Program of 3rd AMOC Meeting
April 16 – April 19, 2018

MONDAY, April 16, 2018			
7:30 – 9:00	**Registration**		
Session A			
9:00 – 9:10		**Attila Császár** (Budapest, Hungary)	Chair: Lauri Halonen (Helsinki, Finland)
		Official opening of AMOC 2018	
9:10 – 9:35		**Kaoru Yamanouchi** (Tokyo, Japan)	Chair: Lauri Halonen (Helsinki, Finland)
		Intense field molecular dynamics and spectroscopy	
9:35 – 10:00		**Tucker Carrington** (Kingston, Canada)	Chair: Lauri Halonen (Helsinki, Finland)
		A variational method for computing vibrational spectra of molecules with up to 18 atoms	
10:00 – 10:30	*Coffee break*		
Session B			
10:30 – 10:55		**Agapi Emmanouilidou** (London, United Kingdom)	Chair: Edit Mátyus (Budapest, Hungary)
		Controlling electron-electron correlation in frustrated double ionization in molecules with orthogonally polarized laser fields	
10:55 – 11:20		**Markus Kitzler-Zeiler** (Vienna, Austria)	Chair: Edit Mátyus (Budapest, Hungary)
		Measurement and control of electron and nuclear dynamics in molecules	
11:20 – 11:45		**Yohann Scribano** (Montpellier, France)	Chair: Edit Mátyus (Budapest, Hungary)
		An efficient sparse-grid scheme for the quantum dynamics of confined molecular hydrogen	
11:45 – 12:00		**Marcin Buchowiecki** (Szczecin, Poland)	Chair: Edit Mátyus (Budapest, Hungary)
		Ro-vibrational coupling in high temperature thermochemistry of the BBr molecule	
12:00 – 13:30	*Lunch break*		
Session C			
13:30 – 13:55		**Lauri Halonen** (Helsinki, Finland)	Chair: Michel Herman (Brussels, Belgium)
		High precision laser double resonance infrared spectroscopy with optical frequency combs	
13:55 – 14:20		**Peter Radi** (Villigen, Switzerland)	Chair: Michel Herman (Brussels, Belgium)
		Unraveling the complex electronic structure of diatomic molecules by nonlinear spectroscopy	
14:20 – 14:45		**Luis Bañares** (Madrid, Spain)	Chair: Michel Herman (Brussels, Belgium)
		Shaping fragment spatial distributions in photodissociation by strong laser fields	

14:45 – 15:10		**Frédéric Merkt** (Zürich, Switzerland)	Chair: Michel Herman (Brussels, Belgium)
		Precision spectroscopic measurements in H_2, H_2^+, He_2 and He_2^+	
15:10 – 15:40	*Coffee break*		
Session D			
15:40 – 16:05		**Edit Mátyus** (Budapest, Hungary)	Chair: Gilberte Chambaud (Paris, France)
		Rovibrational states of molecular systems with several large-amplitude motions: recent developments and applications of a general variational approach	
16:05 – 16:30		**Oriol Vendrell** (Aarhus, Denmark)	Chair: Gilberte Chambaud (Paris, France)
		Nonlinear mode coupling in laser-driven C_{60}	
16:30 – 16:55		**David Perry** (Akron, OH, USA)	Chair: Gilberte Chambaud (Paris, France)
		The Jahn-Teller model as a treatment of molecular anharmonicity	
16:55 – 17:20		**Basile Curchod** (Durham, UK)	Chair: Gilberte Chambaud (Paris, France)
		Towards in silico photochemistry using ab initio nonadiabatic molecular dynamics	
18:00 – 20:00	*Dinner and free evening*		

TUESDAY, April 17, 2018			
Session E			
8:30 – 8:55		**Oskar Asvany** (Cologne, Germany)	Chair: Guntram Rauhut (Stuttgart, Germany)
		High-resolution rotational spectroscopy of weakly bound cation-helium complexes	
8:55 – 9:20		**Henrik Koch** (Trondheim, Norway)	Chair: Guntram Rauhut (Stuttgart, Germany)
		New aspects of conical intersections in coupled cluster theory	
9:20 – 9:45		**Magnus Ringholm** (Tromsø, Norway)	Chair: Guntram Rauhut (Stuttgart, Germany)
		Vibrational wave-mixing with Wilson: 2D-IR spectroscopy	
9:45 – 10:00		**Robert Wodraszka** (Kingston, Canada)	Chair: Guntram Rauhut (Stuttgart, Germany)
		Using new collocation and nondirect product basis approaches with the multi-configuration time-dependent Hartree (MCTDH) method to compute vibrational spectra	
10:00 – 10:30	*Coffee break*		
Session F			
10:30 – 10:55		**Luca Dore** (Bologna, Italy)	Chair: Tucker Carrington (Kingston, Canada)
		Anharmonic resonances in the IR spectrum of the interstellar molecule HC_3N	
10:55 – 11:20		**Mirjana Mladenović** (Paris, France)	Chair: Tucker Carrington (Kingston, Canada)
		A new perspective on triatomic molecules: The example of HCO^+ and HOC^+	

11:20 – 11:45		**Bryan Changala** (Boulder, CO, USA)	Chair: Tucker Carrington (Kingston, Canada)
		Structure and rovibrational dynamics of prototypical non-rigid molecules	
11:45 – 12:00		**Jan Šmydke** (Budapest, Hungary)	Chair: Tucker Carrington (Kingston, Canada)
		Rovibrational structure and tunneling dynamics of the vinyl radical	
12:00 – 13:30	*Lunch break*		
Session G			
13:30 – 13:55		**Ágnes Vibók** (Debrecen, Hungary)	Chair: Bill Poirier (Lubbock, TX, USA)
		Light-induced conical intersections	
13:55 – 14:20		**Krzysztof Szalewicz** (Newark, DE, USA)	Chair: Bill Poirier (Lubbock, TX, USA)
		Automated development of physics-based intermolecular potential energy surfaces: from near-spectroscopic accuracy for small dimers to crystal structure predictions for molecules with dozens of atoms	
14:20 – 14:45		**Jiři Vaníček** (Lausanne, Switzerland)	Chair: Bill Poirier (Lubbock, TX, USA)
		On-the-fly ab initio semiclassical evaluation of electronic spectra of polyatomic molecules beyond the Condon approximation	
14:45 – 15:10		**Sergiy Manzhos** (Singapore, Singapore)	Chair: Bill Poirier (Lubbock, TX, USA)
		Rectangular collocation for solution of the Schrödinger equation	
15:10 – 15:40	*Coffee break*		
Session H			
15:40 – 16:05		**Georg Mellau** (Giessen, Germany)	Chair: Ágnes Vibók (Debrecen, Hungary)
		Fourier-transform emission spectroscopy of highly excited molecular states	
16:05 – 16:30		**Riccardo Conte** (Milano, Italy)	Chair: Ágnes Vibók (Debrecen, Hungary)
		Semiclassical vibrational spectroscopy: the importance of quantum anharmonicity in supramolecular systems	
16:30 – 16:55		**András Csehi** (Debrecen, Hungary)	Chair: Ágnes Vibók (Debrecen, Hungary)
		Manipulating photodissociation dynamics by frequency chirped laser pulses	
Session I: Poster session			
17:00 – 19:00	*Poster session*		
19:00 – 21:00	*Dinner*		

WEDNESDAY, April 18, 2018			
Session J			
8:30 – 8:55		**Olivier Pirali** (Paris, France)	Chair: Majdi Hochlaf (Paris, France)
		Exploitation of synchrotron radiation for high resolution molecular spectroscopy in the far-infrared	
8:55 – 9:20		**Michel Herman** (Brussels, Belgium)	Chair: Majdi Hochlaf (Paris, France)
		High resolution spectroscopy of H_2O-Ar/Kr in the 2OH spectral range	
9:20 – 9:45		**Malgorzata Biczysko** (Shanghai, China)	Chair: Majdi Hochlaf (Paris, France)
		Simulation of fully anharmonic vibrational spectra of biomolecular building blocks	
9:45 – 10:00		**Tibor Nagy** (Budapest, Hungary)	Chair: Majdi Hochlaf (Paris, France)
		A novel form of the full- and reduced-dimensional vibrational Hamiltonian and its application to the preparation of quantized ensembles of classical states using adiabatic switching	
10:00 – 10:30	*Coffee break*		
Session K			
10:30 – 10:55		**Gábor Czakó** (Szeged, Hungary)	Chair: Tamás Szidarovszky (Budapest, Hungary)
		Dynamics and novel mechanisms of reactions of atoms and ions with polyatomic molecules	
10:55 – 11:20		**Federica Agostini** (Paris, France)	Chair: Tamás Szidarovszky (Budapest, Hungary)
		Dynamics of electrons and nuclei in molecules: Beyond the Born-Oppenheimer approximation	
11:20 – 11:45		**Joseph Francisco** (Lincoln, NE, USA)	Chair: Tamás Szidarovszky (Budapest, Hungary)
		Sulfur photochemistry in planetary atmospheres	
11:45 – 12:00		**Ricardo Pérez de Tudela** (Bochum, Germany)	Chair: Tamás Szidarovszky (Budapest, Hungary)
		Can one probe the dissociation state of acids in water droplets by measuring their dipole moment? The HCl/water case	
12:00 – 13:30	*Lunch break*		
Session L			
13:30 – 13:55		**Nelson de Oliveira** (Gif sur Yvette, France)	Chair: Joseph Francisco (Lincoln, NE, USA)
		High resolution absorption spectroscopy in the VUV: Probing neutral radicals produced in a plasma discharge	
13:55 – 14:20		**Andras Bodi** (Villigen, Switzerland)	Chair: Joseph Francisco (Lincoln, NE, USA)
		Threshold photoionization as a molecular thermometer: Is anharmonicity the key to harmony?	
14:20 – 14:45		**Arnaud Cuisset** (Dunkerque, France)	Chair: Joseph Francisco (Lincoln, NE, USA)
		Analysis of very congested spectra in the mm-wave domain for environmental and defense applications	

14:45 – 15:10		**Lam Nguyen** (Paris, France)	Chair: Joseph Francisco (Lincoln, NE, USA)
		Microwave spectroscopic studies on large amplitude motions in molecules	
15:10 – 17:30	*Free afternoon*		
17:30 – 23:00	*Budapest bus tour and conference dinner*		

THURSDAY, April 19, 2018			
Session M			
8:30 – 8:55		**Roberto Marquardt** (Strasbourg, France)	Chair: Csaba Fábri (Budapest, Hungary)
		Vibrational anharmonicity and anharmonic couplings in the gas phase and at gas/solid interfaces	
8:55 – 9:20		**Sergiy Bubin** (Astana, Kazakhstan)	Chair: Csaba Fábri (Budapest, Hungary)
		Non-Born-Oppenheimer variational calculations of few-electron molecules	
9:20 – 9:45		**Kalman Varga** (Nashville, TN, USA)	Chair: Csaba Fábri (Budapest, Hungary)
		Basis optimization with imaginary time propagation	
9:45 – 10:00		**Taras Petrenko** (Stuttgart, Germany)	Chair: Csaba Fábri (Budapest, Hungary)
		A general approach for calculating strongly anharmonic vibronic spectra with a high density of states	
10:00 – 10:30	*Coffee break*		
Session N			
10:30 – 10:55		**Christoph Jacob** (Braunschweig, Germany)	Chair: Malgorzata Biczysko (Shanghai, China)
		Efficient calculation of overtones and combination bands in theoretical vibrational spectroscopy with localized modes	
10:55 – 11:20		**Petr Slavíček** (Prague, Czech Republic)	Chair: Malgorzata Biczysko (Shanghai, China)
		Nuclear quantum effects in electronic spectroscopies: From UV to X-ray domain	
11:20 – 11:45		**Bill Poirier** (Lubbock, TX, USA)	Chair: Malgorzata Biczysko (Shanghai, China)
		Large scale vibrational spectroscopy calculations: Massive parallelization and the classical phase space picture	
11:45 – 12:00		**Dariusz Kedziera** (Toruń, Poland)	Chair: Malgorzata Biczysko (Shanghai, China)
		Basis sets for one-electron approximation methods: The curious case of the lithium dimer potential	
12:00 – 12:10	*Closing ceremony*		