

| PROGRAMME TIMETABLE |   |  |  |   |   |   |  |  |
|---------------------|---|--|--|---|---|---|--|--|
| Time                | 19 <sup>th</sup> (Sunday)   | 20 <sup>th</sup> (Monday)  | 21 <sup>st</sup> (Tuesday)   | 22 <sup>nd</sup> (Wednesday)  | 23 <sup>rd</sup> (Thursday)   | 24 <sup>th</sup> (Friday)   |  |  |
| 8:30                |   | Opening Ceremony   |  |   |   |   |  |  |
| 9:00                |   | SURFACES AND INTERFACES  | REACTION INTERMEDIATES   | ASTROPHYSICS AND COMPUTATIONAL  | BIOSPECTROSCOPY   | BIOMEDICAL APPLICATIONS   |  |  |
|                     |   | PL - 1: <b>Mischa Bonn</b> (D) - <i>Novel Terahertz Molecular Spectroscopies</i>   | PL - 3: <b>Robert J. McMahon</b> (USA) - <i>Rotational Spectroscopy, Molecular Structure Determination, and Radioastronomy</i>   | PL - 5: <b>Harold Linartz</b> (NL) - <i>Solid State Spectroscopy in Support of Interstellar Chemistry</i>   | PL - 7: <b>Janina Diekmann</b> (D) - <i>Photo-Addition of Psoralen to DNA Traced by Time Resolved Spectroscopy</i>                            | PL - 8: <b>Klaus Gerwert</b> (D) - <i>Label-Free Tissue Classification by QCL based IR-Imaging</i>  |  |  |
| 10:00               |   | KL-1: <b>André Peremans</b> (B) - <i>Non Linear Optics at Interfaces: Sensitive Probing of Biomolecular Recognition by Sum Frequency Generation and the Quest of Super Resolution Infrared Microscopy of Biological Tissues</i>  | KL-4: <b>Martin Suhm</b> (D) - <i>Vibrational Spectroscopy at the Service of Quantum Chemistry</i>   | KL-18: <b>Andrzej Sobolewski</b> (PL) - <i>Burning Water with Sunlight: Insights from Computational Chemistry</i>   | KL -23: <b>Marco van de Weert</b> (DN) - <i>The Trials and Tribulations of Becoming a Spectroscopy Specialist</i>                             | KL-25: <b>Nancy Pleshko</b> (USA) - <i>Non-Destructive Applications of Infrared Spectroscopy for Assessment of Tissue Pathology and Regeneration</i>  |  |  |
| 10:30               |   | Coffee Break   | Coffee Break   | Coffee Break  | Coffee Break  | Coffee Break  |  |  |
| 11:00               |   | KL-2: <b>Tito Trindade</b> (PT) - <i>Developing the Surface Chemistry of Hybrid Nanomaterials for SERS</i>   | A- LOW TEMPERATURE - DYNAMICS // B- REACTIVE SPECIES // C- GAS PHASE - INTRAMOLECULAR INTERACTIONS   | A- MATERIALS // B- COMPUTATIONAL // C- BIOMEDICAL APPLICATIONS  | KL-24: <b>Markus Arndt</b> (AT) - <i>New Avenues for Matter-Wave Assisted Spectroscopy</i>  | KL-26: <b>Hugh Byrne</b> (IR) - <i>Advancing Vibrational Spectroscopy for Cellular and Subcellular Analysis: Towards in vitro High Content Spectralomic Analysis</i>                        |  |  |
|                     |   |  | KL-5: <b>Nigel Young</b> (UK) - <i>Matrix Isolation Studies of Transition Metal and Main Group Fluorides</i> // KL-8: <b>Mike Ashfold</b> (UK) - <i>Exploring Photoinduced Molecular Ring-Opening in the Gas and Solution Phase</i> // KL-11: <b>Jan Lundell</b> (FIN) - <i>Vibrational Excitation Induced Chemistry</i>   | KL-19: <b>Micahel Oshttrakh</b> (RUS) - <i>Ordinary Chondrites: What Can We Learn Using Mössbauer Spectroscopy?</i> // KL-20 <b>Frederic Merkt</b> (CH) - <i>Precision Spectroscopy in Cold Samples of Few-Electron Molecules</i> // KL-21: <b>Anders Engdahl</b> (SW) - <i>Pre-Plaque Conformational Changes in Alzheimer's Disease-Linked A <math>\beta</math> and APP</i>  |   |   |  |  |
| 11:20               |   | OC1: <b>Andrzej Kudelski</b> (PL) - <i>Plasmonic Nanoparticles with Many Sharp Apexes and Edges as Efficient Nanoresonators for Shell-Isolated Nanoparticle-Enhanced Raman Spectroscopy</i>  | KL-6: <b>Igor Reva</b> (PT) - <i>Calculations of Spectra and Kinetics in the Context of Matrix Isolation</i> // KL-9: <b>Cláudio Nunes</b> (PT) - <i>Spectroscopic Observation of Quantum Tunneling: Discoveries on the Potential Energy Surfaces of Phenylnitrenes</i> // KL-12: <b>Elangannan Arunan</b> (IND) - <i>Microwave Spectroscopic Investigations on Large Amplitude Motions: Intermolecular Bonding in Ar-(H<sub>2</sub>O)<sub>2</sub>, (H<sub>2</sub>S)<sub>2</sub> and CH<sub>3</sub>CN-CO<sub>2</sub></i> | OC24: <b>Irina V. Alenkina</b> (RUS) - <i>Characterization of the Iron Core in Ferrifol(R), a Pharmaceutical Analogue of Ferritin, Using Mössbauer Spectroscopy and Magnetization Measurement</i> // OC29: <b>Franco Egidi</b> (I) - <i>New Avenues for Computational Chiral Spectroscopy</i> // OC34: <b>Katarzyna Marzec</b> (PL) - <i>Raman, FT-IR, AFM and Complementary Techniques in Studies of the Biochemical, Mechanical and Functional Alterations in Red Blood Cells</i> | OC45: <b>Alberto Mezzetti</b> (F) - <i>Photoprotective Mechanisms in Photosynthesis Studied by Time-Resolved FTIR Difference Spectroscopy</i> | KL-27: <b>Herbert Michael Heise</b> (D) - <i>Infrared Spectroscopy for Clinical Chemistry and Medical Diagnostics - Techniques and Chemometrics for a Successful Marriage of Two Fields</i> |  |  |
| 11:40               |   | OC2: <b>Veronika Sutrová</b> (CZ) - <i>Ag Nanosponge Aggregate with Incorporated Hydrophobic Adsorbates as a Sample for Effective SER(R)S Spectral Detection</i>   | KL-7: <b>Nikolay Kotov</b> (CZ) - <i>Investigation of Phase-Behaviour of an Ionic Liquid at Sub-Zero Temperatures in the Presence of Additives</i> // // KL-10: <b>Anna Gudmundsdottir</b> (USA) - <i>Using Transient Spectroscopy to Understand Photosalient Behavior of Vinyl Azides Crystals</i> // KL-13 <b>José Luís Alonso</b> (SP) - <i>Laboratory Millimeter and Submillimeter Wave Studies of Interstellar Molecules</i>  | OC25: <b>Jorge Costa Pereira</b> (PT) - <i>Excitation-Emission Fluorescence Analysis: Resolving Relevant Underlying Contributions</i> // OC30: <b>Bernardo de Souza</b> (BRA) - <i>Predicting Excited State Dynamics from Scratch - A Path Integral Approach Implemented on ORCA</i> // OC35: <b>Martynas Velicka</b> (LT) - <i>ATR-FTIR Apectroscopy: Towards in vivo Detection of Cancerous Tissue Areas</i>  | OC46: <b>Valery Andrushchenko</b> (CZ) - <i>VCD Spectroscopy of Nucleic Acid Supramolecular Structures</i>                                    | KL-28: <b>Luis Arnaut</b> (PT) - <i>Spectroscopic Determinants in Photodynamic Therapy</i>  |  |  |
| 12:00               |   | OC3: <b>Daria Ruth Galimberti</b> (F) - <i>Molecular Organization at Charged Solid-Water Interfaces: vSFG <math>\chi(2)(\omega)</math> Contribution and How to Use them for Revealing Interfacial Structures</i>   | OC13: <b>Joanna Hetmanczyk</b> (PL) - <i>Phase Transition, Structure and Reorientational Dynamics of H2O Ligands and ReO<sub>4</sub><sup>-</sup> Anions in [Ba(H<sub>2</sub>O)<sub>4</sub>](ReO4)2</i> // OC16: <b>Julien Guthmuller</b> (PL) - <i>Theoretical Investigation of Herzberg-Teller Effects in Resonance Raman Spectra</i> // OC19: <b>Sérgio R. Domingos</b> (D) - <i>Sensing Chirality with Rotational Spectroscopy: From Enantiomer Differentiation to Molecular Recognition</i>                          | OC26: <b>Bence Kutus</b> (H) - <i>The Hydrolysis of Mg<sup>2+</sup> Ions in the Presence of Gluconate</i> // OC31: <b>Malgorzata Biczysko</b> (CHI) - <i>Simulation of Fully Anharmonic Vibrational Spectra of Biomolecular Building Blocks</i> // OC36: <b>Czesława Paluszkievicz</b> (PL) - <i>Vibrational Studies of Salivary Glands Tissues</i>   | OC47: <b>Tatsuya Mori</b> (J) - <i>Detection of Fractal Dynamics of Protein by Terahertz Spectroscopy</i>                                     | KL-29: <b>Henry H. Mantsch</b> (CAN) - <i>Spectroscopy in the 21<sup>st</sup> Century: The Future of Molecular Spectroscopy</i>   |  |  |
| 12:20               | OC4: <b>Paula C. Pinheiro</b> (PT) - <i>Magneto-Plasmonic Nanoparticles for Separation and SERS Detection of Antibiotics</i>                                    | OC14: <b>Ivan Giba</b> (RUS) - <i>Spectral Diagnostics of Hydrogen Bonds by <sup>31</sup>P NMR Chemical Shifts</i> // OC17: <b>Kess Marks</b> (SW) - <i>Sum Frequency Generation Spectroscopy Studies of Temperature Dependent Naphtalene Dehydrogenation on Nickel (111)</i> // OC20: <b>Thomas E. Wall</b> (UK) - <i>Mid-IR Detection and Spectroscopy of Polyatomic Molecules Inside a Cryogenic Buffer Gas Cell</i>  | OC27: <b>Seoncheol Cha</b> (D) - <i>Correlation of Hydrogen-Bonding and Catalytic Activity for Diol-Based Asymmetric Organocatalysts</i> // OC32: <b>Elena Yu. Tupikina</b> (RUS) - <i>3D Outer Electronic Shell Visualization by Laplacian of a Helium Chemical Shift</i> // OC37: <b>Maciej Roman</b> (PL) - <i>Raman Spectroscopy of Urine Extracellular Vesicles in Diabetic Patients</i>  | OC48: <b>Jakub Kaminsky</b> (CZ) - <i>Structure and Interactions of Saccharides Studied by Vibrational Optical Activity Methods</i>   | EUCMOS XXXV Presentation  |   |  |  |
| 12:40               | OC5: <b>Petr Praus</b> (CZ) - <i>Metal-Enhanced Fluorescence of Riboflavin Deposited on Spacer-Modified Ag Substrate: Spectral Intensity and Lifetime Study</i> | OC15: <b>Eva Scholtzová</b> (SK) - <i>Beidellite Intercalates and Their Characterization by Means of DFT Method</i> // OC18: <b>Lucia K. Noda</b> (BRA) - <i>Assignment of the Electronic Transition of Phenothiazine Radical Cation in teh Visible Region - A Resonance Raman Spectroscopy and Theoretical Calculation Investigation</i> // OC21: <b>György Tarczay</b> (H) - <i>The Role of Matrix Isolation Spectroscopy in Conformational Studies of Small and Medium Sized Biomolecules</i> | OC28: <b>Svetlana S. Khokhlova</b> (RUS) - <i>Fluorescence Quenching of Xanthone and Xanthione Derivatives in Protic and Aprotic Solvents</i> // OC33: <b>Marco Mendolicchio</b> (I) - <i>The MSR Route to Accurate Equilibrium Molecular Structures Through the Semi-Experimental Approach</i> // OC38: <b>Ewelina Szafraniec</b> (PL) - <i>Raman Imaging Study of Lipid Droplets in Liver Sinusoidal Endothelial Cells Upon Non-Alcoholic Fatty Liver Disease Progression</i>  | OC49: <b>Nadezhda Kudryasheva</b> (RUS) - <i>Coelenteramide-Containing Fluorescent Protein as a Simplest Bioassay for Monitoring Results of Chemical and Radioactive Exposures</i>  | Closing Ceremony  |   |  |  |
| 13:00               |   | Lunch  | Lunch  | Lunch   | Lunch   | Lunch   |  |  |
|                     |   | MATERIALS AND ANALYTICAL   | HIGH-RESOLUTION SYMPOSIUM (A/B)  | A- NEW METHODS // B- ENERGY // C- MIXTURES  | Excursion   |   |  |  |
| 15:00               | PL - 2: <b>Wybren Jan Buma</b> (NL) - <i>Tailoring Photoactive Materials: Light on the Dark Side of the Force</i>   | PL - 4: <b>Luca Evangelisti</b> (I) - <i>Investigation of Non-Covalent Interactions by Microwave Spectroscopy</i>  | PL - 6: <b>Eberhard Riedle</b> (D) - <i>From Lasers to High Power LEDs, From Photochemistry to Photocatalysis</i>  |   |   |   |  |  |
| 16:00               | OC6: <b>Monika Plass</b> (CH) - <i>Thermal Degradation Behaviour of Elastomers</i>  | KL-14: <b>Otto Dopfer</b> (D) - <i>Geometric and Electronic Structure of Flavins</i> // KL-16: <b>Michael Schmitt</b> (D) - <i>Excited State Dipole Moments from High Resolution Spectroscopy</i>  | KL-22: <b>Mustafa Çulha</b> (TR) - <i>Surface-Enhanced Raman Scattering: A Potential Technique to Study Living Single Cells</i>  |   |   |   |  |  |
| 16:20               | OC7: <b>Sven P. K. Koehler</b> (UK) - <i>Characterisation, Coverage and Orientation of Functionalised Graphene Using Sum-Frequency Generation Spectroscopy</i>  | KL-15: <b>Leonardo Alvarez-Valtierra</b> (MX) - <i>Towards High Resolution Phosphorescence Spectroscopy</i> // KL-17: <b>Elena R. Alonso</b> (SP) - <i>The Gas Phase Study of Artificial Sweeteners: Structure-Swetness Connection</i>   | OC39: <b>Omar A. El Seoud</b> (BRA) - <i>Perichromism: A Successful Approach for Probing Molecular Interactions in Different Media</i> // OC41: - <b>Ivan Nêmec</b> (CZ) - <i>Vibrational Spectroscopic Study of NLO Molecular Crystals Based on Aminopyrimidinium Salts</i> // OC43: <b>Johannes Kiefer</b> (D) - <i>Vibrational Spectroscopy of Binary Mixtures of an Ionic Liquid and Propan-1-ol</i>   |   |   |   |  |  |
| 16:40               | OC8: <b>Terao Wakana</b> (J) - <i>Detection of Boson Peak and Fracton of Sodium Carboxymethyl Starch by Terahertz Time-Domain Spectroscopy</i>                  | OC22: <b>Mirko Lindic</b> (D) - <i>Dipole Moments of Anisole in Ground and Excited State via Condensed Phase Thermochromic Spectroscopy and Gas Phase HRLIF Spectroscopy</i> // OC23: <b>América Torres-Boy</b> (MX) - <i>Analysis of the Rotationally Resolved Electronic Spectra of 3CI and Its Water Cluster Through Genetic Algorithms</i>   | OC40: <b>Helena Nogueira</b> (PT) - <i>Raman Imaging in SERS Studies of Silver Loaded Textiles</i> // OC42: <b>Simona Rada</b> (ROM) - <i>The Optimization of Recycled Lead with Manganese Dioxide Contents for Applications on the Automobile Batteries</i> // OC44: <b>Mirosław A. Czarnecki</b> (PL) - <i>Microheterogeneity in Binary Mixtures: Spectroscopic and Chemometric Studies</i>  |   |   |   |  |  |
| 17:00               | Registration  | Coffee Break   | Coffee Break   | Coffee Break  |   |   |  |  |
| 17:30               |   | KL-3: <b>José Gaspar Martinho</b> (PT) - <i>Biphotonic Materials for Imaging</i>   | Poster Session I   | Poster Session II   |   |   |  |  |
| 18:00               |   | OC9: <b>Sylvia Turrel</b> (F) - <i>The What, How and Where in Art and Archaeology: Use of Raman Spectroscopy for the Study of Ceramics, Glasses and Porcelains</i>   |  |   |   |   |  |  |
| 18:20               |   | OC10: <b>Yasmine Schulenburg</b> (D) - <i>Analysis of the Historical Collection of Dyes at the Hochschule Niederrhein Using Infrared Spectroscopy</i>  |  |   |   |   |  |  |
| 18:40               |   | OC11: <b>Dhanya Puthenmadom</b> (B) - <i>Fourier Transform Infrared Microscopic Investigation of Cysteic Acid in Virgin and Damaged Hair</i>   |  |   |   |   |  |  |
| 19:00               | Welcome party   | OC12: <b>Lucia Bonoldi</b> (I) - <i>Thermal Maturity of Organic Matter from Fossil Fuel Fields by Raman Spectroscopy: Spectral Parameters and Chemometric Data Treatment</i>   |  |   |   |   |  |  |
| 20:00               |   |  |  |   |   |   |  |  |
| 21:00               |   |  |  |   |   |   |  |  |
|                     |   |  |  |   | Gala Dinner   |   |  |  |

**Legend:** PL- Plenary Lecture KL- Keynote Lecture OC- Oral Communication