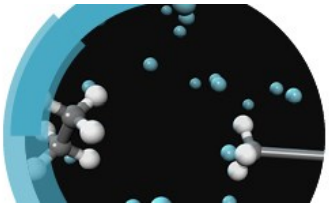
Unimolecular reactions

Faraday Discussion



22–24 June 2022
Oxford, United Kingdom

Wednesday 22 June 2022 (all timings are in BST)

11:30	Registration and refreshments
12:00	Lunch
12:45	**Welcome and introductions** Struan Robertson, *Chair of Scientific Committee*
12:55	**Outline of Discussion format** *Royal Society of Chemistry Publishing Editors*
13:00	**Introductory lecture** (Session chair: Struan Robertson) Stephen J Klippenstein *Argonne National Laboratory, USA*
14:00	Comfort break (no refreshments)
	Session 1: Collisional energy transfer (Session chairs: György Lendvay and Struan Robertson)
14:15	**Predicting third-body collision efficiencies for water and other polyatomic baths** Ahren Jasper* *Argonne National Laboratory, USA*
14:20	**Rotational energy transfer kinetics of optically centrifuged CO molecules investigated through transient IR spectroscopy and master equation simulations** Amy Mullin *University of Maryland, USA*
14:25	**Theoretical Studies on Lennard-Jones Parameters of Benzene and Polycyclic Aromatics Hydrocarbons** Xiaoqing You* *Tsinghua University, China*
14:30	Discussion
15:45	Break
	Session 2: The reaction step (Session chairs: Mike Pilling and Andrew Orr-Ewing)
16:15	**Statistical Theory for the Reaction N + OH ? NO + H Thermal Low-Temperature Rate Constants** Jürgen Troe* *University of Göttingen, Germany*
16:20	**Crossed-beam and theoretical studies of multichannel nonadiabatic reactions: branching fractions and role of intersystem crossing for O(3P)+1,3-butadiene** Carlo Cavallotti *Politecnico di Milano, Italy*
16:25	**Influence of second-order saddles on reaction mechanisms** Upakarasamy Lourderaj *NISER, India*
16:30	Discussion
17:45	Lightning presentations (by invitation of the Scientific Committee)
18:15	Poster session and wine reception

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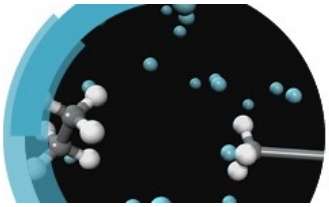

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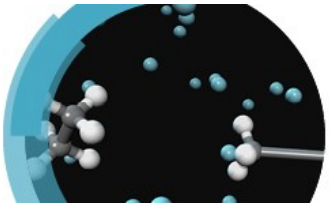
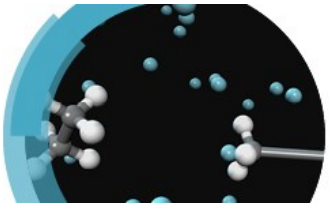
Thursday 23 June 2022 (all timings are in BST)

	Session 2: The reaction step (continued) (Session chairs: David Clary and Claire Vallance)
09:00	**Improved microcanonical instanton theory** Joseph Lawrence *ETH Zürich, Switzerland*
09:05	**Unimolecular Dissociation Dynamics of Electronically Excited HCO( ): Rotational Control of Nonadiabatic Decay** Hua Guo *University of New Mexico, USA*
09:10	Discussion
10:00	Break
10:30	**Quantum resonances and roaming dynamics in formaldehyde photodissociation** Arthur Suits *University of Missouri, USA*
10:35	**Probing the dynamics of the photo-induced decarboxylation of neutral and ionic pyruvic acid** Majdi Hochlaf *Université Paris-Est Marne-La-Vallée, France*
10:40	**Stereoisomer-dependent unimolecular kinetics of 2,4-dimethyloxetane peroxy radicals** Anna Doner *University of Georgia, USA*
10:45	Discussion
12:00	Lunch
	Session 3: The Master equation (Session chairs: Nick Green and Judit Zador)
13:00	**Dissociation-Induced Depletion of High-Energy Reactant Molecules as a Mechanism for Pressure-Dependent Rate Constants for Bimolecular Reactions** Mike Burke *Columbia University, USA*
13:05	**Examining the Accuracy of Methods for Obtaining Pressure Dependent Rate Coefficients** William Green *MIT, USA*
13:10	**Mechanism, Thermochemistry, and Kinetics of the Reversible Reactions: C¬2H3 + H2 ⇌ C2H4 + H ⇌ C¬2H5** Thanh Lam Nguyen *University of Florida, USA*
13:15	**Master Equation Study of Hydrogen Abstraction from HCHO by OH Via a Chemically Activated Intermediate** Xuefei Xu* *Tsinghua University, China*
13:20	Discussion
15:00	Break
15:30	**Master Equation Modelling of Non-equilibrium Chemistry in Stellar Outflows** John Plane *University of Leeds, UK*
15:35	**Modelling Reaction Kinetics of Distonic Radical Ions: A Systematic Investigation of Phenyl-type Radical Addition to Unsaturated Hydrocarbons** Adam Trevitt



	University of Wollongong, Australia
15:40	**The Merit of Pressure Dependent Kinetic Modelling in Steam Cracking** Jeroen Aerssens *Ghent University, Belgium*
15:45	**Cleavage of an aromatic ring and radical migration** *Alexander Mebel** *Florida International University, USA*
15:40	Discussion
17:30	Close of sessions
18:30	Pre-dinner drinks
19:00	Conference dinner



Friday 24 June 2022 (all timings are in BST)

	Session 4: Impact of Lindemann and related theories (Session chair: Dwayne Heard and Paul Seakins)
09:00	**Energy-resolved and time-dependent unimolecular dissociation of hydroperoxyalkyl radicals (•QOOH)** Marsha Lester *University of Pennsylvania, USA*
09:05	**Improved Computational Modeling of the Kinetics of the Acetylperoxy + HO_2 Reaction** Keith Kuwata *Macalester College, USA*
09:10	**An Experimental and Computational Study of the Reaction between Pent-3-en-2-yl Radicals and Oxygen Molecules: Switching from Pure Stabilisation to Pure Decomposition with Increasing Temperature** Arkke Eskola *University of Helsinki, Finland*
09:15	Discussion
10:30	Break
11:00	**Unimolecular isomerisation of 1,5-hexadiyne observed by threshold photoelectron photoion coincidence spectroscopy** David Osborn *Sandia National Laboratories, USA*
11:05	**The unimolecular decomposition of dimethoxymethane: channel switching as a function of temperature and pressure** Matthias Olzmann *Karlsruhe Institute of Technology (KIT), Germany*
11:10	**Electron-induced dissociation dynamics studied using covariance-map imaging** David Heathcote *University of Oxford, UK*
11:15	Discussion
12:30	**Concluding remarks lecture** (Session Chair: Struan Robertson) William H Green *MIT, USA*
13:10	**Acknowledgements and poster prize presentation** Struan Robertson
13:15	**Close of meeting and lunch**

*Presenting virtually