

Solvay Workshop

“Molecular Complexes in our Atmosphere
and Beyond”

20 - 23 April 2010

ULB – Campus Plaine – Salle Solvay
5th Floor, Building NO

Preliminary Programme – January 2010

Sessions

Tuesday 20 April

Afternoon: Experimental investigations in the laboratory

Evening: Free

Wednesday 21 April

Morning: Atmospheric water

Afternoon: Atmospheric chemistry

Evening: Banquet

Thursday 22 April

Morning: Molecular pairs in our atmosphere

Afternoon: Aerosols

Evening: Dining poster session

Friday 23 April

Morning: Astro complexes

INTERNATIONAL SOLVAY INSTITUTES
BRUSSELS

Programme

Tuesday 20 April

11:30 Registration

12:30 – 13:55

Lunch

I - Experimental investigations in the laboratory

Chair: M. Herman

- | | | | |
|-------|-------|-------------------------|--|
| 13:55 | 14:05 | M. Henneaux & M. Herman | <i>Welcome & Introductory Remarks</i> |
| 14:05 | 14:25 | M. Herman
(20) | <i>Experimental investigations in the laboratory: Focus on overtone spectra of acetylene dimers</i> |
| 14:25 | 14:55 | Y. Endo
(30) | <i>Molecular complexes and their intermolecular potentials studied by Fourier-transform microwave spectroscopy</i> |
| 14:55 | 15:25 | A.R.W. McKellar
(30) | <i>High resolution spectroscopy of carbon dioxide clusters</i> |

15:25 – 15:45

Coffee Break

- | | | | |
|-------|-------|---------------------|--|
| 15:45 | 16:15 | M. Suhm
(30) | <i>Hydrogen-bonded complexes in supersonic jets: Can we extrapolate to environmental temperatures?</i> |
| 16:15 | 16:30 | R. Georges
(15) | <i>Direct absorption infrared spectroscopy of molecular complexes using a synchrotron source</i> |
| 16:30 | 16:45 | T. Momose
(15) | <i>Absolute Intensity Determination of Infrared Spectra of Molecular Complexes by Superfluid He Droplet Spectroscopy</i> |
| 16:45 | 17:00 | L Halonen
(15) | <i>Computational study of vibrational spectra of some water containing complexes of atmospheric interest</i> |
| 17:00 | 17:15 | A. Baklanov
(15) | <i>Supramolecular photophysics and photochemistry of the molecular oxygen complexes X-O₂ in atmosphere</i> |

17:15 – 17:25

Short Break

17:25 17:55 Questions and discussion on Session I

Wednesday 21 April

II - Atmospheric water

Chair: R.J. Saykally

9:00	9:20	R.J. Saykally (20')	<i>Towards a Molecular Description of the Evaporation of Water and Aqueous Solutions</i>
9:20	9:50	K. Shine (30')	<i>The UK CAVIAR Consortium: A coordinated theoretical, laboratory and field investigation of the water vapor continuum</i>
9:50	10:20	C. Leforestier (30')	<i>Water Dimer Equilibrium Constant from First-Principles Calculations</i>
10:20 – 10:40		Coffee Break	
10:40	11:10	I. Ptashnik (30')	<i>Water dimers and the water vapor continuum: Recent facts</i>
11:10	11:40	J. Tennyson (30')	<i>Simulating the spectrum of the water dimer in the near infrared and visible</i>
11:40	12:10	P. Bernath (30')	<i>Remote Sensing of Atmospheric Continua from Orbit with the Atmospheric Chemistry Experiment (ACE)</i>

12:10 – 14:00 **Lunch**

III - Atmospheric chemistry

Chair: Y.-P. Lee

14:00	14:20	Y.-P. Lee (20')	<i>Experimental Techniques for Studying Molecular Complexes: Matrix Isolation Using p-H₂, Step-Scan FTIR Absorption, and IR-VUV Time-of-Flight Mass Techniques</i>
14:20	14:50	V. Vaida (30')	<i>Water complexes in atmospheric chemical and photochemical reactions</i>
14:50	15:20	B. Gerber (30')	<i>Atmospherically-Relevant Molecular Reactions in Water and in Ice Clusters</i>
15:20 – 15:40		Coffee Break	
15:40	16:10	J. Francisco (30')	<i>Structure and Reactivity of Radical-Molecule Complexes: New Frontier in Atmospheric Chemistry</i>
16:10	16:25	M. Tretyakov (15')	<i>Observation of water dimer spectrum at equilibrium: problems and perspectives</i>
16:25	16:40	Y. Kasai (15')	<i>Abundance of H₂O–O₂ complex in Earth's atmosphere</i>
16:40	16:55	D. Cappelletti (15')	<i>Experimental and theoretical evidence of charge transfer in the water-hydrogen molecular complex</i>
16:55	17:25	Questions and discussion on Session II and III	

IV - Banquet (Location: Académie Royale de Belgique)

19:30 Drink followed by the banquet

Thursday 22 April

V - Molecular pairs in our atmosphere

Chair: M. Quack

9:00	9:20	M. Quack (20')	<i>On the Role of Symmetry and Symmetry Violations in the Spectroscopy and Dynamics of Molecules and Molecular Complexes</i>
9:20	9:50	J.-M. Hartmann (30')	<i>Inter-molecular interactions in atmospheric spectra</i>
9:50	10:20	A. Vigasin (30')	<i>On the nature of atmospheric absorption caused by weakly interacting molecular pairs</i>
10:20 – 10:40		Coffee Break	
10:40	10:55	L. Frommhold (15')	<i>Infrared Atmospheric Emission and Absorption by Simple Molecular Complexes, from First Principles</i>
10:55	11:10	M.L. Senent Diez (15')	<i>Ro-vibrational inelastic collisions of small astrophysical species with He and H₂</i>
11:10	11:35	Questions and discussions on Session V	
11:35	12:05	J. Langen (30')	<i>ESA's future missions observing Earth's atmosphere</i>
12:05	12:15	Discussion	

12:10 – 14:00

Lunch

INTERNATIONAL SOLVAY INSTITUTES
BRUSSELS

VI - Aerosols

Chair: D. McNaughton

14:00	14:20	D. McNaughton (20')	<i>Infrared and synchrotron infrared spectroscopy of cold molecules and clusters</i>
14:20	14:50	R. Signorell (30')	<i>Properties of Aerosol Particles from Infrared Spectra</i>
14:50	15:20	A. Coustenis (30')	<i>Chemistry and aerosols on Titan and the giant planets</i>
	15:20 – 15:40		Coffee Break
15:40	16:10	E. Dartois (30')	<i>Clathrate hydrates: FTIR spectroscopy for astrophysical remote detection</i>
16:10	16:25	B. Howard (15')	<i>Microwave Studies of the Hydrates of Carboxylic Acids</i>
16:25	16:40	D. Parker (15')	<i>Imaging studies of H₂O-He and H₂O-H₂ complexes: Theory and experiment</i>
16:40	17:10	Questions and discussion on Session VI	
17:40	Bus departure (from Campus Plaine to Campus Solbosch)		
18:00	General picture		
18:10	Poster Session (Campus Solbosch, Hall salle Dupréel, Building S, 1st floor, av. Jeanne)		
18:40	Buffet opening (Campus Solbosch, Hall salle Dupréel, Building S, 1st floor, av. Jeanne)		

Friday 23 April

VII - Astro complexes

Chair: S. Schlemmer

9:10	9:30	S. Schlemmer (20')	<i>On the Formation and Spectroscopy of Weakly Bond Ionic Complexes</i>
9:30	10:00	E. Herbst (30')	<i>Association and Attachment in Interstellar Clouds</i>
10:00	10:30	J. Glosik (30')	<i>Binary and ternary recombination of H_3^+ and D_3^+ ions with electrons in low temperature plasma</i>
10:30 – 10:50		Coffee Break	
10:50	11:20	T. Lee (30')	<i>Theoretical Studies of Cationic Organic Dimers: Astrophysical Implications</i>
11:20	11:35	C. Toubin (15')	<i>Theoretical investigation of water activated formation of complex molecules in space</i>
11:35	12:05	W. Klemperer (30')	<i>Speculations on Complexes of Astronomical Relevance</i>
12:05	12:25	Questions and discussion on Session VII	
12:25	12:55	Chairs : M. Herman and R.J. Saykally Final comments and discussion	
13:10		Lunch	