# **Timetable**

KT: Keynote Talk, IT: Invited Talk, CT: Contributed Talk

### Monday, September $15^{th}$ 2025

8:45	Registration		
9:00–9:10	Opening Early-Career Research Workshop		
		Chair: TBC	
9:15–10:00	KT	Size-filtered Rotational Spectroscopy of Molecular Aggregates Cristóbal Pérez (University of Valladolid, Spain)	
10:00–10:30	IT	Detecting Hydrogen-Bound Complexes at Room Temperature - A Joined Experimental and Theoretical Approach Casper Vindahl Jensen (University of Copenhagen, Denmark)	
10:30–10:50	СТ	Probing Non-Covalent Interactions in Anisaldehyde Homodimers Andres Verde (University of Valladolid, Spain)	
10:50–11:10	СТ	Hydrogen Bonding in Water-Modified Solvate Ionic Liquids Studied by Molecular Dynamics Simulations Jule Kristin Philipp (University of Rostock, Germany)	
11:10–11:40		Coffee Break	
11:40–12:00	СТ	Halogen Bonds in Rotational Spectroscopy: Mesomeric and Inductive Effects Jannes Niels Hasselhorn (Georg-August-Universität Göttingen, Germany)	
12:00–12:20	СТ	Gas-Phase Vibrational Spectroscopy of Fluoride – Hexafluoroisopropanol Complexes: Solvation-Suppressed Proton Transfer and Isotopic Effects Milena Barp (University of Leipzip, Germany)	
12:20–12:40	СТ	Rotational and Vibrational Spectroscopic Characterisation of Hinokitiol and Its Water Complexes Paul Pinillos (University of Bologna, Italy)	
12:40–13:00	СТ	Competition Between NH $\pi$ Hydrogen Bonding and Charge Resonance Interactions in Aromatic Heterodimer Radical Cations revealed by IR spectroscopy  Dashjargal Arildii (Technische Universität Berlin)	
13:00–14:30		Lunch Break	
		Chair: TBC	

14:30–15:00	IT	From Small Substituted Heteroaromatic Rings to Highly Flexible Macrocycles: How Intermolecular and Intramolecular Interactions influence Conformation Charlotte N. Cummings (King's College London, UK)	
15:00–15:20	СТ	Triple Trouble: Hydrogen Bonding at the C≡N Bond Alexander Kanzow (Georg-August-Universität Göttingen, Germany)	
15:20–15:40	СТ	Improving Spectral Interpretation with Learned Vibrational Coordinates Emil Vogt (Center for Free-Electron Laser Science CFEL, Germany)	
15:40–16:00	СТ	Stepwise Microsolvation Study of Prebiotic Aminoacetonitrile by Rotational Spectroscopy: NH <sub>2</sub> CH <sub>2</sub> CN-(H <sub>2</sub> O) <sub>n</sub> (n = 1–5, 7) Ningjing Jiang (Deutsches Elektronen-Synchrotron DESY, Germany)	
16:00–16:30	Coffee Break		
		Chair: TBC	
16:30–17:00	IT	Spectroscopy Studies on Ices of Astrophysical Relevance Christina Tonauer (Deutsches Elektronen-Synchrotron DESY, Germany)	
17:00–17:20	СТ	Vibrational Spectroscopy of Monohydrated Radical Cation Complexes Ruzica Markovic (University of Copenhagen, Denmark)	
17:20–17:40	СТ	Probing Binding-Site Preferences in Propiolic Acid Complexes with Water and H2S inside Helium Nanodroplets Arghya Chakraborty (Ruhr University Bochum, Germany)	
	Break		
18:00	Hbond Conference Welcome Reception		

## Tuesday, September 16<sup>th</sup> 2025

8:45	Registration		
9:00–9:10		Opening HBond conference	
	Chair: TBC		
9:15–10:00	KT	Quantifying Hydrogen Bonding Interactions in Gas Phase Model Systems Using Ion Vibrational Spectroscopy Knut R. Asmis (University of Leipzig, Germany)	
10:00–10:30	IT	Photoreactivity of PAHs as a Function of the Local Hydrogen Bonding Environment, from Isolated Molecules to Clusters and Ices.  Jenny Noble (Centre national de la recherche scientifique CNRS, France)	

СТ	A Photophysical Investigation of Lanthanide Complexes Based on Levofloxacin María Mar Quesada-Moreno (Universidad de Jaén, Spain)
СТ	HCOOH-NH <sub>3</sub> -H <sub>2</sub> O, a Prototypical Acid-Base-Water Cluster Revealed by Rotational Spectroscopy Fan Xie (Univeristy of Science and Technology of China, China)
	Coffee Break
ΙΤ	To Be or Not To Be Hydrogen-bonded: Supercritical Water and (H <sub>2</sub> S) <sub>2</sub> Martina Havenith (Ruhr University Bochum, Germany)
СТ	Kicking off the Second HyDRA Blind Challenge on Microhydration: Challenge Details and First Test Set Announcement Margarethe Bödecker (Georg-August-Universität Göttingen, Germany)
СТ	L-DOPA Autoxidation is Controlled by Water Proteolysis Janez Mavri (National Institute of Chemistry, Slovenia)
СТ	Hydrogen Bonding between Glyco-conjugated Photosensitizer Models, Water Molecules and Receptor Models. Pierre Carcabal (CNRS - Université de Toulouse, France)
Lunch Break	
	Chair: TBC
ΙΤ	TBC Ruth Gschwind (University of Regensburg, Germany)
СТ	OH···NO! Investigating the Interactions between TEMPO and Large Halogenated Alcohols Elisabeth Sennert (Georg-August-Universität Göttingen, Germany)
СТ	Hydrogen Bonding Enables Detection of Elusive Conformers: Interplay between Supersonic Jet Relaxation and Complex Formation in 4-(4-Methoxyphenyl)aniline Pablo Pinacho Morante (University of Valladolid, Spain)
ΙΤ	Chirped-Pulse mmWave Rotational Spectroscopy of Molecules Desorbed from an Ice Surface: Applications to Sublimation Dynamics, Astrochemistry, and Materials Bernadette Broderick (University of Missouri, USA)
Coffee Break	
Chair: TBC	
СТ	Dynamics of Microsolvated (Bio)molecules in General-Chemistry Conditions Jochen Küpper (Center for Free-Electron Laser Science CFEL, Germany)
СТ	Preference of hydrogen bond binding site in 1:1 chromone-methanol complexes in different electronic states Fabian Dietrich (Universidad de La Frontera, Chile)
	CT  CT  CT  CT  CT  CT

17:20–17:40	СТ	Conformer-sensitive Nuclear Dynamics of the Ammonia Dimer Cation Probed by Femtosecond Time-resolved Coulomb Explosion Xiaoyu Mi (CFEL)
		Break
18:00		International Advisory Board Meeting

## Wednesday, September 17<sup>th</sup> 2025

		Chair: TBC	
9:15–10:00	KT	Efficient Quantum Chemical Methods for Non-covalent Interactions Stefan Grimme (University Bonn, Germany)	
10:00–10:30	IT	Decoding Hydrogen-Bonded Clusters: Structural Insights from Rotational Spectroscopy Maria Eugenia Sanz (King's College London, UK)	
10:30–10:50	СТ	Making Hydrogen Bonds: Reaction Kinetics of Heterodimer Formation Alberto Macario Farto (Université Sorbonne Paris Nord, France)	
10:50–11:10	СТ	UV Photochemistry of <i>cis</i> -Pinonic Acid and of its Complexes with O <sub>2</sub> and H <sub>2</sub> O in Cryogenic Matrices Stephane Coussan (CNRS-Aix Marseille University, France)	
11:10–11:40		Coffee Break	
11:40–12:10	IT	The Site of Protonation and Proton Delocalization in Gaseous Molecules Elucidated by IR Spectroscopy Jos Oomens (FELIX Laboratory, Radboud University, Nijmegen, The Netherlands)	
12:10–12:30	СТ	Ligand Exchange in a Supersonic Expansion Beppo Hartwig (Georg-August-Universität Göttingen, Germany)	
12:30–12:50	СТ	H-bond Driven Diastereomer Formation in Chiral Selector Ion Vibrational Spectroscopy of Protonated Amino Acids Francine Horn (Leipzig University / Fritz Haber Institute, Germany)	
12:50–13:10	СТ	Comparative Conformational Analysis of IAM and IAA and Related Compounds: Structural Insights into Their Biological Roles Sofia Municio San Jose (Universidad de Valladolid, Spain)	
13:10–14:30	Lunch Break		
	Chair: TBC		
14:30–15:00	IT	H···H Dihydrogen Bonding in Alkylsilane–Fluoromethane Complexes Observed by Microwave Spectroscopy Weixing Li (Fudan University, China)	

15:00–15:20	СТ	Conformational Preferences of Jet-cooled Gly-Gly-Gly and Ala-Ala-Ala Peptides Vitali Zhaunerchyk (University of Gothenburg, Sweden)
15:20–15:40	СТ	Benchmarking Quantum Methods with Experimental Data: the Rotational Spectroscopy of 3-Fluorobenzylamine and its Water Complexes Sonia Melandri (University of Bologna, Italy)
15:40–16:10	IT	Understanding Non-Covalent Interactions via Mass-Selective Laser Spectroscopy in Jets José A. Fernández (University of the Basque Country)
16:10	Social Activity (planned DESY tour) - Free Afternoon	

## Thursday, September $18^{th}$ 2025

		Chair: TBC	
9:15–10:00	KT	The Twisting World of Chirality: A Molecular Perspective Yunjie Xu (University of Alberta, Canada)	
10:00–10:30	IT	Probing Noncovalent Interactions by Fast Magic-Angle Spinning NMR at 100 kHz and More Thomas Wiegand (RWTH Aachen University, Germany)	
10:30–10:50	СТ	Hydrogen-Bond-Mediated Conformational Locking and Quantum Tunnelling Effects in a Ferrocene Based Molecular Rotor Nuno Campos (University of Coimbra, Portugal)	
10:50–11:10	СТ	Hydrogen Bond Potentials For HCN/HNC Complexes Elangannan Arunan (Indian Institute of Science, India)	
11:10–11:40		Coffee Break	
11:40–12:10	IT	Hydrogen Bonding Motifs in Hydroxy- and Carboxy-functionalized Ionic Liquids Ralf Ludwig (Universität Rostock, Germany)	
12:10–12:30	СТ	Bridging Non-Covalent Interactions in Diverse Cyclic Systems: Insights from Rotational Spectroscopy and Quantum Chemistry Calculations Maider Parra Santamaria (University of the Basque Country)	
12:30–12:50	СТ	Mechanical Tuneability via Water-induced H-bond Change in Sustainable Soft Materials Kai Zhang (Georg-August-Universität Göttingen, Germany)	
13:10–14:30	Lunch Break		

		Chair: TBC	
14:30–15:00	ΙΤ	Invisible Forces, Precise Spectra: A Journey Through Noncovalent Interactions via Gas-Phase Rotational Spectroscopy Camilla Calabrese (Universidad de Valladolid, Spain)	
15:00–15:20	СТ	2D-MolGraphs: a Powerful Tool for Characterizing Hydrogen-Bonding at Aqueous Interfaces. Sana Bougueroua (Université Evry Paris-Saclay, France)	
15:20–15:40	СТ	Peculiarities of Intramolecular Hydrogen Bonds in Porphyrin Isomers Jacek Waluk (Polish Academy of Sciences, Poland)	
15:40–16:00	СТ	IR Spectroscopy of Phosphoric Acid Clusters in Helium Nanodroplets América Torres Boy (Fritz-Haber Institut, Germany)	
16:00–16:30	Coffee Break		
16:30–18:30	Poster Session		
20:00	Conference Dinner		

# Friday, September $19^{th}$ 2025

		Chair: TBC	
9:15–10:00	KT	Short Hydrogen Bonds in the Solid State: New Insights from Computational, Infrared, Inelastic Neutron Scattering and Nuclear Quadruple Resonance Perspective Jernej Stare (National Institute of Chemistry, Slovenia)	
10:00–10:30	ΙΤ	Is water an ultraviscous liquid above 125 K? Experiments on Droplet Coalescence Thomas Loerting (University of Innsbruck, Austria)	
10:30–10:50	СТ	How Water Changes the Photophysics of Small Model Chromophores Sebastian Trippel (Center for Free-Electron Laser Science CFEL, Germany)	
10:50–11:10	СТ	Microwave Spectroscopic Characterization of Furan–Formic Acid Clusters: Large-Amplitude Motions and Noncovalent Interaction Analysis Jingling Hong (Fudan Univeristy, China)	
11:10–11:40	Coffee Break		
11:40–12:10	IT	H-Bonding in Acid-Glycol Switchable Emulsifiers Enlightened with Sum-Frequency Generation Spectroscopy Ellen Backus (University of Vienna, Austria)	

12:10–12:30	СТ	Distinguishing Cavity and Non-cavity Solvation Structures of the Hydrated Electron Benjamin Fingerhut (Ludwig-Maximilians-Universität, Germany)	
12:30–12:50	СТ	Synergy Effect of Hydrogen Bonding and Steric Interactions for Reactivity and Selectivity of Organic, Inorganic and Organometallic Compounds Alexander Antonov (University of Regensburg, Germany)	
12:50	Closing Remarks		
		Departure	