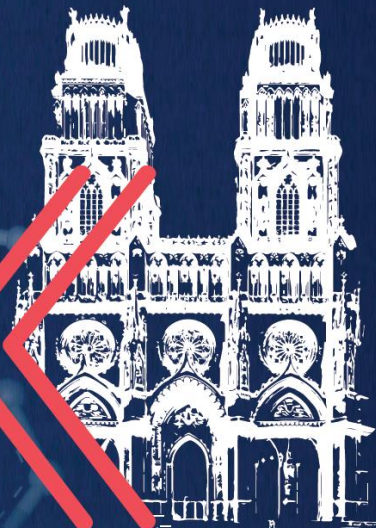


ICCK



11TH INTERNATIONAL CONFERENCE ON CHEMICAL KINETICS

ORLÉANS,
JUNE
23 - 27 2019

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COMBUSTION

CATALYSIS

ATMOSPHERE



Depuis 80 ans, nos connaissances
bâtissent de nouveaux mondes



Monday, June 24	
08:00	Registration
08:20	Welcome and Official Opening
08:30-09:20	Plenary 1 Is Gas Phase Chemical Kinetics Static? Kinetics in the Past, Present, and the Future A.R. Ravishankara, Colorado State University, USA <i>Chair: Georges Le Bras</i>
Move to parallel sessions	
	Session A1 <i>Chairs: C. Cavallotti/Z. Serinyel</i>
	Session B1 <i>Chairs: G. Moortgat/B. Picquet-Varrault</i>
09:30	Accurately Predicting the Kinetics of Complex Reacting Systems: Status Report <i>W.H. Green</i>
09:30	Revisiting the Gas-Phase Rate Coefficient of the OH + SO₂ + M → HSO₃ + M Reaction <i>M. McGillen, H Elothmani, Y. Ren, L. Zhou, M. Idir, S. El Hajjaji, V. Daële, A.R. Ravishankara, A. Mellouki</i>
09:50	Deep Learning of Activation Energies and Automated Reaction Dataset Generation <i>C. Grambow, W.H. Green</i>
09:50	DMS H-Abstraction by OH in Excess in the Absence of O₂ <i>Z. Salta, J. Lupi, O.N. Ventura, V. Barone</i>
10:10	Automated Networks: Harnessing Dynamics, Kinetics and Human Guided VR for Blackbox Mechanism Generation <i>R.J. Shannon, D.V. Shalashilin, D.R. Glowacki</i>
10:10	Kinetic and Mechanistic Study of the Reaction CH₃SO₂NH₂ + OH <i>M. Berasategui, D. Amedro, A. Edtbauer, J. Williams, J. Crowley</i>
10:30	Coffee Break
11:00	Model Analysis Based Experimental Design for Combustion Kinetics <i>B. Yang, J. Wang, Z. Zhou</i>
11:00	Employing pulsed irradiation in photocatalysis <i>T.P. Nicholls, J.C. Robertson, A.C. Bissember</i>
11:25	Benchmarking DFT for Computational Kinetics <i>M.E. Segovia, O.N. Ventura, J. Lupi, Z. Salta, N. Tasinato, V. Barone</i>
11:25	Temperature and Pressure Dependence of the Kinetics of the CH₂OO + CH₃OO Reaction <i>R. Chhantyal Pun, N. Zachhuber, R. Martin, M.A.H. Khan, D.E. Shallcross, A.J. Orr-Ewing</i>
11:45	Ketohydroperoxide Reactions Uncovered by KinBot <i>R. Van de Vijver, J. Zádor, G.B. Marin, K.M. Van Geem</i>
11:45	Kinetic Studies of Self- and Cross-Reactions of Small Peroxy Radicals in the Highly Instrumented Reactor for Atmospheric Chemistry <i>F.F. Østerstrøm, L. Onel, A. Brennan, J. Parr, E. Cooke, L. Whalley, P.W. Seakins, D.E. Heard</i>

Monday, June 24 (continued)		
12:05	Elementary-Reaction Kinetics for Cellulose and Hemicellulose Pyrolysis <i>P.R. Westmoreland, A. Bose, C.J. McGill, A. Raghu</i>	Development and Validation of a New Experimental Set-Up to Study Reactions Between Peroxy RO₂ and HOx Radicals <i>F. Kravtchenko, L. Pillier, S. Batut, B. Calimet, C. Fittschen</i>
12:25	Lunch	
	Session A2 <i>Chairs: C.F. Goldsmith/P.A. Glaude</i>	Session B2 <i>Chairs: C. Fittschen/Y. Bedjanian</i>
13:45	A Systematic Kinetic Modelling Study of Mono-Aromatic Hydrocarbons: Towards the Definition of Reaction Classes and Rate Rules <i>M. Pelucchi, L. Pratali Maffei, R.D. Buetting, W. Pejpichestakul, C. Cavallotti, A. Frassoldati, K.A. Heufer, T. Faravelli</i>	Reactivity of OH Radicals Towards CH₃CHO at T<200 K: Implications in Astrochemistry <i>S. Blázquez, D. González, B. Ballesteros, A. Canosa, J. Albaladejo, E. Jiménez</i>
14:05	Mechanistic Study of thermal degradation of β-1,4-D-xylan <i>M. Goussougli, B. Sirjean, P.A. Glaude, R. Fournet</i>	Pressure-Dependent Rate Constant Caused by Tunneling Effects: OH + HNO₃ as an Example <i>T.L. Nguyen, J.F. Stanton</i>
14:25	An Experimental and Chemical Kinetic Modeling Study of 1,3-Butadiene Combustion: Ignition Delay Time and Laminar Flame Speed Measurements <i>C.W. Zhou, Y. Li, U. Burke, C. Banyon, K.P. Somers, S. Ding, S. Khan, J.W. Hargis, T. Sikes, O. Mathieu, E.L. Petersen, M. AlAbbad, A. Farooq, Y. Pan, Y. Zhang, Z. Huang, J. Lopez, Z. Loparo, S.S. Vasu, H.J. Curran</i>	Reaction Between Peroxy and Alkoxy Radicals Can Form Stable Adducts <i>M. Rissanen, S. Iyer, T. Kurtén</i>
14:45	Group Additive Kinetic Modeling for the Pyrolysis of Cyclic Species <i>F.H. Vermeire, R. Van de Vijver, G.B. Marin, K.M. Van Geem</i>	Pressure Dependent Kinetics of the Reaction Between CH₃O₂ and OH: Triox Formation <i>C. Yan, L.N. Krasnoperov</i>
15:05	The Criegee Intermediate Reaction Network in Ethylene Ozonolysis <i>N. Hansen, A.C. Rousso, A.W. Jasper, Y. Ju</i>	Pressure-Dependent Kinetics of the Reaction Between CH₃O₂ and OH Focusing on the Product Yield of Methyltrioxide (CH₃OOOH) <i>F. Zhang, C. Huang</i>
15:30	Coffee Break	

Monday, June 24 (continued)		
16:00	<p>Modeling PAH Formation using RMG: From Acetylene to Three Rings <i>M. Liu, T.C. Chu, A. Jocher, M.C. Smith, W.H. Green</i></p>	<p>Reaction Products of Fuel Derived CH Radical Reactions with Ammonia and Substituted Amines by Using SVUV Photoionization Coupled to Time-of-Flight Mass Spectrometry <i>J. Bourgalais, K. Caster, O. Durif, D. Osborn, S. Le Picard, F. Goulay</i></p>
16:20	<p>Direct Measurements of PAH Formation and Growth by Addition of Phenyl and Naphthyl Radicals to Acetylene <i>M.C. Smith, T.C. Chu, J. Yang, A. Uwagwu, M. Liu, W.H. Green</i></p>	<p>Reaction OH + OH → H₂O + O Revisited <i>X. Zhang, M. Sangwan, C. Yan, P.V. Koshlyakov, E.N. Chesnokov, L.N. Krasnoperov</i></p>
16:40	Move to plenary session	
16:50-17:40	<p>Plenary 2</p> <p>Quantum Chemical Modeling of Mechanisms and Selectivities in Homogeneous Catalysis F. Himo, Stockholm University</p> <p><i>Chair: Vicent Moliner</i></p>	
19:00	<i>Reception at Hôtel Grosloot</i>	
20:00	End of Day	

Tuesday, June 25	
08:00	Registration
08:20	Daily announcements
08:30-09:20	Plenary 3 Chemical Kinetics of Multiphase Atmospheric Chemistry V. Faye McNeill, Columbia University, USA <i>Chair: Hartmut Herrmann</i>
Move to parallel sessions	
	Session A3 <i>Chairs: K. Brezinsky/A. Farooq</i>
	Session B3 <i>Chairs: J. Chen/I. Bejan</i>
09:30	Reactivity Comparison of Linear C4-C6 Alcohol, Aldehyde and Carboxylic Acid Oxidation <i>S. Namysl, M. Pelucchi, O. Herbinet, T. Faravelli, F. Battin-Leclerc</i>
09:50	Detailed Experimental and Kinetic Modeling Study of 3-Carene Pyrolysis <i>J. Zhang, F.H. Vermeire, R. Van de Vijver, O. Herbinet, F. Battin-Leclerc, M.F. Reyniers, K.M. Van Geem</i>
10:10	A Theoretical and Kinetic Analysis of Phenol Pyrolysis <i>L. Pratali Maffei, M. Pelucchi, T. Faravelli, C. Cavallotti</i>
10:30	Coffee Break
11:00	Ignition Phenomena in Diethyl Ether/Air Mixtures: Elementary Steps, Mechanism, and Transport <i>J. Eble, J. Kiecherer, C. Bansch, M. Olzmann</i>
11:25	Effect of Methyl Group Substitution on the Kinetics of Vinyl Radical Oxidation <i>S.P. Joshi, T.T. Pekkanen, R.S. Timonen, A.J. Eskola</i>
11:45	Kinetics of the Competing C-O Bond-Fission Reactions of Dimethoxymethane <i>L. Golka, D. Gratzfeld, I. Weber, M. Olzmann</i>
11:00	Biomass-Burning Related Atmospheric Aqueous-Phase Chemistry: Kinetics, Photochemistry and Modelling <i>H. Herrmann, T. Scafefer, L. He, T. Felber, A. Tilgner, E.H. Hoffmann</i>
11:25	Effect of Surface/Bulk Partitioning on the Heterogeneous Kinetics of Aqueous Droplets <i>F. Goulay, H Fan, T.W. Massaya</i>
11:45	Atmospheric Chemistry of Iodous and Iodic Acids <i>S. Taamalli, D. Khiri, S. Khanniche, S. Suliman, M. Ribaucour, I. Cernusak, L. Cantrel, F. Louis</i>

Tuesday, June 25 (continued)		
12:05	On the Kinetics of Ammonia Oxidation <i>P. Dagaut</i>	Shielding of Aerosol-Borne Pesticides Against OH Radicals <i>L. Han, C. Zetzsch</i>
12:25	Lunch	
	Session A4 <i>Chairs: M. Olzmann/R. Fournet</i>	Session B4 <i>Chairs: K. Noda/V. Belandria</i>
13:45	Ignition Delay Times of Dibutylether in a Rapid Compression Machine <i>F. Khaled, Z. Serinyel, G. Dayma, F. Foucher</i>	Polymer Mixtures Thermal Degradation Kinetic Analysis <i>J. Briceno, M.A.N.D.A. Lemos, F. Lemos</i>
14:05	CO Formation from Dimethyl-Carbonate Pyrolysis Behind Reflected Shock Waves <i>O. Mathieu, C.R. Mulvihill, E.L. Petersen</i>	Theoretical and Experimental Studies of the Thermal Oxidation of Epoxy-Amine Systems <i>R. Delannoy, E. Richaud, V. Tognetti</i>
14:25	Shock Tube Study of the Pyrolysis Kinetics of Di- and Trimethoxy Methane <i>M. Döntgen, M.E. Fuller, C.F. Goldsmith</i>	Thermal and Catalytic Degradation of Polypropylene with VGO and UCO <i>T. Godinho, M.A.N.D.A. Lemos, H. Carabineiro, L. Tarelho, F. Lemos</i>
14:45	Oxidation of an Iso-Paraffinic Alcohol-to-Jet Fuel and Heptane Mixture: An Experimental and Modelling Study <i>J. Guzman, G. Kukkadapu, K. Brezinsky, C. Westbrook</i>	Fundamentals of Polymer Fouling in Ethylene Crackers <i>M. Forsuelo, D. Ranasinghe, H.W. Pang, L. Lai, M.C. Smith, M. Goldman, W.H. Green</i>
15:05	Reaction Kinetics of Hydroxyl Radicals with Dienes <i>A. Farooq, B. Giri</i>	Revealing the Origin of the Catalytic Power of Enzymes by Merging Computational Studies and Experiments <i>S. Martí, R. Castillo, K. Świderek, M. Roca, K. Arafet, D. De raffe, N. Serrano, M.A. Galmes, V. Moliner</i>
15:30	Coffee Break	
16:00	Shock-Tube Measurements of CO Concentration Time-Histories During Iso-Octane Oxidation <i>O. Mathieu, S. Cooper, S. Alturaifi, C.R. Mulvihill, E.L. Petersen</i>	TG/DSC Analysis of the Pyrolysis Kinetics of Polystyrene from WEEE <i>R. Kol de Carvalho, B. Rijo, F. Rey, T. Carvalho, F. Lemos, M.A.N.D.A. Lemos</i>

Tuesday, June 25 (continued)		
16:20	Dual-Comb Spectroscopy in Shock Tubes: Mid-Infrared Microsecond-Resolved Spectrometer <i>A. Hugi, M. Geiser, R. Horvath, C.I. Strand, N. Pinkowski, Y. Ding, R.K. Hanson</i>	Catalytic Pyrolysis Kinetics of Polystyrene from WEEE <i>P. Pereira, F. Rey, B. Rijo, T. Carvalho, F. Lemos, M.A.N.D.A. Lemos</i>
16:40	Experimental and Kinetic Modeling Investigation on Laminar Flame Propagation of Engine Fuels in a High-Pressure Constant-Volume Cylindrical Combustion Vessel <i>Y. Li, B. Mei, X. Zhang, W. Li, S. Ma, G. Wang, W. Yuan</i>	Formation Kinetics of Water-Soluble Lanthanide(III) Porphyrins as Potential Biomedical Agents <i>Z. Valicsek, M.P. Kiss, O. Horváth</i>
17:00	Laminar Burning Velocities and LIF Measurements of Nitric Oxide Formation in Flames of Simple Alcohols <i>C. Brackmann, T. Methling, G. Capriolo, M. Lubrano Lavadera, A.A. Konnov</i>	Chemistry Triggered Events of PM2.5 Explosive Growth During Late Autumn and Winter in a Megacity <i>W. Sun, D. Wang, L. Yao, Q. Fu, H. Wang, Q. Li, G. Wange, J. Chen</i>
17:25	Move to plenary session	
17:35-18:25	Plenary 4 High-Temperature Reaction Pathways T. Kasper, Duisburg-Essen University, Germany <i>Chair: Philip R. Westmoreland</i>	
18:30	<i>Poster Session and Cocktail</i>	
22:00	End of Day	

Wednesday, June 26		
08:00	Registration	
08:20	Daily announcements	
08:30-09:20	Plenary 5 Theoretical Studies of the Atmospheric Chemical Mechanisms of Isoprene and its Oxidation Products G. Da Silva, University of Melbourne, Australia <i>Chair: William H. Green</i>	
Move to parallel sessions		
	Session A5 <i>Chairs: K. Van Geem/F. Zhang</i>	Session B5 <i>Chairs: O. Mathieu/A. Frassoldati</i>
09:30	A Kinetic View on Dissociative Electron Attachment Processes <i>J. Troe, A.A. Viggiano</i>	Rate Constant Measurements and RRKM Modeling on Thermal Decomposition of Ethylsilanes and Cyclosiloxanes <i>S. Peukert, P. Sela, Y. Sakai, J. Herzler, M. Fikri, C. Schulz</i>
09:50	Understanding Temperature and Pressure Dependence in the Non-Adiabatic Reactions of Oxygen Atoms with Terminal Alkenes <i>C. Cavallotti, L. Pratali Maffei, A. Caracciolo, N. Balucani, P. Casavecchia</i>	Impact of Correlated Inputs on Computed Branching Ratio <i>C. Huang, Z. Zhou, B. Yang, F. Zhang</i>
10:10	New Phenomenological Reaction Rate Equation for Chemical Catalyst Deactivation (Reversible-Irreversible Case) <i>Z.J.G. Gromotka, G.S. Yablonsky, G.B. Marin, D. Constales</i>	Determination of Bond Additivity Corrections for CBS-QB3 Calculated Standard Enthalpies of Formation of C, H, N, O and S species <i>C.A.R. Pappijn, R. Van de Vijver, F.H. Vermeire, M.F. Reyniers, G.B. Marin, K.M. Van Geem</i>
10:30	Coffee Break	
11:00	Electrode Kinetics of Strongly Adsorbed Molecules on Semiconductors: Isolating Kinetic Constants from Lateral Interactions and Diode Parameters <i>S. Ciampi, Y.B. Vogel, A. Molina</i>	On the Combustion Chemistry of Alkyl Nitrates <i>C.F. Goldsmith, M.E. Fuller, N. Chaumeix</i>
11:25	Comparative Methods of Kinetic Analysis of Calcium Looping for Energy Storage <i>L. Fedunik-Hofman, A. Bayon, W., Lipiński, S.W. Donne</i>	Pyrolysis Mechanism and Kinetics of Isopropyl Nitrate <i>M.E. Fuller, C.F. Goldsmith</i>

Wednesday, June 26 (continued)	
11:45	<p>First-Principles Calculation of Catalytic Activity Modifications with an Electric Field <i>K. Wakamatsu, T. Ogura</i></p> <p>Shock Wave and Modelling Study of the Dissociation Pathways of (C₂F₅)₃N <i>E. Tellbach, C.J. Cobos, L. Sölter, J. Troe</i></p>
12:05	<p>Theoretical Kinetic Study of Formic Acid Catalyzed Keto-Enol Tautomerizations for C₂ And C₃ Enols at Conditions Relevant to Atmospheric and Combustion Chemistry <i>E. Grajales-González, M. Monge-Palacios, S.M. Sarathy</i></p> <p>Reaction Pathways of Cyclopentanone Oxidation Intermediates <i>S. Khanniche, W.H. Green</i></p>
12:25	<p>How Can Cells Detect and Respond to Oxygen Levels? Computer Simulations Studies of Oxygen Diffusion into Prolyl Hydroxylases <i>C. Domene</i></p> <p>The Pyrolysis Chemistry of Propionic Acid and Ethyl Propionate Revealed <i>C. Rogers, K. Cummins, J. Porterfield, J.W. Daily, G.B. Ellison, N.J. Labbe</i></p>
12:50	Lunch Boxes
14:00	Bus departure to the “Château de Chambord”
15:30	Free time and visit
18:30	Cocktail on the Terraces
20:00	Banquet on the 1 st floor around the double helix staircase
23:00	End of Day

Thursday, June 27	
08:00	Registration
08:20	Daily announcements
08:30-09:20	Plenary 6 Reactivity of Biogenic Volatile Organic Compounds with NO₃ Radical B. Picquet-Varrault, University Paris-Créteil, France <i>Chair: Gilles Poulet</i>
Move to parallel sessions	
	Session A6 <i>Chairs: A. Konnov/N. Hansen</i>
	Session B6 <i>Chairs: E. Jiménez/M. McGillen</i>
09:30	Thermal Decomposition of Spray in Plug-Flow Reactor at Atmospheric Pressure <i>M. Gonchikzhapov, T. Kasper</i>
	Gas-Phase Rate Coefficients for the Reaction of the NO₃ Radical with a Series of Aromatic Aldehydes <i>Y. Ren, M. McGillen, A.R. Ravishankara, S.S. Brown, L. Zhou, M. Idir, V. Daële, A. Mellouki</i>
09:50	Preliminary Results on Syngas Kinetic Mechanism Optimization Using the New Opt-D* Algorithm <i>S.M. Ali, S. Varunkumar</i>
	Atmospheric Oxidation Mechanism of Toluene Initiated by OH Radical <i>X. Wu, C. Huang, F. Zhang</i>
10:10	Instabilities of H₂-O₂ System and Effect of Several Bath Gases <i>P. Sabia, M.V. Manna, M. de Joannon, R. Ragucci</i>
	Water Vapor Does Not Catalyze the Reaction Between Methanol and OH Radicals <i>C. Schoemaeker, W. Chao, J.Jr.M. Lin, K. Takahashi, A. Tomas, L. Yu, Y. Kajii, S. Batut, C. Fittschen</i>
10:30	Coffee Break
11:00	Fast Pyrolysis Bio-Oil Combustion Characteristics and Challenges for Kinetic Modeling <i>A. Frassoldati, M. Pelucchi, A.E. Saufi, A. Cuoci, C. Cavallotti, T. Faravelli, E. Ranzi</i>
	Photosensitization in the Air: Bridging Fundamental Bulk Processes with Secondary Organic Aerosol Production <i>C. George</i>
11:25	Experimental and Kinetic Study of 1,2,4-Trimethylcyclohexane Pyrolysis <i>Y.X. Liu, D.X. Tian, C.C. Cao, Z.K. Liu, Y.T. Zhai, Y. Zhang, J.Z. Yang, Z.Y. Tian</i>
	Anthraquinone-2-Sulfonate as a Model for Photoinduced Reactions in Tropospheric Aqueous Aerosol <i>T. Schaefer, J.D. Raff, H. Herrmann</i>
11:45	A Comprehensive Experimental and Kinetic Modeling Study of o-Xylene Combustion <i>W. Yuan, L. Zhao, W. Li, Y. Li, P. Dagaut, F. Qi, J. Yang</i>
	Development and Validation of a Teflon Thermal Regulated Atmospheric Simulation Chamber (THALAMOS). A Versatile Tool for the Study of Atmospheric Relevant Processes <i>N. Osseiran, M.N. Romanias, V. Gaudion, M. Angelaki, V.C. Papadimitriou, A. Tomas, F. Thevenet, P. Coddeville</i>

Thursday, June 27 (continued)		
12:05	High-Temperature Fast-Flow Reactor for the study of Radical-Radical Reactions <i>Y. Lee, F. Goulay</i>	Atmospheric Reactivity of Biogenic Volatile Organic Compounds under the Canopy of a Maritime Pine Forest during the LANDEX Field Campaign <i>K. Mermet, S. Sauvage, S. Dusanter, T. Salameh, T. Léonardis, N. Locoge, P.M. Flaud, E. Perraudin, E. Villenave</i>
12:25	Structure of a Counterflow Flame at Different Operating Conditions <i>S.A. Gómez, V. Zhukov, C.R. de Andrade, A.P. Pimenta</i>	First-Principles Kinetic Monte Carlo Study of Hydrodeoxygenation at the Ru/TiO₂ Interface <i>X. Li, L.C. Grabow</i>
12:45	Lunch	
	Close of conference	

TUESDAY EVENING POSTER SESSION PROGRAM

Poster #1

CHAMBER STUDY OF THE OXALYL CHLORIDE PHOTODISSOCIATION IN SUNLIGHT

Kukui Alexandre, Ren Yangang, Daële Véronique, Mellouki Wahid, Ravishankara A. R.

Poster #2

A NEW KINETICS DATABASE OF ORGANIC OXIDATION REACTIONS FOR USE IN STRUCTURE-ACTIVITY RELATIONSHIP STUDIES

McGillen Max, Orlando John, Mellouki Abdelwahid, Picquet-Varrault Bénédicte, Wallington Timothy, Carter William

Poster #3

EFFECTS OF THE AXIAL LIGANDS ON THE FORMATION KINETICS OF WATER-SOLUBLE CERIUM(III) PORPHYRINS

Valicsek Zsolt, Kiss Melitta, Horvath Otto

Poster #4

GAS PHASE KINETIC STUDY FOR A SERIES OF METHYLATED FURANS WITH CHLORINE ATOMS IN ATMOSPHERIC CONDITIONS

Claudiu Roman, Arsene Cecilia, Olariu Romeo, Bejan Iustinian

Poster #5

GAS PHASE KINETIC STUDY FOR A SERIES OF METHYLATED AROMATICS WITH OH RADICALS

Bejan Iustinian, Gibilisco Rodrigo, Barnes Ian, Wiesen Peter

Poster #6

TROPOSPHERIC DEGRADATION OF BIOMASS BURNING COMPOUNDS: OH RADICAL-INITIATED OXIDATION OF THREE DIMETHOXYBENZENE ISOMERS AND 4-VINYLGUAIACOL.

Gibilisco Rodrigo, Barnes Ian, Bejan Iustinian, Wiesen Peter

Poster #7

GAS PHASE KINETIC AND THEORETICAL APPROACH ON THE CHLORINE ATOM CHEMISTRY OF EPOXIDES

Tovar Carmen, Haack Alexander, Barnes Ian, Bejan Iustinian, Wiesen Peter

Poster #8

IUPAC TASK GROUP ON ATMOSPHERIC CHEMICAL KINETIC DATA EVALUATION

Ammann M., Cox R., Crowley J., Herrmann J., Jenkin M., McNeill V., Mellouki A., Troe J., Wallington T.

Poster #9

KINETIC ANALYSIS OF GROWTH MECHANISM OF PAHS THROUGH C5 RINGS

Pejpichestakul Warumporn, Pelucchi Matteo, Cavallotti Carlo, Frassoldati Alessio, Faravelli Tiziano

Poster #10

TOWARDS A COMMON C0-C2 MECHANISM: A CRITICAL EVALUATION OF RATE CONSTANTS FOR HYDROGEN COMBUSTION KINETICS.

Pelucchi Matteo, Burke Ultan, Cai Liming, Somers Kieran, Glarborg Peter, Turanyi Tamas, Heinz Pitsch, Curran Henry, Faravelli Tiziano, Stephen Klippenstein

Poster #11

REACTION GENERALIZATION OF SINGULAR SITE USING LOCAL SURFACE MODEL

Takata Yasumasa, Ogura Teppei

Poster #12

EXAMINATION OF AUTOMATIC GENERATION ALGORITHM OF CATALYST SURFACE REACTION MECHANISM

Aratani Masato, Ogura Teppei

Poster #13

PRELIMINARY RESULTS ON TRACING AIR POLLUTION AND IMPACT ON OZONE IN DIFFERENT PLUMES USING AIRCRAFT MEASUREMENTS IN DACCIWA EUROPEAN PROJECT

Xue Chaoyang, Krysztofiak Gisèle, Brocchi Vanessa, Stratmann Greta, Sauer Danie, Schlager Hans, Lee James, Hopkins James, Colomb Aurélie, Borbon Agnès, Catoire Valéry

Poster #14

KINETICS OF THE GAS PHASE REACTION BETWEEN THE CRIEGEE INTERMEDIATE CH₂OO AND O₃

Onel Lavinia, Blitz Mark, Seakins Paul, Heard Dwayne, Stone Daniel

Poster #15

DIRECT MEASUREMENTS OF THE KINETICS OF THE REACTION BETWEEN THE CRIEGEE INTERMEDIATE CH₃CHOO AND SO₂

Onel Lavinia, Mortiboy Jennifer, Blitz Mark, Seakins Paul, Heard Dwayne, Stone Daniel

Poster #16

UNIMOLECULAR DECOMPOSITION OF THE ALLYLIC METHYL CROTONATE RADICAL: EXPERIMENTAL AND MODELLING STUDY

Seal Prasenjit, Joshi Satya, Eskola Arkke

Poster #17

GAS-PHASE POSITIVE ION INSIGHTS DURING LABORATORY EUV IRRADIATION OF N₂/CH₄ GAS MIXTURES: IMPLICATIONS FOR TITAN'S IONOSPHERIC CHEMISTRY

Bourgalais Jérémy, Pernot Pascal, Carrasco Nathalie

Poster #18

FIRST PEPICO SPECTROSCOPY INVESTIGATIONS OF N-PENTANE LOW TEMPERATURE OXIDATION IN A JET-STIRRED REACTOR

Bourgalais Jérémy, Battin-Leclerc Frédérique, Herbinet Olivier, Wang Zhandong, Tran Luc-Sy, Vanhove Guillaume, Nahon Laurent, Garcia Gustavo

Poster #19

PHOTODEGRADATION OF A SERIES OF FLUOROESTERS INITIATED BY OH RADICALS AT DIFFERENT TEMPERATURES

Lugo P., Rivella C., Gibilisco Rodrigo, Salgado S., Wiesen Peter, Blanco M. B., Teruel Mariano

Poster #20

GAS-PHASE DEGRADATION OF 2-BUTANETHIOL INITIATED BY CL ATOMS. KINETICS, PRODUCT YIELDS AND MECHANISM AT 298K AND ATMOSPHERIC PRESSURE

L. Cardona Alejandro, Gibilisco Rodrigo, Wiesen Peter, Teruel Mariano

Poster #21

SHOCK WAVE AND THEORETICAL MODELING STUDY OF THE DISSOCIATION OF CH₂F₂ - PRIMARY AND SECONDARY REACTIONS

Soelter Lars, Tellbach Elsa, Cobos Carlos, Troe Jurgen

Poster #22

PREMIXED FLAME STRUCTURE OF ETHYL PENTANOATE: EXPERIMENTAL STUDY AND CHEMICAL KINETIC MODELING

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