

# 25<sup>th</sup> International Symposium on Gas Kinetics & Related Phenomena

22nd - 26th July 2018

Lille, France

### **Royal Society of Chemistry Gas Kinetics Committee**

George Marston Andrew Rickard Terry Dillon Paul Seakins Bénédicte Picquet-Varrault Matthias Olzmann Christa Fittschen

### Local Organizing Committee

Christa Fittschen Coralie Schoemaecker Sébastien Batut Laure Pillier Abderahman El Bakali Florent Louis Anne Burlet-Parendel

# Monday, July 23<sup>rd</sup>, 2018

### **Opening, Chair: Andrew Rickard**

9h00	Introduction
/1100	

- 9h20 <u>Plenary Lecture</u>: A. Ravishankara, Colorado State University Association Reactions: My Associations with Prof. Ian W.M. Smith
- 10h00 Olivier Durif, Institut de Physique de Rennes CRESUSOL, a New Instrument for Determining Kinetics and Branching Ratios of Elementary Processes at low Temperatures
- 10h20 David Bones, University of Leeds Field Observations, Laboratory Measurements and Model Simulations of Ni Ablation and Subsequent Chemical Reactions in the Earth's Mesosphere.
- 10h40 Coffee break

#### Atmospheric Chemistry I, Chair: Stanley Sander

- 11h20 <u>Plenary Lecture</u>: Geoffrey Tyndall, NCAR Boulder Formation of Alkyl Nitrates from Some Mid-Sized Alkanes
- 12h00 Damien Amedro, MPI Mainz Re-evaluation of the Rate Constant for OH + NO<sub>2</sub> – The Effect of H<sub>2</sub>O on one of the Most Important Atmospheric Reactions
- 12h20 Lei Zhu, Wadsworth Center, New York State University Role of 2-Nitrophenol and Methyl-2-nitrophenol Photolysis as Missing Sources of OH and HONO in Some Polluted Environments: Implications from Laboratory Studies

#### 12h40 Presentation of RSC Environment Medal to Dwayne Heard, University of Leeds

12h50 Lunch

#### New Methods, Chair: Aamir Farooq

- 14h10 <u>Plenary Lecture</u>: Sebastien Dusanter, IMT Lille Douai Integrated Measurements of Atmospheric Chemistry: Moving Laboratory Experiments into the Field
- 14h50 Graham Boustead, University of Leeds Development of a Photo-fragmentation Laser Induced Fluorescence Instrument for the Measurement of Nitrous Acid
- 15h10 Aileen Hui, California Institute of Technology Direct Detection of OH Radicals using mid-IR 2-f Frequency Modulation Spectroscopy for Temperature Dependence Studies of  $HO_2 + CH_3C(O)O_2$
- 15h30 Frank Winiberg, Jet Propulsion Laboratory Study of key OH + NOx/NOz reactions under upper troposphere/lower stratosphere conditions
- 15h50 Coffee break and photo on the stairs in the entrance hall

#### **Combustion I, Chair: Gernot Friedrichs**

- 16h30 <u>Plenary Lecture</u>: Frédérique Battin-Leclerc, CNRS Nancy Recent Progress on Hydroperoxide Chemistry during Gas-phase Oxidation of Fuel Components
- 17h10 Zachary Buras, Sandia National Laboratories Using OH and HO<sub>2</sub> Radicals as Markers of Biofuel Ignition Properties
- 17h30 Fethi Khaled, King Abdullah University of Science and Technology On the Reaction Kinetics of Dienes with OH Radicals
- 17h50 One-minute flash presentation of posters presented by PhD students

#### 18h10 Odd numbers Poster session, beer and food All around the plenary hall

# Tuesday, July 24<sup>th</sup>, 2018

#### Structure-Activity Relationship, Chair: Mark Blitz

- 9h00 <u>Plenary Lecture</u>: Tim Wallington, Ford Motor Company Structure Activity Relationships for Atmospheric Models: Current Status and Future Outlook
- 9h40 Mark Goldman, Massachusetts Institute of Technology Fate of Peroxy Radicals in Atmosphere, Combustion, and Everywhere in Between
- 10h00 Max McGillen, University of Bristol An Assessment of Structure-Activity Relationship Performance in Predicting the Gas-Phase Rate Coefficients of Organic Compounds with Hydroxyl, Ozone, Nitrate and Chlorine
- 10h20 Luc Vereecken, Forschungszentrum Jülich Validation and Extension of a Structure-Activity Relationship for Reactions of Criegee Intermediates

10h40 Coffee break

#### Atmospheric Chemistry II, Chair: John Orlando

- 11h20 Jim Lin, Academia Sinica, Taipei Kinetics of Criegee Intermediates
- 10h40 Mohamad Al Ajami, University of Lille ROOOH: the Missing Piece of the Puzzle for OH measurements in low NO Environments
- 12h00 Diego Medeiros, University of Leeds Investigations of OH Recycling in the Isoprene + OH Reaction in the Presence of Oxygen: Shedding Light on the Missing OH
- 12h20 Barbara Nozière, CNRS Lyon Speciated Monitoring of Organic Peroxy Radicals: First Laboratory Applications

12h40 Lunch

#### Astrochemistry, Chair: Sébastien Le Picard

- 14h10Plenary Lecture: Catherine Walsh, University of Leeds<br/>Astrochemistry: Molecule Formation at the Frontier of Physics
- 14h50 Elena Jimenez, University of Castilla La Mancha Ultra-low Temperature Kinetics of the OH-Reaction with Oxygenates in the Interstellar Medium
- 15h10 Niclas West, University of Leeds Low Temperature Gas Phase Reaction Rate Coefficient Measurements: Toward Modeling of Stellar Winds
- 15h30 Xiaofeng Tang, Chinese Academy of Sciences
  Multiplex Synchrotron VUV Photoionization Methods for Radical Reactions in Atmospheric Chemistry: CH<sub>3</sub> + O<sub>2</sub>
- 15h50 Coffee break

#### **Combustion II, Chair: Nathalie Lamoureux**

- 16h30 Te-Chun Chu, Massachusetts Institute of Technology Phenyl Radical Addition to Unsaturated Hydrocarbons: Product Distributions & Rates
- 16h50 Kacee Caster, West Virginia University Investigations into the Reaction of Cyclopentadiene with CH Radicals: A Novel Route to Benzene Formation
- 17h10 Cato Pappjin, Ghent University Thermal Decomposition of Sulfur Compounds: Kinetic Modeling and Experimental Validation
- 17h30 James Thorpe, University of Florida Modeling the Thermal Decomposition of Methyl Acetate: a Study in Combustion
- 17h50 One-minute flash presentation of posters presented by PhD students

#### 18h10 Even numbers Poster session, beer and food All around the plenary hall

# Wednesday, July 25<sup>th</sup>, 2018

#### Multiphase Chemistry, Chair: Khatuna Kakhiani

- 9h00 <u>Plenary Lecture</u>: Barbara d'Anna, CNRS Marseille SOA Formation from Photoxidation of Vehicle Exhaust Emissions
- 9h40 Fabien Goulay, West Virginia University Effect of Dimerization on the OH-Initiated Heterogeneous Oxidation of Saccharide Nanoparticles
- 10h00 Chia Wang, National Sun Yat-sen University, Taiwan Probing the Electronic Structures, Interfacial Solvation Properties and Surface pH of Organic-containing Aqueous Nanoaerosols
- 10h20 Césaire Fotsing Kwetche, University of Lille Combining Quantum Chemistry with Classical Molecular Dynamics for the Theoretical Study of Radical Reactivity at the Surface of Organic Aerosols
- 10h40 Matti Rissanen, University of Helsinki and Zhandong Wang, King Abdullah University of Science and Technology Highly Oxidized Products from Rapid Alkane Autoxidation Part 1 – Implications for Atmospheric Secondary Organic Aerosol Formation Highly Oxidized Products from Rapid Alkane Autoxidation Part 2 – Implications for Ignition in Combustion Science
- 11h10 Coffee break

#### **Combustion III, Chair: Zeynep Serinyel**

- 11h50 Franklin Goldsmith, Brown University Decomposition Kinetics for HONO and HNO<sub>2</sub>
- 12h10 Ruben Van de Vijver, Sandia National Laboratories KinBot: Automated Stationary Point Localization on Potential Energy Surfaces
- 12h30 Ghanshyam Vaghihani, Air Force Research Lab High-level Multi-reference Wave Function and Density Functional Theory Treatment of the N<sub>2</sub>H<sub>3</sub> + NO<sub>2</sub> Reaction
- 12h50 Lunch bag and departure for excursion

# Thursday, July 26<sup>th</sup>, 2018

#### **Elementary processes, Chair: Scott Kable**

9h00	<u>Plenary Lecture</u> , Matt Costen, Heriot-Watt University Inelastic and Reactive Scattering at Gas-Liquid Interfaces
9h40	Jeremy Bougalais, Université de Versailles Saint Quentin en Yvelines Gas-Phase Radical Reactions with Hydrocarbons and Amines Probed by Multiplexed Synchrotron VUV Photoionization Mass Spectrometry
10h00	Mitchio Okumura, California Institute of Technology Kinetic Isotope Effect in the Reactions of OH and O( <sup>1</sup> D) with Isotopologues of Methane
10h20	Adriana Caracciolo, Università degli Studi di Perugia Crossed Molecular Beams and Theoretical Studies of the O( <sup>3</sup> P) + 1,2-Butadiene Reaction: Primary Products, Branching Ratios and Intersystem Crossing

10h40 Coffee break

#### Atmospheric Chemistry III, Chair: Jean-François Doussin

- 11h20 <u>Plenary Lecture</u>: Andreas Hofzumahaus, Forschungszentrum Jülich Atmospheric Simulation Chamber Experiments: Bridging the Gap Between Laboratory and Field Studies
- 12h00 Gabriel Da Silva, University of Melbourne Isomerization and Decomposition of Isoprene's Delta-(Z)-Hydroxyperoxyl Radicals
- 12h20 Rasmus Otkjær, University of Copenhagen Atmospheric Autoxidation is Increasingly Important in Urban and Suburban North America

12h40 Lunch

#### **Chamber Studies, Chair: Alexandre Tomas**

14h10	Peter Wiesen, University of Wuppertal A Gas Kineticist's Life: a Reminiscence to Dr. Ian Barnes
14h30	Mike Newland, University of York The Photolysis Mechanism of Monoaromatic Ring Opening Products - Unsaturated 1,4 Dicarbonyls - from Chamber Experiments
14h50	Iustinian Gabriel Bejan, University "Al. I. Cuza" Iasi Products and Mechanisms for the Atmospheric Oxidation of Dimethylbenzoquinones
15h10	Axel Fouqueau, LISA, University of Paris Est - Créteil Reactivity of $\gamma$ -Terpinene and $\alpha$ -Terpinene with NO <sub>3</sub> Radical: a Comparative Kinetic and Mechanistic Study
15h30	Freja F. Oesterstroem, University of Leeds Kinetic Study of the $CH_3O_2 + HO_2$ Cross-reaction in the Highly Instrumented Reactor for Atmospheric Chemistry

15h50 Coffee break

#### **Combustion IV, Chair: Jürgen Troe**

- 16h30 Rajakumar Balla, Indian Institute of Technology, Madras Cl Atom Initiated Photo-oxidation Reaction Kinetics of Methyl and Ethyl Propionate
- 16h50 Isabelle Weber, Karlsruher Institut für Technology Thermal Decomposition of CH<sub>3</sub>I Revisited: Consistent Calibration of I-atom Concentrations Behind Shock Waves with Dual I-/H-ARAS
- 17h10 Michael Burke, Columbia University Pressure Dependence of Chemically Termolecular Reactions

### 17h30 Polanyi lecture: Barbara Finlayson-Pitts University of California Irvine

#### Multiphase Chemistry in the Atmosphere: It All Starts with Gases

# List of posters

### Odd numbers (in white) will be presented on Monday Even numbers (in grey) will be presented on Tuesday

Poster with yellow or blue names participate in best student poster prize on Monday and Tuesday

No	Presenter's name	Title
1	Mohammed ALABBAD	Reaction Kinetics for the Unimolecular Decomposition of $C_5$ and $C_6$ Cyclic Ketones
2	Mark BLITZ	Determination of the $HOOCH_2OCH_2$ (QOOH) + $O_2$ rate coefficient under propagating / branching conditions
3	Joseph BOZZELLI	Computational Study of $\alpha$ -Acrolein Radical Association Reactions with 3O <sub>2</sub> , Thermochemistry and Kinetics s
4	Adriana CARACCIOLO	Crossed beam studies of the O( <sup>3</sup> P) reaction dynamics with benzene and toluene: primary products and branching ratios
5	Harish CHAKRAVARTY	Theoretical investigation of the kinetics of low-temperature combustion chemistry of propylbenzene
6	Guillaume DAYMA	Experimental and numerical kinetic study of the oxidation of $C_5H_{10}O_2$ esters isomers
7	Hong Quan DO	Experimental study of atmospheric laminar premixed $CH_4/O_2/N_2$ and $CH_4/H_2/O_2/N_2$ flames in sooting conditions
8	Ravi FERNANDES	On the auto-ignition kinetics of ammonia at low temperatures and high pressures
9	Fethi KHALED	A high temperture experimental investigation of allyl self- reaction and allyl + OH
10	Olivier HERBINET	Formation study of $NO_2$ and $NO$ in methane oxidation in flow tube at high temperature (up to 1973 K)
11	Corina JANZER	NO <sub>2</sub> formation in the combustion of n-heptane: Kinetic modeling and comparison to engine measurements with diesel fuel
12	Satya JOSHI	An experimental kinetic study for the reaction between vinyl radicals associated propene molecule and molecular oxygen.
13	Saravanan KUZHANTHAIVEL AN	Computational investigations on the thermochemistry and kinetics for the autoignition of 2-pentanone
14	Sonia LARA GOMEZ	Development of a methodology for the chemical characterization of soluble organic fraction (SOF) of the particles generated from (bio)fuels combustion using GC- MS/MS
15	Benoite LEFORT	A comparative high-pressure shock tube study on the ignition of pentanol isomers: 1-, 2- and 3- pentanol
16	Lorena MARRODAN	Jet-stirred low-temperature oxidation of n-pentane: the effect of NOx addition
17	Lorena MARRODAN	Evaluation of DME as a possible fuel additive through the study of the high-pressure oxidation of its mixtures with acetylene

18	Sylvain NAMYSL	Experimental investigation of butanoic and pentanoic acid oxidation
19	lliyana NAYDENOVA	Kinetic characteristics related to particulate matter formation in biomass combustion
20	Matthias OLZMANN	The complexity of ignition phenomena in diethyl ether/air mixtures
21	David POTTER	Laser photolysis kinetic studies of methyl tert-butyl ether with OH at low temperatures relevant to combustion
22	Zeynep SERINYEL	A comparative high-pressure jet-stirred reactor study on the oxidation of pentanol isomers: 1-, 2- and 3- pentanol
23	Samantha SIME	Kinetic Studies of tert-Butanol under Low Temperature Combustion Conditions
24	Mica SMITH	Acetylene addition to vinyl and aryl radicals: Experimental investigation of HACA and PAH formation pathways
25	Yu SONG	The sensitizing effects of NO <sub>2</sub> and NO on methane low temperature oxidation in a jet stirred reactor
26	Elsa TELLBACH	Experimental and Modelling Study of the Multichannel Thermal Dissociations of CH <sub>3</sub> F and CH <sub>2</sub> F
27	Zhen-Yu TIAN	Experimental and kinetic study of 1,2,4-trimethylcyclohexane under pyrolysis condition
28	Luc-Sy TRAN	High-pressure low-temperature oxidation of diethyl ether compared to n-pentane and their mixture
29	Florence VERMEIRE	The oxidation of furfural in a jet-stirred reactor: a combined experimental and modeling approach
30	Charlotte WHELAN	Kinetics of OH radical reactions with 2,5-dimethylfuran
31	Chao YAN	$HO_2$ Radical and Triox Yields in the Reaction $CH_3O_2$ with OH over the 1-100 bar Pressure Range
32	Emmanuel ASSAF	Rate Constants of the Reactions of $DO_2 + DO_2$ and $HO_2 + DO_2$
33	Simone Thirstrup ANDERSEN	Atmospheric Chemistry of n-CH <sub>3</sub> (CH <sub>2</sub> )xCN ( $x = 0-4$ ) and n-CH <sub>2</sub> =CH(CH <sub>2</sub> )xCN ( $x = 0-4$ ): Kinetics and Mechanisms
34	Josep M. ANGLADA	Atmospheric oxidation of CH <sub>3</sub> OOH and CH <sub>3</sub> OOOH by OH
35	Beatriz CABAÑAS	Kinetic study of saturated alcohols during day-time: Reactivity of 3,3-dimethyl-1-butanol and 3,3-dimethyl-2-butanol
36	William CARTER	Structure-Reactivity Evaluation Panel for Gas-Phase Atmospheric Reactions of Organic Compounds
37	Manuela CIRTOG	Reactivity of NO <sub>3</sub> radical with ramified unsaturated aldehydes: theoretical approach for kinetic and mechanistic studies
38	Theodore DIBBLE	BrHgO•: Predicting the chemistry of a previously-unknown intermediate in atmospheric mercury oxidation
39	Theodore DIBBLE	OH Radical Can Initiate Oxidation of Hg(0) in the Upper Troposphere
40	Terry DILLON	Rate coefficients for OH + VOC reactions by a new, rapid, relative rate technique
41	Kevin DOUGLAS	Atmospheric oxidation chemistry of meteor ablated phosphorous

42	Atallah EL ZEIN	Temporal variability of polycyclic aromatic hydrocarbons and their oxidative derivatives in Beijing, China: wintertime observations.
43	Layal FAYAD	A New Environmental Simulation Chamber (CHARME) to study the Atmospheric Reactivity and the Metrology of the Environment: Design, Characterization and Preliminary Tests
44	Camille FORTIN	Atmospheric fate of iodomethanol, unimolecular decomposition and its reaction with OH radicals
45	Aline GRATIEN	Analysis of gas-phase and particulate reaction products from high-NOx photooxidation of n-dodecane: Influence of temperature and relative humidity on secondary organic aerosol formation
46	Fred GRIEMAN	HO <sub>2</sub> /Acetone Chemistry: Temperature Dependence of Acetonylperoxy and Chaperone Mechanism Rate Constants
47	Asma GRIRA	Reactivity of Green Leaf Volatiles (GLVs) in the atmosphere: Kinetics, products and secondary organic aerosol formation
48	Parth GUPTA	Reactivity of a series of alkanes and alkenes with XO radicals (X=Cl, Br and I): A computational study
49	Takashi IMAMURA	OH Radical Formation from the Reactions of Ozone with Dimethyl and Trimethyl Amines
50	Alexander D. JAMES	A novel, low cost material for automotive catalysis
51	Malte JESPERSEN	Theoretical Rate Constants for the 1,4-Cycloaddition of Singlet Oxygen on Conjugated cis-Dienes
52	Revathy KAIPARA	Oxidation of alkyl esters by OH radicals and Cl atoms: An experimental and computational study
53	Carmen KALALIAN	Atmospheric fate of oxygenated biogenic volatile organic compounds
54	Monali KAWADE	A Kinetic Study of Gas Phase OH Radical Reaction with 2- chloroethyl vinyl ether Using Laser Induced Fluorescence Technique in the Atmospheric Temperature Range
55	Alireza Kharazmi	New Observed Triple Fragmentation Photolytic Pathway of Propanal
56	Dorra KHIRI	Ab initio investigation of thermochemical properties of very- short lived brominated substances (VSLS)
57	Florent KRAVTCHENKO	Development and validation of a new experimental set-up to study reactions between peroxy RO <sub>2</sub> and HOx radicals
58	Avinash KUMAR	Kinetic investigations for gas phase reactions of monochlorinated propanes with Cl atoms: Experimental and computational studies.
59	Thomas LEWIS	Contrasting pathways to Iodine Oxide Particle formation in the presence and absence of water
60	Ernesto MARTINEZ ATAZ	SO <sub>2</sub> -Criegee intermediate reaction's role in the formation of secondary organic aerosols
61	Ernesto MARTINEZ ATAZ	Atmospheric Sinks of Styrene: Rate Coefficient and Mechanism of the Cl Atoms Initiated Degradation.

62	Max MCGILLEN	Direct Studies of Criegee Intermediate Reactions Using Cavity Ring-Down Spectroscopy
63	Zara MIR	CH <sub>2</sub> OO Criegee Intermediate UV Absorption Cross-Sections and Self-Reaction Kinetics
64	Kristian Holten MØLLER	Alkoxy Radical Bond Scissions Explain the Anomalously Low Secondary Organic Aerosol and Organonitrate Yields From $\alpha$ -Pinene + NO <sub>3</sub>
65	Julien MORIN	Experimental Study of Photosensitized reduction of nitrogen dioxide on corn as a source of nitrous acid
66	Julien MORIN	Photocatalytic paints: improving a new binder to reduce VOCs emission
67	Freja F. OESTERSTROEM	Mechanistic Study of the Reaction of $CH_2F_2$ with Cl Atoms in the Absence and Presence of $CH_4$ or $C_2H_6$ : Decomposition of $CHF_2OH$ and Fate of the $CHF_2O$ Radical
68	John ORLANDO	Steady State Continuous Flow Chamber for the Study of Atmospheric Hydrocarbon Oxidation Chemistry under Daytime and Nighttime Conditions – Chamber Characterization and First Results
69	Jari PELTOLA	Time-resolved broadband cavity-enhanced absorption spectrometer for reaction kinetic studies of stabilized Criegee intermediates
70	C B RAMYA	Cl and OH initiated photo oxidation reaction kinetics of methyl butyrate
71	Andrew RICKARD	Mechanisms for Atmospheric chemistry: GeneratioN, Interpretation and FidelitY - MAGNIFY
72	Michael ROLLETTER	Acetylperoxy Radical Revisited - Spectra, Absorption Cross Sections and Kinetics of the Self Reaction
73	Emmanouil ROMANIAS	Development and validation of a THermAL Regulated AtMOspheric Simulation Chamber (THALAMOS)
74	Antoine ROOSE	Uptake of peroxy radicals on organic aerosols : Development of an Aerosol Flow Tube and molecular-level characterization
75	Dharmendra SINGH	Photochemical degradation and production of polycyclic aromatic hydrocarbons and carboxylic acids in Canadian high arctic aerosols (Alert) before and after polar sunrise
76	Vijayakumar SIRIPINA	Hydroxyl radical initiated photo-oxidization of series of butadienes in troposphere: An experimental and computational study
77	Eloise SLATER	Elevated levels of OH observed in haze events during wintertime in Beijing, and the comparison of radical measurements with both steady state calculations and box model simulations.
78	Thomas SPEAK	OH initiated study of the oxidation of N,N'- Dimethylformamide: evidence for QOOH+O <sub>2</sub> forming OH
79	Doddipatla Srinivas	The Experimental and Theoretical Study for Reaction of Hydroxyl Radical with Dimethy Ether and its Atmospheric Implications

80	Daniel STONE	Unimolecular Decomposition Kinetics of the Stabilised Criegee Intermediates CH <sub>2</sub> OO and CD <sub>2</sub> OO
81	Sonia TAAMALi	Unravelling the reaction mechanisms of iodous acid with chlorine atom
82	Mariano Teruel	Products and Mechanisms of the Reactions of a Series of Hydrofluoroalkenes initiated by OH Radicals
83	Lauge THORSEN	Epoxide Formation in the Decomposition of MBO232
84	Carmen Maria TOVAR RAMOS	Rate coefficients for the gas phase reactions of chlorine atoms with a series of epoxy compounds
85	Luís Pedro VIEGAS	Reactivity of hydrofluoropolyethers towards OH: a cost- effective implementation of MC-TST
86	Blair WELSH	Vibrationally Excited Products of Roaming Reactions in the Atmosphere as a Novel Source of Hydroxyl Radicals
87	Frank WINIBERG	Study of key OH + NOx/NOz reactions under upper troposphere/lower stratosphere conditions
88	Pierre WINTER	Microcanonical Instanton Rate Theory Applied to Molecular Reactions
89	María ANTIÑOLO	Kinetics of the Atmospherically Relevant Gas-phase Reactions of Allyl Cyanide
90	Alex BRENNAN	An inter-comparison of FAGE and CRDS for the detection of $HO_2$ and $CH_3O_2$ radicals in a simulation chamber
91	Rodrigo G. GIBILISCO	Atmospheric degradation of (E)-4-methoxy-3-buten-2-one and 1-(E)-1-methoxy-2-methyl-1-penten-3-one initiated by OH radicals: Kinetics and reaction products.
92	Rodrigo G. GIBILISCO	Gas-Phase Oxidation of Aromatic Hydrocarbons: A Kinetic Study of the OH Reaction with Methoxybenzenes at Atmospheric Conditions
93	Lei HAN	Rate Constants for the Reaction of OH Radicals with Hydrocarbons in a Smog Chamber at Lower Atmospheric Temperatures
94	Claudiu ROMAN	Gas phase kinetic study of the OH radical initiated oxidation of alkylfurans at atmospheric pressure and 298±2 K
95	Claudiu ROMAN	Temperature dependence kinetic studies by using the newly thermostated ESC-Q-UAIC chamber
96	Mariano Teruel	Kinetics and product distribution of the gas phase reactions of $\beta$ - ocimene and camphene with Cl atoms at room temperature
97	Khatuna KAKHIANI	Morphology and Reactivity: A DFT Study on curved graphene
98	Julian MÜLLER	Structure-reactivity trend for the ozonolysis of fatty acid monolayers – a molecular dynamics perspective
99	Vladimir AZRIEL	Recombination dynamics in system RCs+ + Br-, where R=Ar, Kr and Xe
100	Vladimir AZRIEL	Excitation functions of two channels of interaction in system $ArCs++Cl-$
101	Maxi BURGOS PACI	Photochemistry of (FCO) <sub>2</sub> at 266nm. UV and IR emission
102	Maxi BURGOS PACI	Photolysis of methyl formate at 248nm, a study on the vibrational relaxation of CO.

103	Gus HANCOCK	Self quenching of NO( $A^2\Sigma_+$ ): evidence for the formation of NO( $a^4\Pi$ )
104	Nozomu KANNO	Theoretical study for the reaction between hydrazine derivatives with OH
105	Artem KOVALENKO	Studying reaction of $N^+$ ions with HD using rf 22 pole trap down to 15 K.
106	Thanh Lam NGUYEN	Three-Dimensional Master Equation (3DME) Approach
107	Vladimir ORKIN	High Accuracy OH Reaction Rate Constant Measurements: Studies of Pressure Dependencies
108	Thomas PRESTON	Aminosilanes from co-pyrolysis of silane and ammonia
109	Zhen-Yu TIAN	Catalytic oxidation of CO on perfect and defective CuO and $Cu_2O$ surfaces
110	Raimo TIMONEN	Kinetics of the Reactions of Ethyl, n-Propyl, and n-Butyl Radicals with Molecular Oxygen
111	Thuy Dung TRAN	Isotopic effects in the interaction of $D_2O+$ with $H_2$ and $D_2$ at low temperatures
112	Ondrej VOTAVA	Detailed reinvestigation of water nuclear spin conversion kinetics in supersonic expansion
113	Fayçal ALLOUTI	Oxydation of a potassium iodide surface by gaseous ozone
114	Witkowski BARTŁOMIEJ	Aqueous-phase oxidation of the monoterpene secondary organic aerosols (SOAs)
115	Raluca CIURARU	Volatile Organic Compounds and Secondary Organic Aerosols from Soil Amendments: laboratory and field comparison
116	Joshua BOOTHROYD	Atomic chlorine generation using a radio-frequency atmospheric pressure plasma for use in the comparative reactivity method
117	Joseph BOZZELLI	Towards Direct Molecular Analysis of Atmospheric Oxidized Mercury
118	Marius DUNCIANU	Development of a mobile photochemical reactor to investigate gas-phase chemistry and aerosol formation in the field
119	Daniel STONE	Time-resolved infrared spectroscopy of reactive intermediates in atmospheric chemistry: Method development and characterisation
120	Thomas SPEAK	An instrument for time resolved HO <sub>2</sub> and OH measurement.
121	Harish CHAKRAVARTY	Application of Chemical Organization Theory to Methane Combustion - A Novel Approach to Identify Hierarchical Structures in Dynamical Combustion Networks
122	Rachid HADJADJ	Detailed molecular network of CO <sub>2</sub> hydrogenation
123	Robin SHANNON	Coupling dynamics and kinetics to automate reaction discovery: ChemDyME
124	Anjitha S. KUMAR GEETHA	Pyrolysis of silanes and silane mixtures - kinetic modelling and experiments using a benchtop recator.
125	James Thorpe	mHEAT: a Pragmatic approach to sub-chemical accuracy
126	Nicolas VIN	A study of chlorobenzene pyrolysis
127	Fiona WHITING	Hydroxyl Radical Production from Reactions of $O_2$ with six $C_3$ – C5 Acyl Radicals

