

**PROGRAMME OF THE SYMPOSIUM**  
(all activities in Ron Cooke Hub unless stated)

**Sunday 17<sup>th</sup> July**

**13:00    16:30    REGISTRATION IN RON COOKE HUB**

**17:00    20:00    ICEBREAKER RECEPTION & REGISTRATION IN DEPT OF CHEMISTRY**

**Monday 18<sup>th</sup> July**

**08:45    09:00            INTRODUCTIONS**

**BENSON LECTURE**

**09:00    09:40            Simplification of complex chemical kinetics: what is essential?**  
*Jürgen Troe*  
Institute for Physical Chemistry, University of Göttingen, Germany

**REACTION DYNAMICS**

**09:40    10:00    RD02    Tunnelling in polyatomic chemical reactions**  
*J. Richardson*  
Department of Chemistry, Durham University, UK

**10:00    10:20    RD03    Collisional quenching of excited NO ( $A^2\Sigma^+$ ) studied by time-resolved FTIR emission spectroscopy**  
*J. Fletcher, G. Hancock, and G. Ritchie*  
Physical and Theoretical Chemistry Laboratory, University of Oxford, UK

**10:20    10:40    RD04    Dynamics of Complex-Forming Bimolecular Reactions**  
*P. Szabó, S. Góger, and G. Lendvay*  
Institute of Chemistry, University of Pannonia, Veszprém, Hungary

**10:40    11:10            Tea Break**

**11:10    11:50    RD01    Non-adiabatic molecular dynamics simulations of photochemical isoprene oxidation intermediates**  
*D. Glowacki, and B. Curchod*  
School of Chemistry, University of Bristol, UK

**11:50    12:10    RD05    Crossed molecular beam studies of the  $O(^3P) + 1$ -butene reaction: Primary products, branching ratios and role of intersystem crossing**  
*G. Vanuzzo, N. Balucani, D. Stranges, S. Falcinelli, and P. Casavecchia*  
Dipartimento di Chimica, Biologia e Biotechnologies, Università degli Studi di Perugia, Italy

**12:10    12:30    RD06    Photochemical Quantum Yields of Enol Production**  
*M. Shaw, A. Kharazmi, K. Lapere, M. Jordan, and S. Kable*  
School of Chemistry, University of Sydney, Australia

**12:30    14:00            LUNCH**

## ATMOSPHERIC CHEMISTRY

- 14:00 14:40 AC01 Theory-based studies on reactions in the troposphere**  
*L. Vereecken, I-H. Acir, T. Brauers, H. Chakravarty, H-P. Dorn, I. Gensch, R. Haeseler, A. Hofzumahaus, M. Kaminski, X. Li, A. Lutz, S. Nehr, A. Novelli, T. Piansawan, F. Rohrer, R. Wegener, A. Kiendler-Scharr, and A. Wahner*  
Institute of Energy and Climate Research, Forschungszentrum Jülich, Germany
- 14:40 15:00 AC03 CH<sub>2</sub>OO Criegee Decomposition Kinetics**  
*D. Stone, S. Sime, M. Blitz, P. Seakins, Z. Decker, K. Au, and L. Sheps*  
School of Chemistry, University of Leeds, UK
- 15:00 15:20 AC04 Kinetic studies of Criegee intermediate reactions with SO<sub>2</sub> and RCOOH**  
*R. Chhantyal-Pun, B. Rotavera, A. Eskola, L. Blacker, M. Ashcroft, M. Khan, D. Osborn, C. Taatjes, C. Percival, D. Shallcross, and A. Orr-Ewing*  
School of Chemistry, University of Bristol, UK
- 15:20 15:40 AC05 Theoretical kinetics of reactions of •HgBr critical to oxidation of atmospheric mercury**  
*Y. Jiao, T. Dibble, and A. Schwid*  
Chemistry Department, State University of New York - College of Environmental Science and Forestry, Syracuse, US

**15:40 16:10 Tea Break**

## EXPERIMENTAL METHODS

- 16:10 16:50 EM01 Multimass imaging of molecular fragmentation processes**  
*C. Vallance*  
Department of Chemistry, University of Oxford, UK
- 16:50 17:10 EM02 Chirped-Pulse in Uniform Flow: Probing the Dynamics of Multichannel Reactions with Pure Rotational Spectroscopy**  
*B. Joalland, C. Abeysekara, L. Zack, N. Ariyasingha, I. Sims, R. Field, and A. Suits*  
Department of Chemistry, Wayne State University, Detroit, US
- 17:10 17:30 EM03 An Experimental and Theoretical Study of the Thermal Decomposition of 1,3-Butadiene**  
*J. Lockhart, C. Goldsmith, J. Randazzo, and R. Tranter*  
Chemical Sciences and Engineering Division, Argonne National Laboratory, US
- 17:30 17:50 EM04 Quantitative Diagnostics of Inductively-coupled Radiofrequency Plasmas in Cl<sub>2</sub>, O<sub>2</sub> and mixtures**  
*J-P.Booth, M. Foucher, A. Gibson, and D. Marinov*  
LPP-CNRS, Ecole Polytechnique-UPMC-UPSud, Palaiseau, France

**18:00 20:00 POSTER SESSION I**

Tuesday 19<sup>th</sup> July

## ELEMENTARY PROCESSES

- |       |       |      |   |
|-------|-------|------|---|
| 09:00 | 09:40 | EP01 | <b>Understanding gas-phase processes via experiments and theory: tools to add further understanding</b><br><u>M. Blitz</u><br>School of Chemistry, University of Leeds, UK  |
| 09:40 | 10:00 | EP02 | <b>The Role of Intramolecular H-Migration in Peroxy Radicals Formed in the Atmospheric Oxidation of Volatile Organic Compounds</b><br><u>S. Wang, and L. Wang</u><br>School of Chemistry & Chemical Engineering, South China University of Technology, Guangzhou, China |
| 10:00 | 10:20 | EP03 | <b>Surprising Energy Transfer Effects in Multi-Channel Complex Reactions in Multi-Component Baths</b><br><u>M. Burke</u><br>Department of Mechanical Engineering, Department of Chemical Engineering, and Data Sciences Institute, Columbia University, New York, US    |
| 10:20 | 10:40 | EP04 | <b>The reaction of diethyl ether with OH radicals: rate coefficient, kinetic isotope effect, and mechanism</b><br><u>C. Bansch, J. Kiecherer, J. Hetzler, M. Szöri, and M. Olzmann</u><br>Institute of Physical Chemistry, Karlsruhe Institute of Technology, Germany   |

10:40 11:10 Tea Break

## ATMOSPHERIC CHEMISTRY

- |       |       |      |   |
|-------|-------|------|---|
| 11:10 | 11:30 | AC06 | <b>Peroxy Radical Kinetics using the <math>\tilde{A} \leftarrow \tilde{X}</math> Transition</b><br><u>M. Smarte, and M. Okumura</u><br>Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, US   |
| 11:30 | 11:50 | AC07 | <b>Gas Phase Reaction of CH<sub>3</sub>O<sub>2</sub> Radicals with OH Studied over the 292 – 526 K Temperature Range</b><br><u>C. Yan, S. Kocevskaja, and L. Krasnoperov</u><br>New Jersey Institute of Technology, Newark, US  |
| 11:50 | 12:10 | AC08 | <b>Atmospheric reactivity of organic nitrates: impact on the long-range transport of NO<sub>x</sub></b><br><u>B. Picquet-Varrault, M. Duncianu, R. Suarez-Bertoa, M. Le Quilleuc, A. Fouqueau, E. Pangui, M. Cazaunau, and J-F. Doussin</u><br>LISA, Universités Paris Est et Paris Diderot, France |
| 12:10 | 12:30 | AC09 | <b>Photo-oxidation of Selected Carbonyl Compounds: Efficiencies of Carboxylic Acid Productions under Atmospheric Condition</b><br><u>A. Chattopadhyay, K. Mondal, and T. Chakraborty</u><br>Department of Physical Chemistry, Indian Association for the Cultivation of Science, Kolkata, India     |

12:30 14:00 LUNCH

## COMPLEX SYSTEMS

14:00	14:40	CS01	<b>Effective strategies for collectively improving the robustness of chemical kinetic models</b> <i>A. Tomlin</i> School of Chemical and Process Engineering, University of Leeds, UK
14:40	15:00	CS02	<b>Evaluate the parametric uncertainty of RRKM/Master Equation rate constants</b> <i>Z. Wang, S. Li, B. Yang, and F. Zhang</i> National Synchrotron Radiation Laboratory, University of Science and Technology of China, Anhui, China
15:00	15:20	CS03	<b>Progress towards Accurate Predictive Gas Kinetics</b> <i>W. Green,</i> Dept. of Chem. Eng., Massachusetts Institute of Technology, Cambridge, US
15:20	15:40	CS04	<b>Prompt Dissociations of Small Combustion Radicals</b> <i>N. Labbe, R. Sivaramakrishnan, J. Miller, and S. Klippenstein</i> Argonne National Laboratory, USA
15:40	16:10	<b>Tea Break</b>	

## ELEMENTARY PROCESSES

16:10	16:30	EP05	<b>Analysis of <math>\text{NH}_2 + \text{H}_2\text{O}_2 \rightleftharpoons \text{NH}_3 + \text{HO}_2</math> and <math>\text{NH}_2\text{O} + \text{O}_2 \rightleftharpoons \text{HNO} + \text{HO}_2</math> Kinetics and Modeling</b> <i>I. Alecu, Y. Gao, Y. Song, H. Hashemi, J. Munkholt Christensen, C. Zou, P. Marshall, and P. Glarborg</i> Department of Chemistry, University of North Texas, US
16:30	16:50	EP06	<b>Activation Energies for the Reaction Rates of Muonium with Alkanes: the <math>\text{Mu} + \text{C}_3\text{H}_8 \rightarrow \text{MuH} + \text{C}_3\text{H}_7</math> Reaction</b> <i>D. Fleming, S. Cottrell, and J. Peck</i> STFC Rutherford Appleton Laboratory, Harwell Campus, UK
16:50	17:10	EP07	<b>The impact of oxygen encounter complexes on photophysics of molecular oxygen and some other atmospheric molecules</b> <i>A. Pyryaeva, V. Goldort, A. Kochubei, and A. Baklanov</i> Voevodsky Institute of Chemical Kinetics and Combustion Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russian Federation

## ATMOSPHERIC CHEMISTRY

17:10	17:30	AC10	<b>Water enhancement of OH recycling pathways in isoprene oxidation</b> <i>R. Shannon, and D. Glowacki</i> Department of Chemistry, University of Bristol, UK
17:30	17:50	AC11	<b>Catalytic effect of water on the <math>\text{CH}_3\text{OH} + \text{OH}</math> reaction under quasi-real atmospheric conditions</b> <i>R. Jara Toro, F. Hernández, R. Taccone, S. Lane, and G. Pino</i> INFIQC (UNC-CONICET), Universidad Nacional de Córdoba, Argentina

## 18:00 20:00 POSTER SESSION II

Wednesday 20<sup>th</sup> July

## COMBUSTION CHEMISTRY

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|-------|-------|------|---|
| 09:00 | 09:40 | CC01 | <b>Product Detection and Kinetic Studies of Combustion Intermediates: The Case of the Substituted-Phenyl's Oxidation.</b><br><i>Adam J. Trevitt, Matthew B. Prendergast, John D. Savee, Stephen Blanksby, Craig A. Taatjes, David. L. Osborn, G. da Silva</i><br>University of Wollongong, Australia  |
| 09:40 | 10:00 | CC02 | <b>Detection of hydroperoxide chain-branching agents in the low-temperature oxidation of alkanes</b><br><i>Olivier Herbinet, Anne Rodriguez, Zhandong Wang, Fei Qi, Christa Fittschen, Philip R. Westmoreland and Frédérique Battin-Leclerc</i><br>LRGP, CNRS, Université de Lorraine, Nancy, France  |
| 10:00 | 10:20 | CC03 | <b>Temperature- and pressure-dependent competition among reaction pathways from first- and second-O<sub>2</sub> additions in THF oxidation</b><br><i>Ivan O. Antonov, Judit Zádor, Brandon Rotavera, Ewa Papajak, David L. Osborn, Craig A. Taatjes, and Leonid Sheps</i><br>Combustion Research Facility, Sandia National Labs, Livermore, CA, USA |
| 10:20 | 10:40 | CC04 | <b>Experimental and kinetic investigation of n-decane/1,3,5-trimethylbenzene oxidation</b><br><i>Zhen-Yu Tian and Bing-Yin Wang</i><br>Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing, China  |

10:40    11:10    **Tea Break**

## COMPLEX SYSTEMS

- |       |       |      |   |
|-------|-------|------|---|
| 11:10 | 11:30 | CS05 | <b>Conceptual simplification of mechanism complexity: a new paradigm for understanding the tropospheric ozone budget</b><br><i>P. Edwards, and M. Evans</i><br>Wolfson Atmospheric Chemistry Laboratories, Department of Chemistry, University of York, UK                        |
| 11:30 | 11:50 | CS06 | <b>Atmospheric evolution of individual organic compounds: an explicit modeling of organic species sources and sinks</b><br><i>M. Camredon, R. Valorso, G. Siour, S. La, V. Lannuque, and B. Aumont</i><br>LISA, Universités Paris-Est Créteil et Université Paris Diderot, France |
| 11:50 | 12:10 | CS07 | <b>Modelling and Measuring Silane Gaseous Growth Pathways in Pilot-Scale Silicon Production Reactors</b><br><i>T. Preston, G. Wyller, H. Klette, Ø. Nordseth, W. Filtvedt, E. Marstein, D. Lindholm, and T. Mongstad</i><br>Institute for Energy Technology, Kjeller, Norway      |
| 12:10 | 12:30 | CS08 | <b>A computational approach to the kinetics and dynamics of energy flow in large gas volumes</b><br><i>A. McCaffery</i><br>Department of Chemistry, University of Sussex, UK  |

**PACKED LUNCH, EXCURSIONS & FREE EVENING IN YORK**

Thursday 21<sup>st</sup> July

## ATMOSPHERIC CHEMISTRY

- |       |       |      |  |
|-------|-------|------|--|
| 09:00 | 09:40 | AC02 | <b>Atmospheric chemistry at the ocean surface: Connecting the laboratory to the field</b><br><i>L. Carpenter, S. Swift, X. Pang, A. Lewis, A. Saint, M. Shaw, D. Stone, S. Arnold, D. Heard, D. Cryer, T. Ingham, H. Walker, and L. Whalley</i><br>Wolfson Atmospheric Chemistry Laboratories, Department of Chemistry, University of York, UK |
| 09:40 | 10:00 | AC12 | <b>Estimating N<sub>2</sub>O<sub>5</sub> uptake coefficients using ambient measurements of N<sub>2</sub>O<sub>5</sub>, ClNO<sub>2</sub> and particle properties</b><br><i>J. Crowley, G. Phillips, J. Thieser, M. Tang, N. Sobanski, J. Fachinger, F. Drewnick, and J. Lelieveld</i><br>Max-Planck-Institute for Chemistry, Mainz, Germany     |
| 10:00 | 10:20 | AC13 | <b>Production of OH from Organic Peroxy Radical Photolysis: Absorption Cross-Sections, Quantum Yields, and Atmospheric Implication</b><br><i>R. Hansen, T. Lewis, L. Graham, M. Blitz, D. Heard, P. Seakins, and L. Whalley</i><br>School of Chemistry, University of Leeds, UK  |
| 10:20 | 10:40 | AC14 | <b>Rate coefficient for the OH radical reaction with HONO<sub>2</sub> under UT/LS conditions</b><br><i>F. Winiberg, Y. Liu, and S. Sander</i><br>Jet Propulsion Laboratory, California Institute of Technology, US   |

10:40    11:10    **Tea Break**

## COMBUSTION CHEMISTRY

- |       |       |      |   |
|-------|-------|------|---|
| 11:10 | 11:30 | CC05 | <b>Low-Temperature Oxidation studies of Butanone</b><br><i>R. Caravan, B. Rotavera, K. Ramasesha, D. Osborn, and C. Taatjes</i><br>Combustion Research Facility, Sandia National Laboratories, Livermore, US  |
| 11:30 | 11:50 | CC06 | <b>Development of a Computational Chemical Kinetic Model for Cyclopentanone Combustion: H-atom Abstraction and Radical Decomposition</b><br><i>C-W. Zhou, J. Simmie, W. Pitz, and H. Curran</i><br>Combustion Chemistry Centre, National University of Ireland Galway, Ireland                                |
| 11:50 | 12:10 | CC07 | <b>High-Temperature Shock Tube Kinetic Study for the Branching Ratios of Isobutene + OH Reaction</b><br><i>F. Khaled, B. Giri, and A. Farooq</i><br>Clean Combustion Research Center, Physical Science and Engineering Division, King Abdullah University of Science and Technology, Saudi Arabia             |
| 12:10 | 12:30 | CC08 | <b>Implications of Radical Ring-Opening Reactions on Ketohydroperoxide Formation: Cyclohexane and Tetrahydropyran</b><br><i>B. Rotavera, R. Caravan, K. Ramasesha, I. Antonov, J. Zádor, L. Sheps, D. Osborn, and C. Taatjes</i><br>Combustion Research Facility, Sandia National Laboratories, Livermore, US |

12:30    14:00    **LUNCH**

## NANOPARTICLES AND AEROSOLS

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|-------|-------|------|--|
| 14:00 | 14:40 | NA01 | <b>Does the physical phase of organic aerosols matter when atmospheric processes are considered?</b><br><i>A. Virtanen, A. Pajunoja, T. Yli-Juuti, M. Ehn and I. Riipinen</i><br>Department of Applied Physics, University of Eastern Finland, Kuopio, Finland   |
| 14:40 | 15:00 | NA02 | <b>Molecular-level measurement and modelling of heterogeneous chemistry in organic aerosols</b><br><i>P. Gallimore, P. Griffiths, F. Pope, and M. Kalberer</i><br>Department of Chemistry, University of Cambridge, UK   |
| 15:00 | 15:20 | NA03 | <b>Heterogeneous reaction of HO<sub>2</sub> with airborne TiO<sub>2</sub> particles, production of HOx by UV-irradiated photocatalytic airborne TiO<sub>2</sub> particles and implications for climate change mitigation strategies</b><br><i>D. Moon, T. Ingham, G. Taverna, C. Canto, L. Whalley, M. Baeza-Romero, P. Seakins, M. Chipperfield, and D. Heard</i><br>School of Chemistry, University of Leeds, UK |
| 15:20 | 15:40 | NA04 | <b>Detailed soot modelling in laminar methane flames</b><br><i>D. Aubagnac-Karkar, A. El Bakali, and P. Desgroux</i><br>Laboratoire PC2A, UMR CNRS, Villeneuve d'Ascq, France  |
| 15:40 | 16:10 | NA05 | <b>Low temperature reaction kinetics of molecular cluster formation of interest for planetary atmospheres</b><br><i>J. Bourgalais, V. Roussel, M. Capron, A. Bénidar, A. Jasper, S. Klippenstein, L. Biennier, and S. Le Picard</i><br>Institut de Physique de Rennes, CNRS-Université de Rennes 1, France   |

16:10 16:30 Tea Break

### *Symposium photo*

## POLANYI LECTURE

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|-------|-------|--|
| 17:30 | 18:15 | <b>Kinetics of Free Radical Catalytic Photochemistry: Mapping the Molecular Scale to the Global Scale in the Context of Climate Change.</b><br><i>James G. Anderson</i><br>Department of Chemistry and Chemical Biology, Harvard University, Cambridge, US |
|-------|-------|--|

## SYMPOSIUM BANQUET

- |       |       |  |
|-------|-------|--|
| 18:15 |       | <b>Depart by coach for the National Railway Museum</b> |
| 19:00 | 23:30 | <b>Gala Banquet at the National Railway Museum</b>     |

Friday 22<sup>nd</sup> July - DEPART