

## PROGRAMME IN DETAILS

WEDNESDAY, September 26		
8:30 – 9:15	REGISTRATION <i>(Institute of Organic Chemistry, Polish Academy of Sciences)</i>	
9:15 – 9:45	OPENING CEREMONY <b>Jarosław Jaźwiński</b> <i>(Chairman of the Organizing Committee)</i> <b>Sławomir Jarosz</b> <i>(Director of the Institute of Organic Chemistry, Polish Academy of Sciences)</i>	
<b>SESSION I</b> (Chairman: Sławomir Jarosz)		
9:45 – 10:30	<b>Jürgen Senker</b> , C.S. Zehe, C.B.L. Tschense, M. Schmidt, G. Maurin, K. Kreger, R. Siegel, V. Daebel, A.L. Goodwin, H.-W. Schmidt <i>(Inorganic Chemistry III, University of Bayreuth, Germany)</i>  NMR CRYSTALLOGRAPHY – A TOOL FOR STUDYING STRUCTURE, DISORDER AND FUNCTION OF MATERIALS	<b>FL-1</b>
10:30 – 11:15	<b>Nikodem Kuźnik</b> <i>(Silesian University of Technology, Gliwice, Poland)</i>  MRI CONTRAST AGENTS BASED ON IRON COMPLEXES	<b>FL-2</b>
11:15 – 11:30	<b>Jan Novotný*</b> , P. L. Bora, K. Ruud, S. Komorovsky, R. Marek <i>(CEITEC, Masaryk University, Brno, Czechia)</i>  PARAMAGNETIC NMR OF METALLOCOMPLEXES – SYNERGY BETWEEN EXPERIMENT AND DFT CALCULATIONS	<b>C-3</b>
11:30 – 11:45	<b>Katarzyna Jakubowska*</b> , M. Jaszuński, M. Pecul-Kudelska <i>(University of Warsaw, Faculty of Chemistry, Warsaw, Poland)</i>  CALCULATION OF NUCLEAR SPIN-SPIN COUPLING CONSTANTS IN SERIES OF ACETYLENE DERIVATIVES $\text{HC}\equiv\text{CXH}_3$ , WHERE X = C, Si, Ge, Sn, Pb	<b>C-4</b>
11:45 – 12:15	Coffee break	
<b>SESSION II</b> (Chairman: Jürgen Senker)		
12:15 – 13:00	<b>Gaël De Paëpe</b> <i>(CEA, CNRS, University Grenoble Alpes, France)</i>  DYNAMIC NUCLEAR POLARIZATION ENHANCED SOLID-STATE NMR: NATURAL ISOTOPIC ABUNDANCE AND CLOSED-LOOP CRYOGENIC HELIUM SAMPLE SPINNING	<b>FL-5</b>

13:00 – 13:15	<b>Natalia Olejnik-Fehér*</b> , S. Badoni, M. Jędrzejewska, M. Wolska-Pietkiewicz, D. Lee, G. De Paëpe <i>(Institute of Physical Chemistry PAS, Warsaw, Poland)</i>	<b>C-6</b>
	DYNAMIC NUCLEAR POLARIZATION ENHANCED SOLID-STATE NMR AS A POWERFUL TOOL FOR PROBING THE SURFACE OF NANOMATERIALS WITH SUB-ÅNGSTRÖM RESOLUTION	
13:15 – 13:30	<b>Nicole Sudžukovič*</b> , L. Brecker <i>(Department of Organic Chemistry, Univeristy of Vienna, Austria)</i>	<b>C-7</b>
	PICTET-SPENGLER REACTION IN THE SPOTLIGHT. AN <i>IN SITU</i> NMR INVESTIGATION.	
13:30 – 15:00	Lunch	
<b>SESSION III (Chairman: Gaël De Paëpe)</b>		
15:00 – 15:45	<b>Krzysztof Kazmierczuk</b> <i>(Centre of New Technologies, University of Warsaw, Poland)</i>	<b>FL-8</b>
	ALTERNATIVE PROCESSING TECHNIQUES FOR SERIAL NMR EXPERIMENTS	
15:45 – 16:15	<b>Radek Marek</b> <i>(CEITEC, Masaryk University, Brno, Czechia)</i>	<b>L-9</b>
	HYPERFINE NMR EFFECTS IN PARAMAGNETIC Ru(III) COMPLEXES	
16:15 – 16:30	<b>Teobald Kupka</b> , X. Tian, Y. Nie, H.-M. Lin, M. Jewgiński, S.P.A. Sauer, Sz. Mycer <i>(Faculty of Chemistry, University of Opole, Poland)</i>	<b>C-10</b>
	RELATIVISTIC, ELECTRON CORRELATION AND BASIS SET EFFECTS IN THE CALCULATION OF Se CHEMICAL SHIFTS	
16:30 – 17:00	Break	
17:00 – 21:00	<b>CONFERENCE MIXER</b>	

**THURSDAY, September 27**

**SESSION IV** (Chairman: Graham A. Webb)

9:15 – 10:00	<p><b>Jean-Paul Amoureux</b> (UCCS, University of Lille, France)</p> <p>RECENT NEW SOLID-STATE NMR METHODS</p>	<b>FL-11</b>
10:00 – 10:45	<p><b>Marek Potrzebowski</b> (Centre of Molecular and Macromolecular Studies PAS, Łódź, Poland)</p> <p>VERY FAST MAS SOLID-STATE NMR IN SERVICE OF PHARMA – METHODS FOR CONTROLLING OF PREPARATION AND STRUCTURE ELUCIDATION OF PHARMACEUTICAL COCRYSTALS AND APIs EMBEDDED INTO DRUG DELIVERY SYSTEMS</p>	<b>FL-12</b>
10:45 – 11:15	<p><b>Satoshi Sakurai</b> (JEOL U.K. Ltd, Welwyn Garden City, United Kingdom)</p> <p>HOW DO YOU ASSOCIATE WITH FLUORINE COMPOUNDS BY NMR?</p>	<b>L-13</b>
11:15 – 11:30	<p><b>Piotr Paluch*</b>, J. Trébosc, O. Lafon, M. Potrzebowski, J.-P. Amoureux (Centre of Molecular and Macromolecular Studies PAS, Łódź, Poland)</p> <p>DETAILED ANALYSIS OF <math>^1\text{H}\{-\text{X}\}</math> D-HMQC FOR SPIN <math>\frac{1}{2}</math> IN CASE OF EXTREMELY LARGE ANISOTROPIC INTERACTIONS</p>	<b>C-14</b>
11:30 – 11:45	<p><b>Dariusz Gołowicz*</b>, M. Urbańczyk, A. Shchukina, K. Kazimierczuk (University of Warsaw, Poland)</p> <p>SWEPT COHERENCE TRANSFER (SCOT) METHOD FOR IMPROVING QUANTITATIVENESS OF HETERONUCLEAR 2D NMR</p>	<b>C-15</b>
11:45 – 12:15	Coffee break	
<b>SESSION V</b> (Chairman: Marek Potrzebowski)		
12:15 – 13:00	<p><b>Wiktor Koźmiński</b> (Faculty of Chemistry, Biological &amp; Chemical Research Centre, University of Warsaw, Poland)</p> <p>HIGH DIMENSIONALITY AND HIGH RESOLUTION NMR EXPERIMENTS</p>	<b>FL-16</b>
13:00 – 13:15	<p><b>Alexandra Shchukina*</b>, M. Urbańczyk, K. Kazimierczuk (Centre of New Technologies, University of Warsaw, Poland)</p> <p>OVERCOMING LINE BROADENING IN REAL TIME PURE-SHIFT NMR SPECTROSCOPY</p>	<b>C-17</b>

13:15 – 13:30	<b>Jan Stanek*</b> , T. Schubeis, L. Andreas, A. Marchanka, T. Carlomagno, G. Pintacuda <i>(University of Warsaw, Poland)</i>  NEW METHODS TO ASSIGN RESONANCES IN PROTEINS AND RNA IN THE SOLID-STATE AT MAS ABOVE 100 kHz	<b>C-18</b>
13:30 – 15:00	Lunch	
<b>SESSION VI</b> ( <i>Chairman: Michał Jaszuński</i> )		
15:00 – 15:45	<b>Stanislav Komorovsky</b> , J. Vícha, M. Repisky, R. Marek, M. Straka <i>(Institute of Inorganic Chemistry SAS, Bratislava, Slovakia)</i>  SPIN-ORBIT HEAVY ATOM ON THE LIGHT ATOM NMR CHEMICAL SHIFTS EXPLAINED	<b>FL-19</b>
15:45 – 16:15	<b>Xxxxx</b> <i>(BRUKER)</i>  -----	<b>L-20</b>
16:15 – 16:30	Break	
16:30 – 17:30	POSTER SESSION	
17:30 – 18:00	<i>Announcement of the results of the <b>Young Scientists Contest</b></i>	
18:00 – .....	<b>FREE EVENING ☺</b>	

\* – *Young Scientists Contest* presentations

FRIDAY, September 28		
<b>SESSION VII</b> ( <i>Chairman: Karol Jackowski</i> )		
9:15 – 10:00	<b>William S. Price</b> , T. Stait-Gardner, A. Gupta, R. Masuda, A. Torres, S.A. Willis, G. Zheng, Y. Aihara <i>(Nanoscale Group, Western Sydney University, Penrith, NSW, Australia)</i> RECONSIDERING NMR DIFFUSION MEASUREMENTS	<b>FL-21</b>
10:00 – 10:45	<b>Poul Erik Hansen</b> , O. Hammerich, S.P.A. Sauer, F.S. Kamounah, K. Coutinho, E. Lacerda, R.S. Elias, B.A. Saeed <i>(Department of Science &amp; Environment, Roskilde University, Denmark)</i> HOW TO FIND THE NEEDLE IN THE HAYSTACK? A THEORETICAL NMR STUDY.	<b>FL-22</b>
10:45 – 11:15	<b>Dominik Wójcik</b> <i>(IKA Poland Ltd.)</i> APPLICATIONS OF ELECTROCHEMISTRY IN ORGANIC CHEMISTRY	<b>L-23</b>
11:15 – 11:45	Coffee break	
<b>SESSION VIII</b> ( <i>Chairman: Poul Erik Hansen</i> )		
11:45 – 12:30	<b>Karol Jackowski</b> , M. Misiak, P. Garbacz, W. Makulski <i>(Faculty of Chemistry, University of Warsaw, Poland)</i> NMR STUDIES OF ATMOSPHERIC GASES	<b>FL-24</b>
12:30 – 13:00	<b>Piotr Garbacz</b> <i>(Faculty of Chemistry, University of Warsaw, Poland)</i> DIRECT DETERMINATION OF THE ABSOLUTE CONFIGURATION BY MEANS OF THE DIPOLAR CROSS-CORRELATED RELAXATION PERTURBED BY AN ELECTRIC FIELD	<b>L-25</b>
13:00 – 13:30	CLOSING REMARKS <b>Jarosław Jaźwiński</b> <i>(Chairman of the Organizing Committee)</i> <b>Sławomir Jarosz</b> <i>(Director of the Institute of Organic Chemistry, Polish Academy of Sciences)</i>	
13:30 – 15:30	Lunch	