

<b>Monday, May 22</b>			
08:00	<b>Registration</b>		
08:20	<b>Welcome and Official Opening</b>		
08:30-09:20	<b>Plenary 1</b> <b>Active Thermochemical Tables: A Divertimento in Thermochemistry for the 21st Century</b> Branko Ruscic, Argonne National Laboratory, USA  <i>Chair: Margaret S. Wooldridge, University of Michigan, USA</i>		
<b>Move to parallel presentations</b>			
	<b>Session A1 (Illinois A/B)</b> Chairs: Judit Zádor Phillip Westmoreland	<b>Session B1 (Cardinal)</b> Chairs: Brandon Rotavera Nabiha Chaumiex	<b>Session C1 (White Oak A/B)</b> Chairs: Ravi Fernandes Steven Pyl
09:30	A1-01 MUQ002 D. H. Bross, L. B. Harding, B. Ruscic <b>Partition functions for non-rigid molecules</b>	B1-01 COM019 S. Thion, C. Togbé, Z. Serinyel, G. Dayma, P. Dagaut <b>A chemical kinetic study of dibutyl-ether oxidation in a jet-stirred reactor</b>	C1-01 CHE001 K. Li, K. Liu, H. Lin <b>Catalytic combustion of lean methane assisted by electric field over Pd-Ce-Zr catalyst at low temperature</b>
09:55	A1-02 COM018 G. Dayma, S. Thion, M. Lailliau, Z. Serinyel, P. Dagaut <b>On the influence of the position of the ester function for biodiesel combustion</b>	B1-02 COM001 Z. Wang, B. Chen, K. Moshhammer, D. M. Popolan-Vaida, D. Vuilleumier, T. Tao, L. Ruwe, E. Bräuer, N. Hansen, P. Dagaut, S. M. Sarathy <b>Probing cool flame intermediates from jet-stirred reactor auto-oxidation of alkanes</b>	C1-02 CHE002 S. P. Pyl, M. R. Harper, R. J. Quann <b>Heavy oil hydroconversion: Modeling composition and chemistry</b>
10:20	<b>Coffee Break</b>		
10:50	A1-03 GPH015 C. Cavalotti, M. Pelucchi, Y. Georgievskii, S. J. Klippenstein <b>From electronic structure calculations to temperature and pressure dependent rate constants: a new computational environment</b>	B1-03 TGP007 S. Y. Mohamed, A. C. Davis, M. J. Al Rashidi, S. M. Sarathy <b>High-pressure rate rules for hydroperoxyalkylperoxy radicals isomerization reaction</b>	C1-03 CHE003 Y. Li, Y. Wang, D. Wang <b>Hydrocarbon pool co-catalyst in the methanol-to-olefins reactions also causes deactivation</b>
11:15	A1-04 GPH032 L. Lei, M. P. Burke, <b>Exploring representations of multi-component pressure dependence of complex-forming reactions in mixtures</b>	B1-04 COM030 A. J. Eskola, I. O. Antonov, L. Sheps, R. L. Caravan, D. L. Osborn, C. A. Taatjes <b>Kinetic measurements and simulations of product formation in neopentane and n-pentane oxidation experiments: investigating autoignition chemistry</b>	C1-04 CHE005 L.-N. Wu, Z.-Y. Tian <b>A comparative DFT study on the CO oxidation mechanism on CuO (111), Cu<sub>2</sub>O (111), Co<sub>3</sub>O<sub>4</sub> (110), and Mn<sub>3</sub>O<sub>4</sub> (110) surfaces</b>

<b>Monday, May 22 (continued)</b>			
11:40	A1-05 TGP010 W. H. Green, A. Grinberg Dana, R. Gillis, Y. Chung, B. Slakman, R. H. West <b>Challenges in predicting chemical kinetics</b>	B1-05 COM036 Y. Zhang, A. Kéromnès, H. J. Curran <b>An experimental and kinetic modelling study of ethanol/DME mixtures auto-ignition</b>	C1-05 CHE008 R. E. Smith, K. Brezinsky, M. J. Castaldi <b>Elucidation of the catalytic partial oxidation of methane reaction sequence via catalytic shock tube testing</b>
12:05	A1-06 COM034 E. S. Blurock, M. de Joannon, G. Skevis <b>Towards efficient data exchange within the Combustion Community</b>	B1-06 COM031 K. Zhang, C. Conroy, J. Bugler, W. J. Pitz, H. J. Curran, M. Mehl, S. Wagnon, G. Kukkadapu <b>An experimental and kinetic modeling study of n-butylcyclohexane and its mixture with n-heptane</b>	C1-06 POL001 J. C. Hernández-Ortiz, P. Van Steenberge, J. N. E. Duchateau, K. Remerie, C. Toloza, A. L. Vaz, F. Schreurs, M.-F. Reyniers, G. B. Marin, D. R. D'hooge <b>A tracking of the complete microstructural evolution of individual polymer chains during polymer modification reactions</b>
12:30	<b>Lunch</b>		
14:00 14:50	<b>Plenary 2</b>  <b>How Charge Transforms Chemical Bonds at Solid-Liquid Interfaces</b> Tanja Čuk, University of California, Berkeley, USA  <i>Chair: Kevin van Geem, University of Ghent, Belgium</i>		
	<b>Move to parallel sessions</b>		
	<b>Session A2 (Illinois A/B)</b> Chairs: Subith Vasu Michael Burke	<b>Session B2 (Cardinal)</b> Chairs: Franklin Goldsmith John Barker	<b>Session C2 (White Oak A/B)</b> Chairs: Arkke Eskola Luc Vereecken
15:00	A2-01 COM026 N. D. Harms, B. L. Slakman, J. Cain, R. H. West <b>Automated transition state theory calculations of abstraction by OOH from novel biofuels</b>	B2-01 GPH034 Y. Li, C.-W. Zhou, H. J. Curran <b>Theoretical kinetic study of H- atom addition to 1,3-butadiene and relative reactions on the C<sub>4</sub>H<sub>7</sub> potential</b>	C2-01 TOT002 T. Frankcombe <b>Dissociation of methane on catalytic surfaces: 15D dynamics from DFT</b>
15:25	A2-02 TGP004 J. Zádor, M. D. Fellows, J. A. Miller <b>Initiation reactions in acetylene pyrolysis</b>	B2-02 COM009 C. Huang, B. Yang, F. Zhang <b>Initiation mechanism of 1,3- butadiene and its effect on soot precursors</b>	C2-02 TOT003 N. Kumioshi, K. Anzai, A. Fuwa <b>Estimation of rate coefficients for simulation of silicon epitaxial growth processes</b>
15:50	Coffee Break		

<b>Monday, May 22 (continued)</b>			
16:20	A2-03 COM013 N. Atef, G. Issayev, Z. Wang, A. Farooq, S. M. Sarathy <b>Shock tube ignition and detailed kinetic modelling of 2,2,3-trimethylbutane</b>	B2-03 GPH024 J. P. A. Lockhart, C. F. Goldsmith, J. B. Randazzo, B. Ruscic, R. S. Tranter <b>A detailed study of the pyrolysis of C<sub>4</sub>H<sub>6</sub> isomers: experiment and theory</b>	C2-03 GPH033 P. Marshall <b>Formation of sulfuric acid from equilibrium and non-equilibrium sulfur trioxide</b>
16:45	A2-04 GPH020 M. Pelucchi, C. Cavallotti, T. Faravelli, S. J. Klippenstein <b>Ab initio and kinetic modelling study of toluene oxidation</b>	B2-04 GPH002 J. Lopez, Z. Loparo, O. Pryor, S. Barak, S. Vasu <b>Kinetics of 1,3-butadiene oxidation at high temperatures in a shock tube</b>	C2-04 ACM002 E. Assaf, C. Schoemaeker, L. Sheps, L. Whalley, D. Heard, C. Fittschen <b>The reaction of RO<sub>2</sub> radicals with OH and its impact in remote environments</b>
17:10	A2-05 GPH030 R. Sivaramakrishnan, S. J. Klippenstein <b>Probing variational effects in the thermal decomposition kinetics of hydroxyalkyl radicals</b>	B2-05 GPH026 J. B. Randazzo, R. S. Tranter <b>The thermal decomposition of organic nitrites and their use as radical precursors</b>	C2-05 TGP006 L. Vereecken, A. Novelli, D. Taraborrelli <b>The concentration of Criegee intermediates in the troposphere</b>
17:35	A2-06 GPH027 T. Speak, L. James, M. Blitz, D. de Jesus Medeiros, P. Seakins, A. Bunkan <b>OH initiated study of the oxidation of N,N'-dimethylformamide: evidence for QOOH+O<sub>2</sub> forming OH</b>	B2-06 COM020 C. F. Goldsmith <b>The decomposition kinetics of HONO and HNO<sub>2</sub></b>	C2-06 TGP002 M. Pfeifle, Y.-T. Ma, A. W. Jasper, W. L. Hase, S. J. Klippenstein <b>Nascent energy of Criegee intermediates: Is the statistical assumption valid for primary ozonide dissociation?</b>
18:00	<b>End of Day</b>		

<b>Tuesday, May 23</b>			
08:00	Registration		
08:25	Daily announcements		
08:30-09:20	Plenary 3		
	<b>Strategies for Collectively Improving the Robustness of Chemical Kinetic Models for Practical Applications in Combustion</b> Alison S. Tomlin, University of Leeds, UK  <i>Chair: Henry J. Curran, NUI Galway, Ireland</i>		
	Move to parallel sessions		
	<b>Session A3 (Illinois A/B)</b> Chairs: Andrea Comandini Zeynep Serinyel	<b>Session B3 (Cardinal)</b> Chairs: Ahren Jasper William Pitz	<b>Session C3 (White Oak A/B)</b> Chairs: Olivier Mathieu Nils Hansen
09:30	A3-01 COM028 M. J. Davis, R. Sivaramakrishnan <b>Global sensitivity analysis of the ignition of a mixture of n-heptane and methylbutanoate</b>	B3-01 MUQ001 M Liu, K. Han, W. H. Green <b>Going bigger: Capturing PAH chemistry in RMG</b>	C3-01 GPH001 P. Sela, S. Peukert, J. Herzler, M. Fikri, C. Schulz <b>High-repetition-rate time-of-flight mass spectrometry and single-pulse shock-tube study of the decomposition of tetramethylsilane</b>
09:55	A3-02 COM023 M. Tao, P. Zhao, A. Laich, P. T. Lynch <b>On the interpretation and correlation of high temperature ignition delays in reactors with varying thermodynamic conditions</b>	B3-02 MUQ004 B. Weber, K. Niemeyer <b>ChemKED: a human- and machine-readable data standard for chemical kinetics experiments</b>	C3-02 GPH016 M. E. Fuller, J. B. Randazzo, R. S. Tranter, <b>Shock tube experimental investigation of pyrolysis of propyl nitrite</b>
10:20	Coffee Break		
10:50	A3-03 COM007 C. Barraza-Botet, M. S. Wooldridge <b>Effects of blends of iso-octane and ethanol on ignition and reaction pathways</b>	B3-03 CFD001 E. S. Blurock <b>Chemconnect2016: Data repository with interconnected searchable network of combustion data</b>	C3-03 GPH023 O. Skrebkov, S. Kostenko, A. Smirnov <b>Inhibition of the hydrogen-oxygen reaction by polyatomic gas admixtures</b>
11:15	A3-04 COM006 S. Richter, T. Kick, M. Braun-Unkhoff, C. Naumann, U. Riedel <b>An experimental and modeling study on isopropanol oxidation - ignition delay time and burning velocity</b>	B3-04 CFD007 D. Combs, B. Akih-Kumgeh <b>Enhancing chemical kinetic simulations through combined chemical Langevin equations and model reduction</b>	C3-04 COM025 C. D. Needham, P. R. Westmoreland <b>F-atom chemistry in a hydrogen-starved tetrafluoropropene flame</b>

<b>Tuesday, May 23 (continued)</b>			
11:40	A3-05 COM035 D. Kang, A. Fridlyand, S. S. Goldsborough, M. Mehl, S. Wagnon, W. J. Pitz, M. J. McNenly <b>Chemical kinetic interactions of ethanol with a full boiling range gasoline and its surrogates at engine conditions</b>	B3-05 CFD008 Y. Wu, P. Pal, S. Som, T. Lu <b>A skeletal chemical kinetic mechanism for gasoline and gasoline/ethanol blend surrogates for engine CFD applications</b>	
12:05	<b>Lunch</b>		
13:30-14:20	<b>Plenary 4</b>  <b>High-accuracy Quantum Chemical Methods for Kinetics: Some Recent Developments</b> John F. Stanton, University of Florida, USA  <i>Chair: Carlo Cavallotti, Politecnico di Milano, Italy</i>		
<b>Move to parallel sessions</b>			
	<b>Session A4 (Illinois A/B)</b> Chairs: Scott Goldsborough Pieter Reyniers	<b>Session B4 (Cardinal)</b> Chairs: Raghu Sivaramakrishnan Peter Glarborg	<b>Session C4 (White Oak A/B)</b> Chairs: Sebastian Peukert Nicole Labbe
14:30	A4-01 CFD002 P. A. Reyniers, D. J. Van Cauwenberge, G. B. Marin, K. M. Van Geem <b>Towards large eddy simulations with detailed kinetics</b>	B4-01 COM002 N. Hansen, A. W. Jasper, K. Moshhammer, H. Wang, Z. Wang, D. M. Popolan-Vaida, P. Dagaut, S. M. Sarathy <b>The low-temperature oxidation of tetrahydrofuran investigated by experiment, theory, and modeling</b>	C4-01 COM008 F. Zhang, C. Huang <b>Kinetic study of methyl oxidation and its impact to methane ignition</b>
14:55	A4-02 CFD004 G. Vaghjiani, S. D. Chambreau, J. G. Reuster, A. H. Kawasaki, C. A. Taatjes <b>Improved pyrolysis micro-reactor design via computational fluid dynamics simulations</b>	B4-02 COM010 B. R. Giri, F. Khaled, M. Szőri, J. R. Barker, A. Farooq <b>A combined experimental and theoretical kinetic study of the reaction of OH radicals with tetrahydropyran</b>	C4-02 GPH010 C. Yan, L. Krasnoperov <b>Reaction of CH<sub>3</sub> radicals with HO<sub>2</sub> over the 292 – 558 K temperature range</b>
15:20	Coffee break		
15:50	A4-03 CFD006 S. R. Kulkarni, L. A. Vandewalle, P. A. Reyniers, K. M. Van Geem, G. B. Marin <b>Computational fluid dynamics simulations of biomass fast pyrolysis in a gas-solid vortex reactor</b>	B4-03 GPH014 M.-W. Chen, B. Rotavera, W. Chao, J. Jr-Min Lin, J. Zádor, C. A. Taatjes <b>Direct measurement of OH and HO<sub>2</sub> formation in R + O<sub>2</sub> reactions of cyclohexane and tetrahydropyran: influence of oxygenation in cyclic hydrocarbons</b>	C4-03 ACH002 M. I. Jacobs, K. R. Wilson <b>Studying the kinetics of reactions in microdroplets using a linear electrodynamic balance</b>

<b>Tuesday May 23 (continued)</b>			
16:15	A4-04 CFD005 C. Druzgalski, S. Lapointe, M. J. McNenly <b>Quantifying reaction rates sensitivity and discoverability in a millimeter-scale flow reactor</b>	B4-04 GPH022 H. Wang, S. M. Sarathy <b>A detailed cyclic ether oxidation mechanism for tetrahydrofuran radicals: A theoretical study</b>	C4-04 GPH031 D. Zaleski, K. Prozument <b>Dynamic time-resolved chirped-pulse rotational spectroscopy of vinyl cyanide photoproducts in a room temperature flow reactor</b>
16:40	A4-05 COM003 Y. Zhang, L. Wang, P. Liu, Z. He, H. Lin <b>Experimental and kinetic study of the effects of CO<sub>2</sub> and H<sub>2</sub>O addition on PAHs formation in laminar premixed C<sub>2</sub>H<sub>4</sub>/O<sub>2</sub>/AR flames</b>	B4-05 COM012 F. Vermeire, H.-H. Carstensen, O. Herbinet, F. Battin-Leclerc, K. Van Geem <b>Experimental and modeling study of the pyrolysis and combustion of dimethoxymethane</b>	C4-05 GPH025 T. Q. Bui, B. J. Bjork, O. H. Heckl, P. B. Changala, B. Spaun, M. Okumura, J. Ye <b>Time-resolved frequency comb measurement of OD + CO reaction kinetics and product branching yields</b>
17:05	<b>End of Oral Presentation</b>		
17:30	<b>Poster Session</b>		
19:00	<b>End of Day</b>		

<b>Wednesday, May 24</b>			
08:00	<b>Registration</b>		
08:25	<b>Daily announcements</b>		
08:30-09:20	<b>Plenary 5</b> <b>Low Temperature Kinetics in Uniform Supersonic Flows: Rate Constants, Branching Ratios and Energy Transfer</b> Ian R. Sims, University of Rennes, France  <i>Chair: Stephen J. Klippenstein, Argonne National Laboratory, USA</i>		
<b>Move to parallel sessions</b>			
	<b>Session A5 (Illinois A/B)</b> Chairs: Feng Zhang Frederik Ossler	<b>Session B5 (Cardinal)</b> Chairs: James Lockhart Kirill Prozument	<b>Session C5 (White Oak A/B)</b> Chairs: Richard West Binod Giri
09:30	A5-01 COM011 A. J. Vervust, M. R. Djokic, S. S. Merchant, A. E. Long, G. B. Marin, W. H. Green, K. M. Van Geem <b>Detailed experimental and kinetic modeling study of the pyrolysis of cyclopentadiene in the presence and absence of ethene</b>	B5-01 GPH003 S. Gudiyella, Z. Buras, T. Chu, I. Lengyel, S. Pannala, W. H. Green <b>A modeling study of high temperature pyrolysis</b>	C5-01 CHE004 K. Alexopoulos, M. John, M.-F. Reyniers, G. B. Marin <b>Decoding the complexity of zeolite catalyzed alcohol dehydration by microkinetic modeling</b>
09:55	A5-02 GPH004 Z. J. Buras, T.-C. Chu, A. Jamal, N. Yee, W. H. Green <b>Phenyl radical + propene as a prototypical reaction surface for aromatic-catalyzed resonance stabilized radical formation</b>	B5-02 GPH012 V. Burkle-Vitzthum, R. Bounaceur, P.-M. Marquaire <b>Kinetic model of the thermal cracking of 78 n- and iso-alkanes in the saturated fraction of oils</b>	C5-02 CHE006 C. F. Goldsmith, R. H. West <b>Computer generated microkinetics: a case study for methane dry reforming</b>
10:20	<b>Coffee Break</b>		
10:50	A5-03 TGP005 A. Comandini, N. Chaumeix <b>PAH growth by o-benzyne cycloaddition</b>	B5-03 TGP008 A. F. Wagner, R. Chitsazi <b>Pressure effects on the vibrational rotational relaxation of OH(v,j) in argon bath</b>	C5-03 GPH019 M. AlAbbad, B. R. Giri, J. R. Barker, A. Farooq, <b>High temperature unimolecular decomposition of cyclopentanone</b>
11:15	A5-04 ACH003 F. Ossler <b>In-situ soot/nanoparticle formation and interactions studies based on X-ray and neutron diagnostics</b>	B5-04 TGP011 G. Guillon, T. R. Rao, S. Mahapatra, P. Honvault <b>Permutation symmetry and isotope effects in the xO + yO<sub>2</sub> exchange processes</b>	C5-04 GPH013 V. Burkle-Vitzthum, R. Michels, V. P. Nguyen, N. C. Leguizamon-Guerra, C. Lorgeoux, A. Randi, R. Bounaceur, P.-M. Marquaire <b>Influence of H<sub>2</sub>S on thermal cracking of hydrocarbons at 70 MPa and 473-623 K</b>
<b>Wednesday, May 24 (continued)</b>			

11:40	A5-05 GPH006 F. Goulay, J. Bourgalais, D. L. Osborn, S. D. Le Picard. <b>Reactions of atomic carbon with unsaturated hydrocarbons</b>	B5-05 TOT004 S. Han, X. Li, M. Zheng, F. Nie, L. Guo <b>Reactivity Differences of a 3- component surrogate and a 24- component model for RP-1 fuel pyrolysis evaluated by ReaxFF MD</b>	
12:15- 13:05	<b>Plenary 6</b>  <b>Fast Reactions in Aqueous Nanodrops</b> Evan R. Williams, University of California, Berkeley, USA  <i>Chair: Christa Fittschen, CNRS-University of Lisle, France</i>		
13:15	<b>Lunch and afternoon in Chicago</b>		
18:30	<b>Banquet at Moxee &amp; Mad Mouse</b>		
21:00	<b>End of Day</b>		



Thursday, May 25			
08:00	Registration		
08:25	Daily announcements		
08:30-09:20	Plenary 7 <b>Controlling Phenolic Hydrodeoxygenation by Tailoring M-O Bond Strength Via Specific Catalyst Metal Type and Particle Size Selection</b> Daniel E. Resasco, University of Oklahoma, USA  <i>Chair: William H. Green, Massachusetts Institute of Technology, USA</i>		
<b>Move to parallel sessions</b>			
	<b>Session A6 (Illinois A/B)</b> Chairs: Paul Marshall Sang Soo Lee	<b>Session B6 (Cardinal)</b> Chairs: David Bross Patrick Lynch	<b>Session C6 (White Oak A/B)</b> Chairs: Al Wagner John Randazzo
09:30	A6-01 ION001 S. S. Lee, P. Fenter, K. L. Nagy, N. C. Sturchio <b>Real-time observations of monovalent cation exchange processes at the muscovite (001) – water interface</b>	B6-01 GPH018 M. Abián, J. Giménez-López, M. U. Alzueta, C. T. Rasmussen, P. Glarborg <b>High pressure oxidation of C<sub>2</sub>H<sub>2</sub>/NO mixtures</b>	C6-01 COM004 Y. Huang, H. Yang, <b>Mathematical modelling of the pyrolysis of a large and high ash coal particle</b>
09:55	A6-02 SLK001 R. Khattak, I. I. Naqvi <b>Kinetics and mechanism of the redox reactions between dicyanobis(PHEN/BPY)Iron(III) and hexacyanoferrate(II)</b>	B6-02 COM005 S. Wang, D. F. Davidson, R. K. Hanson <b>A shock tube study of CH<sub>2</sub>O oxidation via simultaneous laser absorption measurements of OH and CO</b>	C6-02 GPH005 S. Peukert, M. Fikri, C. Schulz <b>Experimental and theoretical high temperature rate constants for bimolecular reactions of silicon-organic precursors for nanoparticle synthesis</b>
10:20	<b>Coffee Break</b>		
10:50	A6-03 SLK004 P. P. Plehiers, G. B. Marin, C. V. Stevens, K. Van Geem <b>Automated reaction family generation and analysis using cheminformatics</b>	B6-03 COM024 R. A. Schwind, A. B. Mansfield, M. S. Wooldridge <b>The impact of organic silicon compounds on syngas auto-ignition behavior</b>	C6-03 TGP009 L. A. Rivera-Rivera, A. F. Wagner <b>Normal mode analysis on the relaxation of an excited nitromethane molecule in argon bath</b>
11:15	A6-04 SLK007 F. Yan, N. D. Dhumal, H. J. Kim <b>CO<sub>2</sub> capture in ionic liquid 1-ethyl-3-methylimidazolium acetate: A concerted mechanism without carbene</b>	B6-04 COM017 C. K. Westbrook, M. Mehl, W. J. Pitz, G. Kukkadapu, K. Zhang, S. Wagnon <b>Use of familiar kinetics experiments to predict octane parameters of SI engine fuels</b>	C6-04 TGP003 A. Teplukhin, D. Babikov <b>Quantum mechanical study of ozone recombination</b>

<b>Thursday, May 25 (continued)</b>			
11:40	A6-05 SLK008 M. Ochmann, I. von Ahnen, A. C. Cordones, J. H. Lee, K. Hong, K. Adamczyk, R. W. Schoenlein, T. K. Kim, O. Vendrell, N. Huse <b>Early timescale            photofragmentation kinetics of            a disulfide model system            investigated by time-resolved            X-ray spectroscopy</b>	B6-05 COM033 S. S. Goldsborough, J. Santner, D. Kang, M. J. McNenly <b>Chemical kinetics of engine            knock, revisited.</b>	C6-05 CFD003 T. Tankaria, E. Santos, M.A.N.D.A. Lemos, F. Lemos <b>Kinetic analysis of            thermochemical process            (pyrolysis) for dried cattle            dung</b>
12:05	<b>Close of conference</b>		

## Posters

P01_TGP001	<b>Rate constants for five sensitive reactions during the oxidation process of 1,2,4-trimethylbenzene at low temperature</b> D. Yu, J.-J. Weng, L.-Dong Zhang, Z.-Y. Tian
P02_GPH008	<b>Kinetics of Hydroxyl and Other Small Free Radical Reactions with Cyclopentadiene</b> K. L. Caster, J. Lee, P. Orndorff, K. Hinkelman, F. Goulay
P03_GPH011	<b>Kinetics of OH + ketohydroperoxides in the low-temperature oxidation of n-pentane: Multi-path variational transition state theory</b> L. Xing, J. L. Bao, F. Zhang, D. G. Truhlar
P04_GPH035	<b>On the reactivity of mono-lignol derivatives</b> S. Gorugantu, J. Van Overloop, D. C. Vargas, H.-H. Carstensen, K. M. Van Geem, G. B. Marin
P05_ACH001	<b>Effect of dimerization on the OH-initiated heterogeneous oxidation of saccharide nanoparticles</b> H. Fan, M. R. Tinsley and F. Goulay
P06_GPH028	<b>Reactions of the Simplest Criegee Intermediate with Inorganic Acids and Alcohols</b> S. V. Tadayon, E. S. Foreman, K. M. Kapnas, C. Murray
P07_COM032	<b>Shock-Tube Studies of Diisopropyl Methylphosphonate</b> O. Mathieu, W. D. Kulatilaka, E. L. Petersen
P08_GPH017	<b>Reactions of hex-5-en-1-yl radicals</b> M. Liszka, K. Brezinsky, X. Han
P09_COM022	<b>High temperature pulsed flow reactor studies of radical species at high temperature</b> Y. Lee, K. Caster, K. Hinkelman, F. Goulay
P10_COM027	<b>Autoignition of liquefied natural gas (LNG) in shock tube and rapid compression machine</b> V. Patel, M. Al-Abbad, S. K. Vallabhuni, A. Lucassen, K. Moshhammer, A. Farooq, R. Fernandes
P11_COM029	<b>Experimental and kinetic modeling study of ammonia autoignition</b> S. K. Vallabhuni, A. Lucassen, M. Wahab, G. Issayev, A. Farooq, R. Fernandes
P12_COM014	<b>Shock tube studies of propulsion fuels at low temperatures</b> J. Guzman, K. Brezinsky
P13_CHE009	<b>Kinetics and mechanism of catalytic coke gasification by air/CO<sub>2</sub></b> M.A.N.D.A. Lemos, S.A.C. Carabineiro, L.F. Bobadilla, M.A. Centeno, E. Santos, F. Lemos and L.S. Lobo
P14_EXP001	<b>Product distributions from fast pyrolysis of 10 Ecuadorian agricultural residual biomass samples</b> D. C. Vargas, S. Gorugantu, H.-H. Carstensen, D. A. Streitwieser, K. M. Van Geem, G. B. Marin
P15_GPH029	<b>Identifying broadband rotational spectra with neural networks</b> D. Zaleski, K. Prozument
P16_MUQ005	<b>An improved algorithm for automatic mechanism generation</b> M. S. Johnson, W. H. Green
P17_MUQ006	<b>Automatic kinetic model generation: a combination of the rule-based and rate-based termination criteria</b> R. Van de Vijver, F. Vermeire, K. Van Geem
P18_COM037	<b>High accuracy thermochemical kinetics for <math>H + CH_3 (+N_2) \rightleftharpoons CH_4 (+N_2)</math></b> N. J. Labbe, A. W. Jasper, R. Sivaramakrishnan, S. J. Klippenstein, J. A. Miller, B. Ruscic
P19_COM038	<b>Predictive automated thermochemistry for combustion</b> M. Keçeli, A. W. Jasper, C. Cavallotti, Y. Georgievskii, Y.-P. Li, J. M. Wozniak, T. Lu, J. Zádor, R.A. Bair, W. H. Green, A. F. Wagner, S. J. Klippenstein
P20_COM015	<b>Shock tube study of the pyrolysis of the jet fuels JP10 and Jet A2</b> X. Han, M. Liszka, K. Brezinsky
P21_GPH009	<b>Reaction <math>CH_3 + Cl</math> studied over the 292 – 558K temperature and 1 – 100 bar pressure ranges</b> C. Yan, L. N. Krasnoperov
P22_GPH036	<b>Kinetics of reactions of atomic chlorine with ketones</b> T. N. Herath, E. C. Clinch, I. Orozco, P. Marshall
P23_GPH037	<b>Time resolved HO<sub>2</sub> and OH measurements provide evidence for the formation of OOQOOH</b> T. Speak, L. James, M. Blitz, P. Seakins
P24_MUQ003	<b>RMG-Py version 2: New Capabilities &amp; Demonstration</b> A. M. Payne, W. H. Green