. For deuterated glycosides, a shift of some oscillations is observed, which is due to isotopic substitution. Spectral analysis has shown that Raman spectroscopy can be used to distinguish between different groups of glycosides and to confirm the synthesis results.

References
1. P. Nykiel, *Biul. Wydz. Farm. Warsz. Univ. Med.*, 11.4 (2013) 27.
2. G. Zonios, et al. *Gastrointest. Endosc.*, 4.43 (1996) 307.
3. V. Kren, et al., *Curr. Med. Chem.*, 8.11 (2001) 1303.
4. P. Lafite, et al.,*Mol. Catal.*, 479 (2019) 110631.

Acknowledgements: This study was supported by the subsidiary research part of Jagiellonian University Faculty of Chemistry, Krakow, Poland from the Ministry of Science and Higher Education, Poland.

Non-linear Dielectric Effect in Solutions of Menthol

Kewin Żmigrodzki, Kazimierz Orzechowski
Faculty of Chemistry, University of Wrocław, Fryderyka Joliot-Curie 14, 50-383 Wrocław, Poland
334224@uwr.edu.pl

Non-linear dielectric effect (NDE) is the one of the techniques used in dielectric experiments, in which is measured the NDE increment as a difference between an electric permittivity obtained at strong and week electric fields [1]. According to Debye–Langevin theory, in simple dipolar liquids, the nonlinear dielectric effect increment should be negative and proportional to the square of the electric field strength. However, in certain liquids—such as nitrobenzene, 1,2-dichloroethane, and higher alcohols—a positive NDE increment has been observed. This deviation is attributed to conformational changes in the case of 1,2-dichloroethane, or to structural changes in intermolecular complexes, as seen in nitrobenzene and alcohols, induced by the strong electric field.
In the paper we discuss the case of menthol. Both in a liquid state (temperature higher than the melting temperature) and for solutions with p-xylene the NDE increment is positive. We doubt that the change of conformation could be responsible for the positive NDE effect. We suspect, that the effect is related to the movement of association equilibrium from cyclic to linear form under the influence of a strong electric field. Alcohols form associations by forming hydrogen bonds in their structures, so we can divide them into those that have a dipole moment, i.e. linear (open), and those without a dipole moment - cyclic (closed). When alcohols are applied to an electric field, their dipole moments align in the direction of the field - i.e. the equilibrium shifts towards linear associates. [3,4]

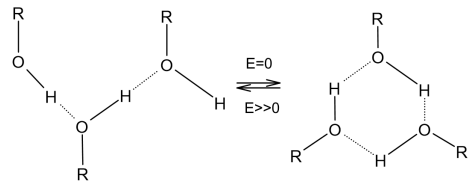


Figure 5 – Formation of associations in alcohols

Electric permittivity, density and refractive index were also measured to compare Onsager model predictions with experimental data

References

1. T. Chełkowski, *Dielectric Physics* Warszawa: PWN, 1980.
2. J. Małecki, *Chem. Phys. Lett.*, 297 (1998) 29.
3. K. Orzechowski, M. A. Czarnecki, *J. Mol. Liq.*, 279 (2019) 540.

Excited State and Charge Transfer Dynamics in Metal-Ligand Coordination Polymers for Synapse-Mimicking Memristors

M. A. Thottappali[a], Y. Panthi[a], A. Pandey[a], A. Chernyshev[b], J. Zedník[b], J. Vohlídal[b], J. Pfleger[a]
[a]*Institute of Macromolecular Chemistry CAS, Prague, 16200, Czech Republic.*
[b]*Department of Physical and Macromolecular Chemistry, Charles University, 12800, Czech Republic.*
thottappali@imc.cas.cz

Recent studies have demonstrated that the metallo-supramolecular coordination polymer ($[CoU]_n$) made of bisterpyridine phenylcarbazole unimer (U) and Co(II) ions exhibits multimodal resistance changes mimicing synaptic plasticity, whereas thin films of the unimer display non-volatile bistable memory behavior[1]. To gain deeper insight into the underlying excited-state charge transfer mechanisms, femtosecond transient absorption (TA) spectroscopy was employed. Upon photoexcitation, the unimer (U) exhibits a broad excited-state absorption (ESA) with the longest-lived component persisting for 3.4 ns, indicative of a well-defined intramolecular charge transfer (ICT) state (Figure 1b). In contrast, the TA spectrum of the polymer $[CoU]_n$ shows a prominent ground-state bleach (GSB) corresponding to the metal-to-ligand charge transfer (MLCT) band, along with a blue-shifted ESA (shifting from 585 nm to 558 nm, with a shoulder at 517 nm), and a significantly longer excited state lifetime that extends beyond the experimental detection window (>6 ns). The ICT state observed in the unimer signifies a stable, charge separated configuration and reflects a relatively simple excited state landscape. This discrete ICT state facilitates binary electronic switching behavior, correlating well with the non-volatile, bistable memory performance observed in U. In contrast, the polymer $[CoU]_n$ displays a more complex excited state landscape (Figure 1c), shaped by the incorporation of Co(II) centers, as evidenced by the MLCT associated GSB. It enables multimodal, analog-like resistance modulation, providing a mechanistic basis for the observed neuromorphic-like functionality.

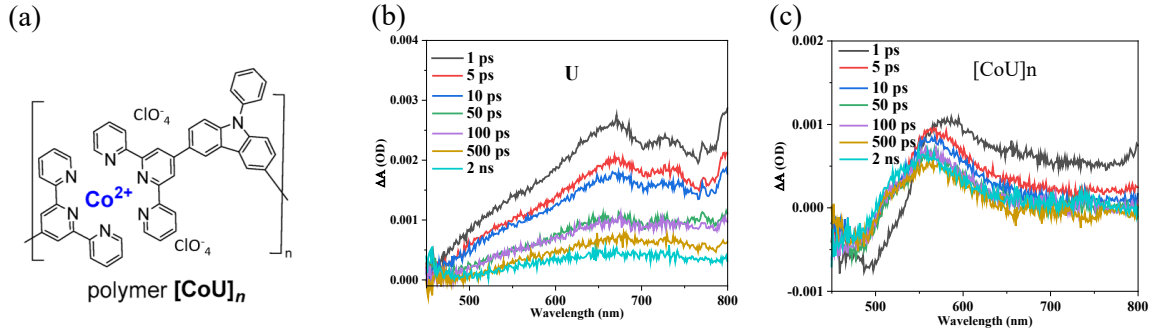


Figure 1 – (a) Scheme of metallo-supramolecular polymer $[CoU]_n$, (b) and (c) Time evolution of transient absorption spectra of thin film of U and $[CoU]_n$ complex, respectively

References

1. A. Pandey, A. Chernyshev, Y.R. Panthi, J. Zedník, A. Šturcová, M. Konefał, O. Kočková, S.H. Foulger, J. Vohlídal, J. Pfleger, *Polymers,* 16 (2024) 542.

Acknowledgments: The authors thank the Czech Science Foundation, project No. 24-10384S, for funding.

Autor Index

Autor Index

Plenary **L**ecture (PL), **O**ral **C**ontribution (OC), **P**oster (P)

Clausen	Morten Rahr		P-9
Contreras-Cáceres	Rafael		OC-1
Coriani	Sonia		P-8
Cukras	**Janusz**	janusz.cukras@uw.edu.pl	**P-8**
Czaja	**Tomasz Pawel**	tomasz.czaja@food.ku.dk	**OC-35, P-9**
Czaja	Kacper		P-4
Czarnecki	Mirosław A.		OC-9, P-40
Dabrowska	**Alicja**	alicja.dabrowska@tuwien.ac.at	**OC-56**, PL-15
Dannenberg	Lars		P-47
Davydova	N. A.		P-13
Dawiec	**Patrycja**	patrycja.dawiec@doctoral.uj.edu.pl	**OC-11**
Dendisová	Marcela		OC-47, P-28
Detert	**Heiner**	detert@uni-mainz.de	**P-10**
Długoń	Elżbieta		OC-30
Doni	Daryna		P-11
Dopieralski	**Przemysław**	przemyslaw.dopieralski@uwr.edu.pl	**OC-27**, P-2
Dovbeshko	**Galyna**	matinelli@gmail.com	**OC-64, P-11, P-12**, P-43
Drăgoi	Brîndușa		OC-6, P-48
Drahos	L.		OC-17, P-43
Drozd	**Marek**	m.drozd@intibs.pl	**OC-24, P-13, P-14**
Ďuríšková	**Lucia**	lucia.duriskova722@student.cuni.cz	**P-15**, OC-25
Dutkiewicz	**Natalia**	ndutkiewicz@ichf.edu.pl	**OC-41**, P-19
Dybaś	**Jakub**	jakub.dybas@uj.edu.pl	**OC-15**, OC-10
Dymińska	L.		P-31, P-32, P-35, P-36
Ehrlich	Hermann		P-5
Engelsen	**Søren Balling**	se@food.ku.dk	**PL-12**, OC-35, P-9
Eshel	Yotam D.		OC-18
Fatafta	Hebah		P-6
Fausto	**Rui**	rfausto@ci.uc.pt	**PL-1**, P-25
Ferguson	Dougal		PL-5
Fischer-Fodor	Eva		P-17
Fiser	B.		OC-17
Focsan	Monica		P-17
Forte-Castro	Arantxa		OC-1
Frandsen	Benjamin N.		P-44
Fu	Y.		P-23
Furter	**Jasmine S.**	jasmine.furter@hu-berlin.de	**P-16**
Gabryelczyk	Agnieszka		P-45
Găină	Ioana-Luiza		P-3, P-17
Gajewska	Agnieszka		OC-43
Gál	**Emese**	emese.gal@ubbcluj.ro	**P-17**, P-3
Galimberti	Daria Ruth		OC-60, P-55
Gardner	**Peter**	peter.gardner@manchester.ac.uk	**PL-5**
Garg	**Shivangi**	shivangi.garg@pwr.edu.pl	**P-18**, OC-59
Gastaldo	Michele		OC-48
Gavrilko	Tetiana		P-14
Gaweł	Przemysław		OC-41
Gerwert	**Klaus**	klaus.gerwert@ruhr-uni-bochum.de	**PL-4**
Ghasemi	**Shiva**	shivaghasemi805@gmail.com	**OC-57**
Gieroba	**Barbara**	barbaragieroba@umlub.pl	**OC-12**
Gnatyuk	Olena		OC-64, P-11,P-12, P-43

Gnatyuk	Ivan		P-11, P-14
Godlewska	P.		P-36
Golec	**Barbara**	b.golec@uksw.edu.pl	**OC-55**, OC-41, OC-43, P-19
Golin Almeida	**Thomas**	tga@chem.ku.dk	**OC-20**
Gomory	A.		OC-17, P-43
Gordel-Wójcik	**Marta**	marta.gordel-wojcik@uwr.edu.pl	**OC-13**, P-34
Gorski	**Aleksander**	agorski@ichf.edu.pl	**P-19**,OC-41,OC-43,OC-55
Góbi	**Sándor**	sandor.gobi@ttk.elte.hu	**OC-34**, P-27
Grabska	**Justyna**	Justyna.Grabska@uibk.ac.at	**OC-52**
Graham	Duncan		OC-4
Grdadolnik	**Jože**	joze.grdadolnik@ki.si	**OC-58**
Gritsevich	María		P-33
Grygier	Anna		OC-9
Gyepes	Róbert		OC-19
Hansen	**Poul Erik**	poulerik@ruc.dk	**PL-17**
Hansen	**Vera Staun**	vsh@chem.ku.dk	**OC-39**
Hansen	Bjørn Niels		P-9
Hanuš	Jan		OC-51
Hanuza	Jerzy		P-31, P-32, P-35, P-36
Haque	Shabnam		P-26
Hart	Claire A.		PL-5
Haupa	**Karolina A.**	karolina.haupa@bruker.com	**OC-28**
Havránek	Jakub		P-28
Hebestreit	Marie-Luise		PL-8
Heise	**Herbert M.**	heise.h@fh-swf.de	**PL-6,P-20,P-21,P-22,P-23**
Helscher	**Sara**	333205@uwr.edu.pl	**P-24**
Horak	Daniel		OC-16
Huck	Christian W.		OC-52
Huleihel	Mahmoud		OC-18
Ilchenko	O.		OC-64
Ildiz	**Gulce O.**	g.ogruc@iku.edu.tr	**P-25**
Isokov	Timur		P-11
Iyer	Anisha		OC-39
Iyer	Siddharth		P-44
Jakubowska	Justyna		OC-11, P-1
Janicki	Mikołaj		OC-59
Janissek	P.R.		P-20
Jarczewska	Karolina		P-29
Jensen	**Casper Vindahl**	CVJ@chem.ku.dk	**OC-29**, OC-39
Jezierska	Aneta		P-58
Jílek	**Štěpán**	stepan.jilek@matfyz.cuni.cz	**OC-63**, OC-25, P-15
Jin	Jiaye		P-26
Jochem	Matthias		P-10
Johnson	Magnus		P-53
Kalbáč	Martin		OC-48
Kalisz	Grzegorz		OC-12
Kamecka	Anna		P-39
Kapelushnik	Joseph		OC-18
Kapitán	Josef		OC-25, OC-63
Kapusta	Šimon		OC-36

Karakhim	S.		P-12
Karmakar	**Hrittik**	hrittik.karmakar@uni-leipzig.de	**P-26**
Kazimierczak	Paulina		OC-12
Kazimierczuk	Katarzyna		P-39
Kaźmierski	**Wojciech**	wojciech.kazmierski@bruker.com	BRUKER
Keresztes	**Barbara**	barbi1226@gmail.com	**P-27**, OC-34
Khalavka	Maryna		OC-12
Kjaergaard	**Henrik G.**	hgk@chem.ku.dk	**PL-14**,OC-20,OC-21, OC-23,OC-29,OC-31, OC-32, OC-39
Kjaersgaard	Alexander		OC-32
Kkadan	Mohammed S.P.		OC-63
Kmetík	**Matěj**	kmetikm@vscht.cz	**P-28**, OC-47
Knechtel	**Fabian**	Fabian.Knechtel@bruker.com	**BRUKER**
Kneipp	Janina		P-16, P-47
Koch	**Joanna**	joanna.koch@chemland.pl	**CHEMLAND**
Kočišová	**Eva**	eva.kocisova@matfyz.cuni.cz	**OC-36**, OC-51
Kolesnyk	D.		OC-64, P-12
Kolniak-Ostek	Joanna		OC-8
Kołkowski	Radosław		OC-13
Kołodziej	**Anna**	anka.kolodziej@uj.edu.pl	**OC-16**, OC-30
Komisar	D.		OC-64
Kopal	**Ivan**	kopal@ufe.cz	**OC-47**, P-28
Kopeć	**Monika**	monika.kopec@p.lodz.pl	**P-29**, OC-3, P-52
Korona	**Wiktoria**	wiktoria.korona@doctoral.uj.edu.pl	**OC-14**, PL-3
Kosendiak	Iwona		P-30
Kosevich	M.		P-43
Kowalczyk-Głowacka	**Agnieszka**	kowalczyk@qd-europe.com	***Quantum Design GmbH***
Kowalska	Dorota		OC-44
Kowalski	Jarosław		P-19
Królikowska	Agata		OC-53
Krupa	**Justyna**	justyna.krupa@uwr.edu.pl	**P-30**
Kucharska	**Edyta**	edyta.kucharska@ue.wroc.pl	**P-31, P-32**, P-35, P-36
Kucharska	Martyna		P-60
Kułacz	**Karol**	karol.kulacz@uwr.edu.pl	**OC-49**
Kupka	Teobald		OC-22, P-6
Kurek	Aleksandra		P-59
Kuzmina	**Veranika**	vkuzmina@ichf.edu.pl	**OC-54**
Kwasnowska	Elżbieta		P-56
Kylián	Ondřej		OC-36, OC-51
Lafite	Pierre		P-60
Lapidot	Itshak		OC-18
Larsen	Jon		P-33
Lebowa	W.		OC-15
Lech	Barbara K.		P-18
Lendl	**Bernhard**	bernhard.lendl@tuwien.ac.at	**PL-15**, OC-56
Limbach	Daniel		P-10
Lindenbauer	Leopold		PL-15
Listkowski	Arkadiusz		OC-43
Lopez-Ramirez	**Maria Rosa**	mrlopez@uma.es	**OC-1, P-33**
Lundell	**Jan**	jan.lundell@helsinki.fi	**PL-9**, P-30

Lüttschwager	Nils O. B.		OC-46
Lwin	Eaindra		OC-29
Lwin	**Eaindra**	eaindra.lwin@uni-goettingen.de	**OC-46**
Machowski	Jakub		OC-2
Magoulas	Ilias		PL-16
Măirean	Ciprian-Paul		P-48
Majdecki	Maciej		OC-41
Majzner	Katarzyna		OC-4, OC-11, P-1
Malik	**Magdalena**	magdalena.malik@pwr.edu.pl	**P-34**
Mariusz Pietrzak			OC-54
Marković	**Ružica**	ftq203@alumni.ku.dk	**OC-21**
Markussen	Sofie		OC-39
Marx	Dominik		OC-27
Marynowski	Leszek		P-54
Masternak	Joanna		P-39
Matulková	Irena		OC-19
Mazur	Tomasz		P-34
Mazurek	**Sylwester**	sylwester.mazurek@uwr.edu.pl	**OC-8**
Mazuryk	Olga		OC-11
Mączka	Mirosław		OC-38
Mbakara	Idaresit		OC-43
Meuwly	**Marcus**	m.meuwly@unibas.ch	**PL-10**
Michalski	**Jacek**	jacek.michalski@ue.wroc.pl	**P-35, P-36**, P-31, P-32
Mielke	Zofia		P-50
Minofar	B.		OC-17
Miskin	Hagit		OC-18
Misztal	Oliwier		P-8
Młynarski	Wojciech		OC-11
Møller	Kristian H.		OC-20
Monastyrskyi	G.		OC-64, P-12
Moraru	Vanda-Gianina		P-48
Mordechai	Shaul		OC-18
Moskal	Paulina		P-56
Mozgova	Olena		OC-12
Mucha	**Karolina**	karolina.mucha@uwr.edu.pl	**P-37**
Muhieddine	**Ali**	alimuhydine@gmail.com	**OC-37**
Musiał	**Karolina**	karolina.musial@uwr.edu.pl	**P-38**, OC-9
Myllys	Nanna		P-44
Nagaj	Aleksandra		P-59
Najgebauer	**Piotr**	122217@student.uni.opole.pl	**OC-22**
Němec	**Ivan**	ivan.nemec@natur.cuni.cz	**OC-19**
Němec	Petr		OC-19
Nogueira	Bernardo A.		P-25
Nosach	Liudmyla		OC-12
Novák	David		OC-36
Nowakowska	Anna		PL-3, OC-14, P-1
Nowakowski	Robert		OC-12
Nyk	Marcin		OC-13
O'Faolian	Liam		PL-15
Oćwieja	Magdalena		OC-26
Okła	**Karol**	karol.okla@onet.pl	**P-39**
Olariu	Dragos		P-48

Olenchuk	M.		OC-64, P-12
Olivares-Fernández	Lucas		OC-1
Olivera	Pedro		PL-5
Olsztyńska-Janus	**Sylwia**	sylwia.olsztynska-janus@pwr.edu.pl	**P-40, P-41**
Onaciu	Anca		OC-6
Orzechowska	Barbara		PL-3, OC-14
Orzechowski	**Kazimierz**	kazimierz.orzechowski@uwr.edu.pl	**OC-42**, OC-49, P-24, P-61
Osmólska	Julia		OC-44
Ostrowska	Kinga		OC-11
Ozarowski	Andrew		P-34
Pagacz-Kostrzewa	Magdalena	magdalena.pagacz-kostrzewa@uwr.edu.pl	**P-42**, P-37
Pajda	Maria		OC-30
Pal	**Dhritabrata**	dp@chem.ku.dk	**OC-32**, OC-29
Palko-Łabuz	A.		OC-33
Palounek	David		OC-47
Pandey	A.		P-62
Pandey	Siddharth		OC-61
Panek	Agnieszka		OC-26
Panthi	Y.		P-62
Paramasivam	S.		PL-6, P-21
Pashynska	**Vlada**	vlada.pashynska@gmail.com	**OC-17, P-43**
Pasik	**Dominika**	dominika.pasik@helsinki.fi	**P-44**
Pastorczak	Agata		OC-11
Paszkowski	M.		P-41
Pfleger	J.		P-62
Piecuch	**Piotr**	piecuch@chemistry.msu.edu	**PL-16**
Pieczara	**Anna**	anna.pieczara@uj.edu.pl	**OC-2**, PL-3, OC-14
Pielorz	Sonia		OC-8
Piergies	**Natalia**	natalia.piergies@ifj.edu.pl	**OC-26**
Pięta	Izabela S.		OC-12
Piliarik	Marek		OC-47
Plšek	Jan		OC-48
Płowaś-Korus	**Iwona**	iwplowas@ifmpan.poznan.pl	**OC-45, P-45**
Pocheć	**Michał**	michal.pochec@pwr.edu.pl	**P-46**
Pogoda	Katarzyna		OC-26
Poulsen	**Andras Sun**	ansp@chem.ku.dk	**OC-40**
Procházka	**Marek**	marek.prochazka@matfyz.cuni.cz	**OC-51**, OC-36
Profant	**Václav**	vaclav.profant@matfyz.cuni.cy	**OC-25**, OC-63, P-15
Przekora	Agata		OC-12
Pshenichnikov	**Maxim S.**	m.s.pchenitchnikov@rug.nl	**PL-7**
Ptak	**Maciej**	M.Ptak@intibs.pl	**OC-44**, OC-38, P-31, P-32, P-35, P-36
Punko	Timofey		P-56
Pyra	Anna		P-31, P-32
Rahman	**Fariha Binte**	fariha.binte.rahman@hu-berlin.de	**P-47**
Rasmussen	Morten Arendt		OC-35
Ratajczyk	Tomasz		OC-54
Renata	**Septila**	septila01@gmail.com	**P-48**, OC-6
Ropuszyńska-Robak	P.		P-35
Rudzińska	Magdalena		OC-9
Ryazanova	**Olga**	ryazanova@ilt.kharkov.ua	**P-49**

Rząca	Marek		OC-42
Rzepiela	Kacper		P-6
Sacha	T.		OC-15
Sachdeva	Ashwin		PL-5
Saladino	**Maria Luisa**	marialuisa.saladino@unipa.it	**PL-2**
Salman	**Ahmad**	ahmad@sce.ac.il	**OC-18**
Salo	**Vili-Taneli**	vili@chem.ku.dk	**OC-31**
Saldyka	**Magdalena**	magdalena.saldyka@uwr.edu.pl	**P-50**, P-7
Samoć	Marek		OC-13
Sanchez	Diego F.		PL-5
Sangwan	**Anjali**	sipandey@chemistry.iitd.ac.in	**OC-61**
Sąsiadek	W.		P-31, P-32, P-35, P-36
Schmitt	**Michael**	mschmitt@uni-duesseldorf.de	**PL-8**
Schneiker	Anita		OC-34, P-27
Schulenburg	R.		P-22
Shafizadeh	Niloufar		OC-37
Sharaha	Uraib		OC-18
Shcherban	Natalia		P-14
Shen	Jun		PL-16
Shorabadi	Reza		OC-57
Sieradzki	Adam		OC-44
Sitkowski	Jerzy		P-39
Skovbo	Tine Elmelund		OC-32
Skóra	Grzegorz		P-8
Smeliková	**Valerie**	valerie.smelikova@jh-inst.cas.cz	**OC-48**, OC-47
Smółka	**Szymon**	s.smolka@intibs.pl	**OC-38**, OC-44
Sobczyk	Marcin		P-57
Soep	Benoît		OC-37
Solyanik	G.		OC-64, P-12
Soorkia	Satchin		OC-37
Sørensen	Klavs Martin		OC-35
Sozańska	**Agnieszka**	agnieszka.sozanska@renishaw.com	**OC-50**
Spedalieri	Cecilia		P-47
Sroka-Bartnicka	Anna		OC-12
Staś-Bobis	Monika		OC-22
Stefański	Mariusz		OC-44
Stelmaszek	P.A.		P-41
Stiufiuc	**Rares-Ionut**	rares.stiufiuc@umfcluj.ro	**OC-6**, P-48
Știufiuc	Gabriela		OC-6
Stoean (Vasile)	Bianca		P-3, P-17
Stopka	Gabriela		P-59
Stoppelkamp	S.		PL-6
Strodel	Birgit		P-6
Styopkin	Viktor		P-14
Suhm	Martin A.		OC-46
Surmacki	**Jakub M.**	jakub.surmacki@p.lodz.pl	**P-51, P-52**, OC-3
Svecova	**Marie**	svecovam@vscht.cz; svecova@kth.se	**P-53**
Szabla	**Rafał**	rafal.szabla@pwr.edu.pl	**OC-59**, P-18, P-46
Szczepanek–Dulska	Monika		OC-26
Szczęsny-Małysiak	**Ewa**	ewa.szczesny@uj.edu.pl	**OC-10**, OC-15
Szewczyk	Marta		OC-11
Szewczyk	Jakub		P-8

Szostak	Roman		OC-8
Szybowicz	Mirosław		P-5
Szymańska	**Aleksandra**	a.szymanska40@uw.edu.pl	**OC-53**
Szymański	Damian		OC-44
Śmiszek-Lindert	**Wioleta**	wioleta.smiszek-lindert@us.edu.pl	**P-54**
Środa-Pomianek	K.		OC-33
Świderska-Mocek	Agnieszka		P-45
Świętek	Małgorzata		OC-16, OC-30
Świtlicka	Anna		P-34
Tarasenko	Alla		P-11
Tarczay	György		OC-34, P-27
Targosz-Korecka	M.		OC-15
Tarnowski	Antoni		P-8
Tchaya	**Maxime**	Maxime.TCHAYA@oxinst.com	**OXFORD**
Teisseyre	**Andrzej**	andrzej.teisseyre@umw.edu.pl	**OC-33**
Thottappali	**M. A.**	thottappali@imc.cas.cz	**P-62**
Tipping	William		OC-4
Tokaji	Gy. M.		OC-17
Toma	Valentin		OC-6
Tomasetig	Daniela		PL-15
Tommasini	Matteo		P-25
Turrell	**Sylvia**	sylvia.turrelljones@gmail.com	**PL-18**
Tyshkovets	O.		P-22
Uryga	A.		OC-33
Valášková	Martina		OC-25
van de Ven	**Roel**	roel.vandeven@ru.nl	**OC-60, P-55**
Verevka	Serhij		P-11
Vivcharenko	Vladyslav		OC-12
Vogt	Emil		OC-32
Vohlídal	J.		P-62
Vosough	Faraz		OC-7
Waluk	**Jacek**	jwaluk@ichf.edu.pl	**OC-43**,OC-54,OC-55**,**P-19
Wesełucha-Birczyńska	**Aleksandra**	birczyns@chemia.uj.edu.pl	**OC-30, P-56**,OC-16, P-59, P-60
Wichrowski	Mikołaj		OC-45
Widdowson	W.		PL-6
Wielgus	Ireneusz		OC-41
Wiercigroch	**Ewelina**	ewelina.wiercigroch@jci.pl	
Wierzejewska	Maria		P-30, P-37, P-42
Włodarski	**Jakub**	jakub.wlodarski@uwr.edu.pl	**P-57**
Wojtkowiak	**Kamil**	kamil.wojtkowiak2@uwr.edu.pl	**OC-62, P-58**
Wrona	**Emilia**	emilia.wrona@doctoral.uj.edu.pl	**P-59, P-60**
Wróbel	Piotr		OC-53
Yuwono	Stephen H.		PL-16
Zedník	J.		P-62
Zhang	Z.		OC-64, P-12
Zoloff Michoff	Martin		OC-27
Zupančič	Barbara		OC-58
Żmigrodzki	**Kewin**	334224@uwr.edu.pl	**P-61**

Advanced Research and QA/QC Solutions based on Infrared, Near Infrared and Raman Spectroscopy.

Our selection of near, mid and far infrared and Raman spectrometers is unrivalled across the industry. Our portfolio includes compact, portable routine as well as powerful research spectrometers. Our solutions cover the entire spectral range from near infrared, mid infrared, far infrared to THz applications.

- FT-IR Spectrometers
- FT-NIR Spectrometers
- Raman Spectrometers
- Process Monitoring
- Remote Sensing
- FT-IR Research Spectrometers
- FT-IR Microscopes
- Raman Microscopes
- Dairy Analyzers
- Gas Analyzers
- Silicon Analyzers
- Software Solutions

For more information please visit www.bruker.com/optics

Bruker Polska Sp.z o.o.
Budziszyńska 69
60-179 Poznań
Tel. +48 61 868 90 08
Fax. +48 61 868 90 96
Email: bruker.polska@bruker.com

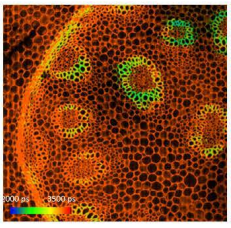
Innovation with Integrity

RENISHAW
apply innovation™

Discover Renishaw's innovative Raman spectrometers

Our range of Raman systems include research-grade confocal microscopes, benchtop laboratory analysers and portable fibre-optic analysers for in-situ measurements. Our Raman instruments can be easily integrated with other instruments for multimodal analysis including SEM, AFM, FLIM and CARS.

Innovative technologies, high-quality instruments and expert support. Scientists across the world choose to partner with us for these reasons. Find out how our product range can help you achieve your research goals.



https://www.renishaw.com/raman

Renishaw Sp. z o.o., ul. Osmańska 12, 02-823 Warszawa, Polska | +48 22 577 11 80 | poland@renishaw.com

ChemLand®

Being a market leader has been our standard for over 30 years.

Over **6 000 m²** Storage area

Over **60** team members

Over **22 000** available products

Our Offer

Laboratory Equipment

Incubators, ovens, dryers, circulating thermostats, water baths, stirrers, mills, heating mantles, benches, heating blocks, hot plates, measuring instruments, laboratory balances, centrifuges, vacuum evaporators, shakers, laminar flow cabinets, ultrasonic cleaners.

Laboratory Glassware

Basic, volumetric, specialist glassware and custom-made glassware

Chemical Reagents

We offer chemical reagents under our own PureLand brand. Thanks to our own modern laboratories, we guarantee the highest quality.

Filtration Materials

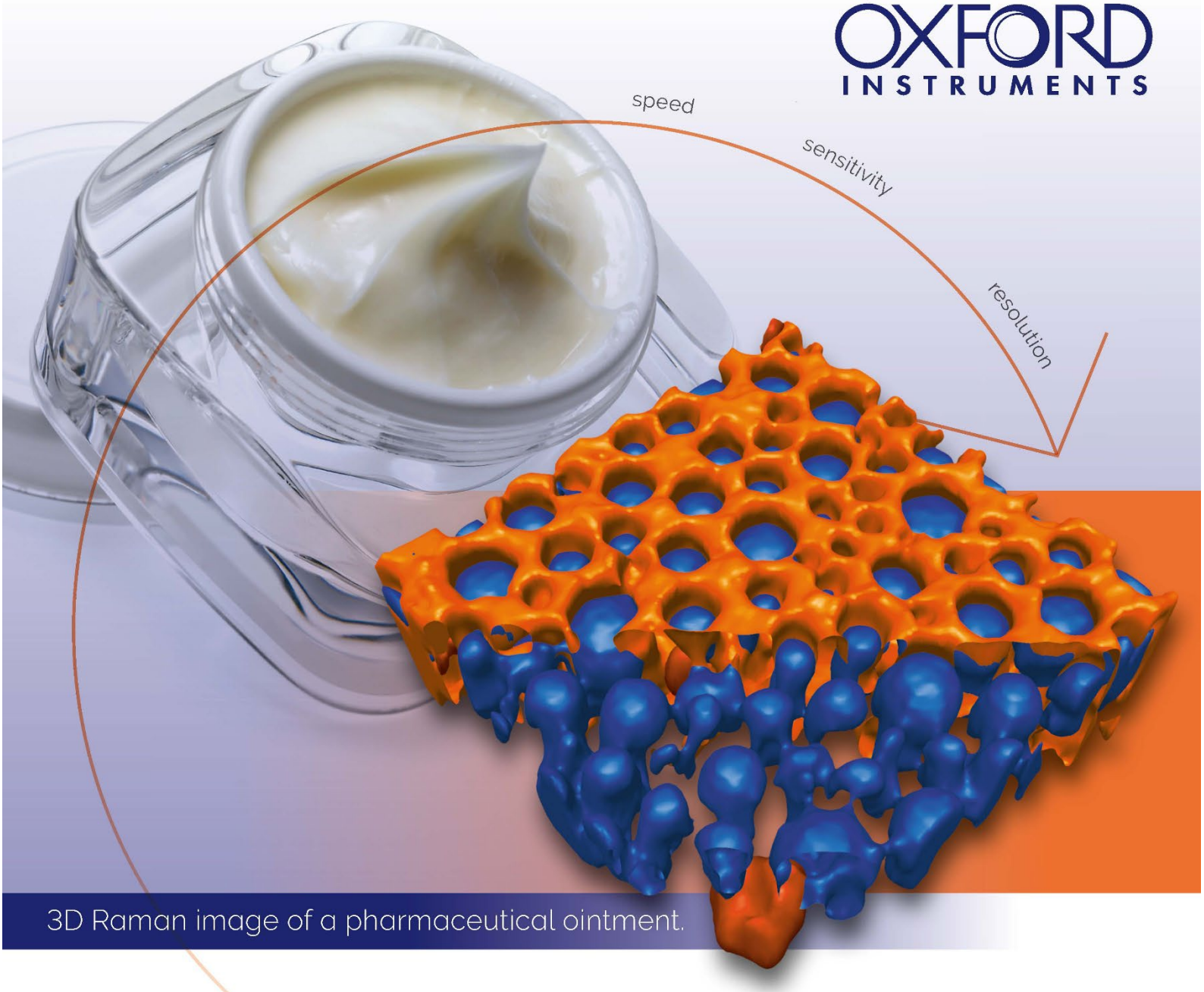
Filter papers, cellulose thimbles, extraction sleeves, membrane filters, pH strips

Custom Projects

We create custom-made products tailored to your individual needs. Our team of experts designs and manufactures orders using modern technologies, including 3D printing.

ul. Usługowa 3, 73-110 Stargard
tel: +48 691 443 533
oferty@chemland.pl
www.sklep-chemland.pl

OXFORD INSTRUMENTS



3D Raman image of a pharmaceutical ointment.

3D Raman Imaging

Turn ideas into discoveries

Let your discoveries lead the scientific future. Oxford Instruments WITec's confocal 3D Raman microscopes enable cutting-edge chemical imaging, Raman-based particle analysis and correlative integration with SEM, AFM, SNOM or optical profilometry. Discuss your ideas with us at **info.witec@oxinst.com**.

Raman • AFM • SNOM • RISE

OXFORD INSTRUMENTS | WITec

https://raman.oxinst.com

EUCMOS 2025 PROGRAMME TIMETABLE

Time	Sunday	Monday	Tuesday	Wednesday		Thursday		Friday
	Chemistry	Library LH III	Library LH III	Library LH III	Library LH IV	Library LH III	Library LH IV	Library LH III
09:00		Opening	Gardner	Lundell		Buchner		Piecuch
09:30		Fausto	Heise	Meuwly		Kjaergaard		Hansen
10:00		Saladino	Pshenichniko	Biczysko		Lendl		Turrell
10:30		coffee	coffee	coffee		coffee		Closing
11:00		Barańska	Schmitt	Engelsen		Waluk		coffee & snacks
11:10								
11:20						Ptak		
11:30		Gerwert	Gieroba	Drozd				
11:40			Gordel-W.			Płowaś-K.		
11:50			Korona	Profant				
12:00		López-R.	Dybas			Lwin		
12:10		Pieczara	Kołodziej	Piergies		Kopal		
12:20			Pashynska			Smeliková		
12:30		Abramczyk	Salman	Dopieralski		Kułacz		
12:40				Haupa		Sozańska		
12:50		Adamczyk						
13:00		LUNCH	LUNCH	LUNCH	Bruker WS2	LUNCH	BrukerWS3	
13:55								
14:00	Registration							
14:55								
15:00		Brożek-P.	Němec	Jensen	Czaja	Procházka	Grdadolnik	
15:10								
15:20		Stiufiuc	Golin Almeida	Weselucha-B.	Kočišová	Grabska	Szabla	
15:30			Marković					
15:40		Barth	Najgebauer	Salo	Muhieddine	Szymańska	van de Ven	
15:50			Christensen		Smółka	Kuzmina	Sangwan	
16:00		Mazurek	Posters - flash	Pal	Hansen V.	Golec	Wojtkowiak	
16:10					Poulsen		Jilek	
16:20		Cieślik-B.		Teisseyre	Dutkiewicz	Dabrowska	Dovbeshko	
16:30					Orzechowski			
16:40		Szczęsny-M.		Góbi		Ghasemi		
16:50		Dawiec						
17:00		coffee	Poster session coffee	coffee		coffee		
17:30								
18:30								
19:00	Get-together party	Barbecue		Concert		Dinner		
19:30								
20:00								
21:00								

Bruker WS1

LH - Lecture hall, WS- workshop, lecture colors: Green – Plenary Lecture (25+5 min discussion); Orange – Oral Contribution (18+2 min); Yellow – Oral Contribution (8+2 min).

ISBN 978-83-60043-45-5