

Solvay Workshop on

Atomic and molecular collision mechanisms - ACME

Collisions: astrophysics, atmospheric, dynamics, reactivity, spectroscopy, theory
(March 30 – April 2, 2015)

Program

Monday 30 March

11:00 12:00 REGISTRATION

12:00 13:45 LUNCH

Session 1 - In honour of J. Liévin (Chair - D. Gauyacq)

13:45 14:00 Welcome speeches by Marc Henneaux, Director of the Solvay Institutes
Nathalie Vaeck, co-organizer and Dolorès Gauyacq, session chairwoman

14:00 14:35 C. Lauzin *High resolution pulsed-field-ionization zero-kinetic-energy photoelectron spectroscopic study of water*

14:35 15:10 S. Boyé-Péronne *VUV photoionization of cyanoacetylene: towards a better characterization of the cation vibronic structure*

15:10 15:45 P. Cassam-Chenaï *The generalized mean field configuration interaction method: how far a direct product wave function ansatz can go*

15:45 16:05 COFFEE BREAK

16:05 16:40 J. Bowman *The central role of the potential in reaction dynamics and energy transfer*

16:40 17:15 H.-J. Werner *Accurate calculation of molecular properties using explicitly correlated wave functions*

Tuesday 31 March

Session 2 - Half collisions (Chair – J. De Keyser)

9:00 9:35 J. Loreau *Bound states and scattering of NH₃-noble gas complexes*

9:35 9:50 *Contributed talk*
Y. Scribano et al *Quantum trajectory capture for complex-forming reactions*

9:50 10:25 M. Herman *High-resolution overtone spectroscopy and dynamics of van der Waals complexes*

10:25 10:45 COFFEE BREAK

10:45 11:20 A. Van der Avoird *Collision-induced spectra of hydrogen and nitrogen from quantum calculations with an anisotropic potential*

11:30	12:05	D. Nesbitt	<i>Atomic and Molecular Collisions at the Gas-Liquid Interface: From Energy Transfer to Stereodynamics</i>
12:05	12:10	Group Photo	
12:10	13:45	LUNCH	

Session 3 - *Cold ions, molecules and collisions* (Chair – S. Hogan)

13:45	14:20	E. Narevicius	<i>Chemistry with Cold Molecules: from Universality to Quantum Resonances</i>
14:20	14:55	F. Merkt	<i>Collisional and spectroscopic experiments with cold samples of one-, two- and three-electron molecules</i>
14:55	15:30	T. Softley	<i>Cold collisions of decelerated molecules and laser cooled ions</i>
15:30	16:00	COFFEE BREAK	
16:00	17:00	Colloquium Solvay (Chair – A. Sevrin)	
		J. Ye	<i>Ultracold molecules - New frontiers in quantum & chemical physics</i>

Session 4 - *Poster session /Buffet* at the UAE Restaurant (ULB, Campus Plaine)

18:00 20:00 **Poster session**

Wednesday 1 April

Session 5 - *Intramolecular events and control*

9:00	9 :35	D. Cappelletti	<i>Catching the role of chemical interactions in neutral complexes of helium and neon by molecular beam experiments and charge displacement calculations</i>
9:35	9:50	<i>Contributed talk</i> A. Canosa et al	<i>Experimental and theoretical study of the CN + CH₃CN reaction at very low temperature: Evidence of a competition between tunnelling and adduct stabilization at temperatures below 160 K?</i>
9:50	10:25	P. De Natale	<i>Novel sources and spectroscopic techniques for precision spectroscopy of cold molecules</i>
10:25	10:45	COFFEE BREAK	
10:45	11:20	C. Koch	<i>Non-resonant light control of ultracold collisions</i>
11:20	11:35	<i>Contributed talk</i> A. Bergeat et al	<i>Crossed-beam inelastic scattering experiments at energies approaching the cold regime</i>
11:35	12:10	A. Ross	<i>Efficient collisional energy transfer in electronic spectra of small polar molecules</i>
12:10	14:00	LUNCH	

Session 6 - *Planetary atmospheres* (Chair - Pascal Quinet)

14:00	14:35	J. Vander Auwera	<i>Line shape parameters from Fourier transform infrared spectra</i>
14:35	14:50	<i>Contributed talk</i> S. Hoekstra et al	<i>Ultracold trapped SrF molecules - for precision spectroscopy and as a platform for quantum simulation</i>
14:50	15:25	J.-M. Hartmann	<i>Infrared probing of molecule-wall collisions in/and porous media</i>
15:25	15:45	COFFEE BREAK	
15:45	16:20	R. Ciurylo	<i>Spectral line shapes affected by collisions in theory and experiment</i>
16:20	16:55	R. Signorell	<i>Photoemission from aerosol particles: from nanosolutions to electron mean free paths</i>
19:30		BANQUET	

Thursday 2 April

Session 7 - *The interstellar medium* (Chair – X. Urbain)

9:15	9:50	T. Momose	<i>Nuclear spin conservation and interstellar chemistry</i>
9:50	10:05	<i>Contributed talk</i> D. W. Savin et al	<i>Merged Beams Studies for Astrobiology</i>
10:05	10:40	S. Schlemmer	<i>Spectroscopy of Cold Molecular Ions</i>
10:40	11:00	COFFEE BREAK	
11:00	11:35	E. Herbst	<i>Complex Molecules in Regions of Stellar and Planetary Formation</i>
11:35	12:10	T. Oka	<i>Interplay between collisions and radiative effects in the analyses of diffuse interstellar bands</i>
12:10	12:25	M. Herman, N. Vaeck, T. Softley	Closing
12:25		LUNCH	

Poster Session - Tuesday 31 March 2015 (6:00 to 8:00 p.m.)

- POSTER PANEL 1 *Experimental Studies on the Chemical Reactivity of Small Oxygenates towards OH radicals at the Ultra-Low temperatures in the Dense Molecular Clouds of the Interstellar Medium - M. Antiñolo, B. Ballesteros, E. Jiménez, A. Canosa, G. El Dib and J. Albaladejo*
- POSTER PANEL 2 *Studying the formation of product isomers in ion-molecule reactions with Velocity Map Imaging - E. Carrascosa, M.A Kainz, M. Bawart, M. Stei, F. Linden, W.D Geppert and R. Wester*
- POSTER PANEL 3 *Non-statistical Fragmentation of Pyrene-based Polycyclic Aromatic Hydrocarbons in collisions with He - N. de Ruelle, M. H. Stockett, L. Adoui, J. D. Alexander, T. Chen, R. Delaunay, M. Gatchell, L. Giacomozzi, B. A. Huber, P. Rousseau, H. T. Schmidt, V. Vizcaino, H. Zettergren and H. Cederquist*
- POSTER PANEL 4 *Photo-dissociation Resonances of Jet-Cooled NO₂ at the Dissociation Threshold by CW CRDS - P. Dupré*
- POSTER PANEL 5 *Chemistry inside a comet coma: ROSINA/DFMS measurements onboard Rosetta - J. De Keyser, F. Dhooche, R. Maggiolo, H. Gunell, N. Vaeck, A. Gibbons, K. Altwegg, U. Calmonte, S. Fuselier, M. Hässig, J. Berthelier, U. Mall, T. Gombosi and B. Fiethe*
- POSTER PANEL 6 *Simulation of inelastic collisions and rotational cooling of ammonia in a 4 K helium buffer gas cell - C. J. Rennick, O. Schullian, J. Loreau, N. Vaeck, T. P. Softley*
- POSTER PANEL 7 *Buffer-gas cooled velocity selected molecular beams combined with ion trapping for studying cold chemistry – E. Steer, K. Twyman, L. Pollum, B. Heazlewood and T. Softley*
- POSTER PANEL 8 *Zeeman deceleration of nitrogen atoms in the metastable ²D_{5/2} state - J. Toscano, K. Dulitz, A. Tauschinsky and T. Softley*
- POSTER PANEL 9 *Complementary cavity-enhanced spectrometers to investigate the OH+CH combination band in trans-formic acid - D. Golebiowski, T. Vanfleteren, T. Földes, J. Liévin, M. Herman and A. Perrin*
- POSTER PANEL 10 *2OH overtone spectroscopy of water-containing dimers - T. Vanfleteren, T. Földes, M. Herman, J. Liévin, J. Loreau, and L. Coudert*
- POSTER PANEL 11 *Modelling Atom Abstraction Dynamics in the Gas Phase and in Solution – J. N. Harvey B. Hornung, A. Ewing and D. Glowacki*
- POSTER PANEL 12 *Electric dipole interactions between Rydberg atoms in beams and in traps – V. S. Zhelyazkova and D. Hogan*
- POSTER PANEL 13 *Applications of Molecular Guides to Studying Chemical Reactions J. Jankunas, B. Bertsche, K. Reisman, A. Osterwalder*
- POSTER PANEL 14 *Collision-induced absorption spectra: improved theory applied to H₂⁺-H₂⁺ and N₂⁺-N₂⁺ - T. Karman, E. Miliordos, K. L. C. Hunt, A. van der Avoird, and G. Groenenboom*
- POSTER PANEL 15 *Copper Fine-Structure K-shell Electron Impact Ionization Cross Sections for Fast-Electron Diagnostic in Laser-Solid Experiments - P. Palmeri, P. Quinet, D. Batani*
- POSTER PANEL 16 *Collisional energy transfer between excited electronic states in NiH - A.J. Ross, P. Crozet, H. Harker, D. Tokaryk*

- POSTER PANEL 17 *Chemical dynamics simulation to suggest possible pathways of formamide synthesis in the interstellar medium - **R. Spezia** and A. Largo*
- POSTER PANEL 18 *Towards cold collisions in a molecular synchrotron - **A.P.P. van der Poel**, P.C. Zieger, S.Y.T. van de Meerakker, and H.L. Bethlem*