

20th International Symposium on Gas Kinetics, Manchester, 20 – 25th July 2008

Day 1: Monday 21st July

0850	Opening Remarks and Welcome. Gas Kinetics Group Chairman and Conference Organisers
Session 1	Dynamics <i>Chair: Dr Martin Levy</i>
0900	Plenary: "Probing Radical Intermediates of Bimolecular Reactions" <i>Professor Laurie Butler</i>
0950	Crossed molecular beam reactive scattering of sulfur atoms: The reaction dynamics of S(¹ D) + C ₂ H ₂ and S(¹ D) + C ₂ H ₄ <i>F. Leonori, R. Petrucci, N. Balucani, K. H. Hickson, W. D. Geppert, M. Hamberg, M. Rosi and P. Casavecchia</i>
1010	Speed Dependent Rotational Angular Momentum Polarization of the O ₂ (a ¹ Δ _g) fragment following Ozone Photolysis in the Hartley Band <i>S. J. Horrocks, G. A. D. Ritchie, T. R. Sharples</i>
1030	Transition State Theory for Roaming Radicals <i>Stephen J. Klippenstein, Yuri Georgievskii, and Lawrence B. Harding</i>
1050	Coffee (Chemistry Foyer)
Session 2	Dynamics (continued) <i>Chair: Dr Matt Costen</i>
1110	Absolute HCO quantum yields for the radical channel of HCHO photolysis measured by the direct detection of the HCO photoproduct <i>S. C. Smith, P. Gorroategui Carbajo, A. L. Holloway, C. A. Smith, F. D. Pope and A. J. Orr-Ewing</i>
1130	The Pressure and Temperature Dependence of Glyoxal Photochemistry in the 382-414 nm Region <i>Robert J. Salter, Mark A. Blitz, Michael J. Pilling, Dwayne E. Heard and Paul W. Seakins</i>
1150	Formaldehyde detection at 325 nm with sub-Doppler resolution <i>Martin Crow, Sarah Taylor, Graham Richmond, Rob Peverall, Grant A. D. Ritchie and Gus Hancock</i>
1210	Overview: Constructing an object-oriented code: MESMER <i>Chi-Hsiu Liang, David Glowacki, Michael Pilling, Struan Robertson, Chris Morley</i>
1220	Conference Photograph (Chemistry Building steps)
1240	Lunch in Alan Turing Building Atrium.
Session 3	Atmospheric Chemistry <i>Chair: Dr Carl Percival</i>
1350	Plenary: "Gas Kinetics in the Solar System" <i>Professor Richard Wayne</i>
1440	Hydroxyethyl-peroxy Radicals in Atmospheric and Combustion Chemistry: Kinetics of the Acetaldehyde and Vinyl Alcohol + HO ₂ Reactions <i>Gabriel da Silva and Joseph W. Bozzelli</i>
1500	Reactivity of Unsaturated Oxygenated VOC with NO ₃ Radical <i>B. Picquet-Varrault, M. Scarfogliero and J-F. Doussin</i>
1520	Rate coefficients for the reaction of OH with Methyl Glyoxal, and NO ₃ with Glyoxal and Methyl Glyoxal <i>Ranjit K. Talukdar, Lei Zhu, Karl Feierabend and James B. Burkholder</i>
1540	Coffee in Chemistry Building Foyer
Session 4	Atmospheric Chemistry <i>Chair: Andrew Horn</i>
1600	Plenary: "From the Poles to the Tropics: Field Measurements of Free Radicals, a Link Between Chemical Kinetics and the Atmosphere" <i>Professor Dwayne Heard</i>
1650	Investigations on the photolysis of ortho-nitroalkylated aromatics: A new gas phase source of HONO <i>I. Bejan, G. Villena Tapia, I. Barnes, Th. Benter, P. Wiesen and J. Kleffmann</i>
1710	Recent laboratory results on the atmospheric chemistry of carbonyl molecules and carbonyl free radicals <i>Sándor Dóbe</i>
1730	Application of the Master Chemical Mechanism (MCM) in assessing photo-oxidation of emissions from well defined refinery sources <i>Sean Ho Man Lam, Sam Saunders, Marisa Ioppolo-Armanios and Allan McKinley</i>
1800	Poster Session 1: Chemistry Building Foyer With wine reception and demonstration from <i>Liang et al.</i>
2000	Close

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Day 2: Tuesday 22nd July

Session 5	Energy Transfer <i>Chair:</i>
0900	Plenary: "Collisional Rotational and Vibrational Energy Relaxation in Diatomic Free Radicals" <i>Professor Paul Dagdigan</i>
0950	The Influence of Amplified Spontaneous Emission in Collisional Energy Transfer Studies Exemplified by E→D Transfer in I ₂ . <i>Robert J. Donovan, Vadim A. Alekseev, Trevor Ridley and Kenneth P. Lawley</i>
1010	Reaction mechanisms involving singlet methylene ¹ CH ₂ : non-reactive, reactive and combinations thereof. <i>Mark Blitz, Kelly Gannon, Mike Pilling and Paul Seakins</i>
1030	Determination of collisional energy transfer distributions in highly vibrationally excited molecules: mesitylene and stilbene studies on the influences of large donor sizes <i>Matthias Hollerbach, Thomas Lenzer and Klaus Luther</i>
1050	Coffee (Chemistry Foyer)
Session 6	Combustion <i>Chair:</i>
1110	Plenary: "On the reactivity of small carbon-containing radicals in combustion" <i>Professor Sean Carl</i>
1200	Chain branching and termination in oxidation of n-alkanes: reaction of n-pentyl radical with O ₂ , isomerization and association with a second oxygen molecule <i>Rubik Asatryan and Joseph W. Bozzelli</i>
1220	Oxidation of CH ₄ /C ₂ H ₆ mixtures under oxy-fuel conditions <i>J. Giménez, A. Millera, R. Bilbao, M.U. Alzueta</i>
1240	Lunch in Alan Turing Building Atrium.
Session 7	Combustion Chemistry (cont.) <i>Chair:</i>
1400	Modeling and Experimental study of OH-formation in the Cyclohexyl + O ₂ reaction at elevated pressures <i>Ravi X. Fernandes, Judit Zádor, Leonard E. Jusinski and Craig A. Taatjes</i>
1420	The reaction of vinyl radical with alkenes: measured rates and predicted pressure-dependent product distributions. <i>C. Franklin Goldsmith, Huzeifa Ismail, Paul R. Abel, William H. Green</i>
1440	Shock Tube Study of Cyclohexane and 1-Hexene Decomposition <i>J. H. Kiefer, K. S. Gupte, L. B. Harding and S. J. Klippenstein</i>
1500	Shock tube measurements of high temperature rate constants for OH + cycloalkanes <i>R. Sivaramakrishnan and J. V. Michael</i>
1540	Coffee in Chemistry Building Foyer
Session 8	Combustion Chemistry (cont.) <i>Chair:</i>
1600	Reaction paths, thermochemical properties and kinetic analysis for the reaction of secondary vinylic 1,2/1,3 diene radicals with O ₂ <i>L. Rutz, G. da Silva, J. Bozzelli and H. Bockhorn</i>
1620	A Diaphragm-less Shock Tube/Laser Schlieren Study of the Dissociation of C ₆ H ₅ I and the Self Reaction of C ₆ H ₅ Radicals <i>Robert S. Tranter</i>
1640	A New Method for Determining Mechanisms and Rate Constants for the Oxidation of Fuel Radicals Under Combustion Conditions <i>Wing Tsang</i>
1700	From PAH molecules to carbonaceous nanoparticles in the laboratory, in soot formation, and in space <i>Hassan Sabbah</i>
1900	Civic Reception from the City of Manchester Manchester Town Hall
2000	Close

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Day 3: Wednesday 23rd July

Session 9	Extreme Environments <i>Chair:</i>
0900	Plenary: "Ion-molecule reaction dynamics at sub-Kelvin temperatures" <i>Professor Tim Softley</i>
0950	Pushing the frontiers of low temperature reaction kinetics <i>Ian R. Sims, Sébastien Morales, Coralie Berteloite, Sebastien D. Le Picard, André Canosa and Bertrand R. Rowe</i>
1010	VUV Photoionization of jet-cooled radicals using synchrotron radiation and electron/ion coincidences <i>G. A. Garcia</i>
1030	FTIR Studies of Pre-ignition Products Formation and Mechanisms in the Reaction of Nitric Acid with Ionic Liquids <i>Ghanshyam L. Vaghjiani, S. D. Chambreau and C. J. Gallegos</i>
1050	Coffee (Chemistry Foyer)
Session 10	General Kinetics <i>Chair:</i>
1110	OH recycling via the reactions of peroxy radicals <i>Terry J. Dillon and John N. Crowley</i>
1130	Determination of the Low Pressure Three-Body Rate Constant for $\text{NH}_2(\text{X}^2\text{B}_1) + \text{NH}_2(\text{X}^2\text{B}_1) \rightarrow \text{Products}$ in CF_4 , N_2 and Ar at 293 K. <i>Mi-Kyung Bahng and R. Glen Macdonald</i>
1150	Study of the self and cross reactions of resonance-stabilized radicals by synchrotron photoionization mass spectrometry <i>Talitha M. Selby, David Osborn, Craig A. Taatjes, and Giovanni Meloni</i>
1210	On the direct detection of HO_2 radicals after 248nm irradiation of benzene C_6H_6 in the presence of O_2 by laser photolysis / cw-CRDS <i>Christa Fittschen, Alina Aluculesei, Coralie Schoemacker and Alexandre Tomas</i>
1230	Overview to Poster presentation: Modeling butanol combustion: Automated mechanism generation utilizing the Process Informatics Model (PrIME) data depository <i>Michael R. Harper and William H. Green</i>
1240	Depart in buses for Tours / Packed lunches will be provided.
1800	Poster session II, Chemistry Building Foyer Wine reception.
2000	Close

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Day 4: Thursday 24th July

Session 11	Atmospheric Chemistry <i>Chair:</i>
0900	Plenary: "Heterogeneous Atmospheric Chemistry: Concepts, Methods and Results" <i>Professor Reinhard Zellner</i>
0950	Generation and detection of OH radicals in the Leeds HIRAC chamber <i>T. Malkin, D. Glowacki, A. Goddard, K. Hemavibool, T. Ingham, D. Heard, M. Pilling and P. Seakins</i>
1010	Mechanisms for the Formation of Organic Acids in Terpene Ozonolysis <i>Yan Ma, Rachel Porter and George Marston</i>
1030	Structure-activity relationship (SAR) for the prediction of gas-phase ozonolysis rate coefficients: an extension towards heteroatomic olefinic species. <i>Max R. McGillen, Carl J. Percival, Alex T. Archibald and Dudley E. Shallcross</i>
1050	Coffee (Chemistry Foyer)
Session 12	General Kinetics <i>Chair:</i>
1110	Characterisation of Ionic Emissions from Alkali Ion Sources and Long Term Removal of Impurities in a Lithium Attachment Mass Spectrometer <i>M Benvezzar and R S Mason</i>
1130	Recombination Reactions of SiH ₂ with a Series of Alkenes: Experiments and Modelling <i>Gernot Friedrichs, Mustapha Fikri, Friedrich Temps</i>
1150	Vibrational nonequilibrium of HO ₂ radical in the reaction of hydrogen with oxygen; 1000 < T < 1200 K <i>Oleg V. Skrebkov, Sergey P. Karkach</i>
1210	Competing reactions in the atmospheric conversion of SO ₂ into H ₂ SO ₄ <i>Núria González-García and Matthias Olzmann</i>
1240	Lunch in Alan Turing Building Atrium.
Session 13	Dynamics <i>Chair:</i>
1400	Plenary: "Significant OH Radical Reactions in the Lower Atmosphere: A New View" <i>Professor Marsha Lester</i>
1450	Collisional Evolution of Rotational Orientation and Alignment of OH with simple partners <i>Grant Paterson, Sarandis Marinakis, Matthew L. Costen and Kenneth G. McKendrick</i>
1510	Theoretical Studies of the Reactions of OH+NH <i>Lawrence B. Harding, Stephen J. Klippenstein and Stephen K. Gray</i>
1530	Non-adiabatic processes in gas-phase reactions <i>Wenfang Hu, György Lendvay, Biswajit Maiti and George C. Schatz</i>
1550	Back to Halls of Residence
1700	Polanyi Lecture and Medal Presentation 2008 Lecture Theatre, <i>Professor Piergiorgio Casavecchia</i>
1900	Conference Dinner Old Trafford Football Ground
2300	Close

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Day 5: Friday 25th July

Session 14	Heterogeneous Processes <i>Chair:</i>
0930	Plenary: "Modelling the formation of secondary organic aerosol" <i>Professor Dudley Shallcross</i>
1020	Interaction of RC(O)OH, H ₂ O ₂ and HO ₂ with Ice Surfaces <i>Nicolas Pouvesle, Matthias Kippenberger, Philipp v. Hessberg and John N. Crowley</i>
1040	An FTIR study of the ozonolysis reactions of 2-butenedioic acid isomer aerosols <i>Juan J. Nájera, Deborah Last, Carl J. Percival and Andrew B. Horn</i>
1100	Coffee (Chemistry Foyer)
Session 15	Heterogeneous Processes (cont.) <i>Chair:</i>
1120	Photodesorption Processes involving Model Interstellar Ices <i>J. D. Thrower, D. J. Burke, M. P. Collings, A. Dawes, P. J. Holtom, F. Jamme, P. Kendall, W. A. Brown, I. P. Clarke, H. J. Fraser, M. R. S. McCoustra, N. J. Mason and A. W. Parker.</i>
1150	Dynamics of Inelastic Scattering of OH Radicals from Inert and Reactive Liquid Surfaces <i>Carla Waring, Paul A. J. Bagot, Matthew L. Costen and Kenneth G. McKendrick</i>
1210	Numerical Kinetic Model of Particle Nucleation and Growth: Application to Rapid Expansion of Supercritical Solutions <i>Evgeni N. Chesnokov, Takuya Matsunaga, Andrei V. Chernyshev, and Lev N. Krasnoperov</i>
1230	Closing Remarks.