

Publications of Dr. Thomas Zeuch

Communications, letters, reviews, hot articles, papers in journals with high impact factor.

Hot article:

K. Hoyermann, F. Mauß, T. Zeuch: "A detailed chemical reaction mechanism for the oxidation of hydrocarbons and its application to the analysis of benzene formation in fuel-rich premixed laminar acetylene and propene flames", *Phys. Chem. Chem. Phys.* **6** (2004) 3824-3835.

Hot article:

I. Dauster, M.A. Suhm, U. Buck, T. Zeuch: "Experimental and theoretical study of the microsolvation of sodium atoms in methanol clusters: Differences and similarities to sodium/water and sodium/ ammonia", *Phys. Chem. Chem. Phys.* **10** (2008) 61–75.

Angewandte Chemie communication:

J. L. Wolf, M.A. Suhm, T. Zeuch: "Suppressed particle formation by kinetically controlled ozone removal: Revealing the role of transient-species chemistry during alkene ozonolysis": *Angew. Chem. Int. Ed.* **48** (2009) 2231-2235.

Communication:

R. M. Forck, I. Dauster, Y. Schieweck, T. Zeuch, U. Buck, M. Oncak, P. Slavicek: "Communications: Observation of two classes of isomers of hydrated electrons in sodium-water clusters", *J. Chem. Phys.* **132** (2010) 221102.

Communication:

R. M. Forck, J. M. Dietrich, C.C Pradzynski, A. L. Huchting, R.A. Mata, T. Zeuch: „Structural diversity in sodium doped water trimers“, *Phys. Chem. Chem. Phys.* **14** (2012) 9054-9057.

Science paper:

C. C. Pradzynski, R. M. Forck, T. Zeuch, P. Slavíček, U. Buck: „A Fully Size-Resolved Perspective on the Crystallization of Water Clusters“, *Science*, **2012**, *337*, 1529-1532.

Letter:

J. Lengyel, A. Pysanenko, J. Kočíšek, V. Poterya, C. C. Pradzynski, T. Zeuch, P. Slavíček, M. Fárník: „Nucleation of Mixed Nitric Acid–Water Ice Nanoparticles in Molecular Beams that Starts with a HNO₃ Molecule“, *J. Phys. Chem. Lett.*, **2012**, *3*, 3096–3101.

Communication:

P. T. M. Carlsson, C. Keunecke, B. C. Krüger, M.-C. Maas, T. Zeuch: „Sulfur dioxide oxidation induced mechanistic branching and particle formation during the ozonolysis of β -pinene and 2-butene“, *Phys. Chem. Chem. Phys.* **14** (2012) 15637 - 15640.

Frontiers article (review, front cover):

T. Zeuch, U. Buck: „Sodium doped hydrogen bonded clusters: Solvated electrons and size selection“, *Chem. Phys. Lett.* **579** (2013) 1 - 10.

Angewandte Chemie, hot paper:

J. Ahrens, P. T. M. Carlsson, N. Hertl, M. Olzmann, M. Pfeifle, T. Zeuch: “Infrared Detection of Criegee Intermediates Formed during the Ozonolysis of beta-Pinene and Their Reactivity towards Sulfur Dioxide”: *Angew. Chem. Int. Ed.* **53** (2014) 715-719.

Perspective article (review):

U. Buck, C. C. Pradzysnki, T. Zeuch, J. M. Dieterich, B. Hartke: “A size resolved investigation of large water clusters“, *Phys. Chem. Chem. Phys.* **16** (2014) 6859-6871.

Communication:

C. C. Pradzysnki, C. W. Dierking, F. Zurheide, R. M. Forck, U. Buck, T. Zeuch, S. S. Xantheas: “Infrared detection of $(\text{H}_2\text{O})_{(20)}$ isomers of exceptional stability: a drop-like and a face-sharing pentagonal prism cluster“, *Phys. Chem. Chem. Phys.* **16** (2014) 26691-26696.

Perspective article (review):

K. Hoyer mann, F. Mauß, M. Olzmann, O. Welz, T. Zeuch: “Exploring the chemical kinetics of partially oxidized intermediates by combining experiments, theory, and kinetic modeling“, *Phys. Chem. Chem. Phys.* **19** (2017) 18128-18146.

Other peer reviewed research papers:

W. Hack, K. Hoyer mann, M. Olzmann, T. Zeuch: “Mechanisms and Rates of the Reactions $\text{C}_2\text{H}_5 + \text{O}$ and $1\text{-C}_3\text{H}_7 + \text{O}$ “, *Proc. Combust. Inst.* **29** (2002) 1247-1255.

W. Hack, M. Hold, K. Hoyer mann, J. Wehmeyer, T. Zeuch: “Mechanism and Rate of the Reaction $\text{CH}_3 + \text{O}$ – Revisited“, *Phys. Chem. Chem. Phys.* **7** (2005) 1974-1984.

W. Hack, K. Hoyer mann, M. Olzmann, B. Viskolcz, J. Wehmeyer, T. Zeuch: “The reactions of the branched alkyl radicals iso-butyl and neo-pentyl with oxygen atoms - an experimental and theoretical study“, *Proc. Comb. Inst.* **30** (2005) 1005-1013.

K. Hoyer mann, J. Nothdurft, M. Olzmann, J. Wehmeyer, T. Zeuch: "Formation and decomposition of chemically activated cyclopentoxy radicals from the $c\text{-C}_5\text{H}_9\text{+O}$ reaction", *J. Phys. Chem. A* **110** (2006) 3165-3173.

S. S. Ahmed, G. Moreac, F. Mauß, T. Zeuch: "A comprehensive and compact n-heptane oxidation model derived using chemical lumping", *Phys. Chem. Chem. Phys.* **9** (2007) 1107 – 1126.

T. Zeuch, G. Moréac, S.S. Ahmed, F. Mauss: "A comprehensive skeletal mechanism for the oxidation of n-heptane generated by chemistry-guided reduction", *Combust. Flame* **155** (2008) 651–674.

K. Hoyer mann, F. Nacke, J. Nothdurft, M. Olzmann, J. Wehmeyer, T. Zeuch: "The reaction of allyl radicals with oxygen atoms-rate coefficient and product branching", *Proc. Comb. Inst.* **32** (2009) 157-164.

M. Hold, K. Hoyer mann, I. Morozov, T. Zeuch: " CH_2Cl and CHCl_2 Radical Chemistry: The Formation by the Reactions $\text{CH}_3\text{Cl} + \text{F}$ and $\text{CH}_2\text{Cl}_2 + \text{F}$ and The Destruction by the Reactions $\text{CH}_2\text{Cl} + \text{O}$ and $\text{CHCl}_2 + \text{O}$ ", *Z. Phys. Chem.* **223** (2009) 409-426.

S. S. Ahmed, F. Mauß, T. Zeuch: "The Generation of a Compact n-Heptane / Toluene Reaction Mechanism Using the Chemistry Guided Reduction (CGR) Technique", *Z. Phys. Chem.* **223** (2009) 551-563.

K. Hoyer mann, S. Maarfeld, F. Nacke, J. Nothdurft, M. Olzmann, J. Wehmeyer, O. Welz, T. Zeuch: "Rate coefficients for cycloalkyl plus O reactions and product branching in the decomposition of chemically activated cycloalkoxy radicals: an experimental and theoretical study", *Phys. Chem. Chem. Phys.* **12** (2010) 8954–8968.

K. Hoyer mann, M. Olzmann, O. Welz, T. Zeuch: " The reaction of iso-propyl radicals with oxygen atoms: Rate coefficient, product branching, and relevance for combustion modeling", *Proc. Comb. Inst.* **33** (2011) 283-291.

J. L. Wolf, S. Richters, J. Pecher, T. Zeuch: " Pressure dependent mechanistic branching in the formation pathways of secondary organic aerosol from cyclic-alkene gas-phase ozonolysis", *Phys. Chem. Chem. Phys.* **13** (2011) 10952-10964.

R. M. Forck, I. Dauster, U. Buck, T. Zeuch: "Sodium Microsolvation in Ethanol: Common Features of $\text{Na}(\text{HO-R})_n$ ($\text{R} = \text{H}, \text{CH}_3, \text{C}_2\text{H}_5$) Clusters", *J. Phys. Chem. A* **115** (2011) 6068-6076.

P. Oßwald, K. Kohse-Höinghaus, U. Struckmeier, T. Zeuch, L. Seidel, L. Leon, F. Mauss: "Combustion chemistry of the butane isomers in premixed low-pressure flames", *Z. Phys. Chem.*, **225** (2011), 1029-1054.

R. M. Forck, C.C Pradzynski, S. Wolff, M. Oncak, P. Slavicek, T. Zeuch: "Size resolved infrared spectroscopy of $\text{Na}(\text{CH}_3\text{OH})_n$ ($n=4-7$) clusters in the OH stretching region: unravelling the interaction of methanol clusters with a sodium atom and the emergence of the solvated electron", *Phys. Chem. Chem. Phys.* **14** (2012) 3004-3016.

- P. T. M. Carlsson, J. E. Dege, C. Keunecke, B. C. Krüger, J. L. Wolf, T. Zeuch: „Pressure dependent aerosol formation from the cyclohexene gas-phase ozonolysis in the presence and absence of sulfur dioxide: a new perspective on the stabilisation of the initial clusters“, *Phys. Chem. Chem. Phys.* **14** (2012) 11695-11705.
- E. Goos, C. Sickfeld, F. Mauß, L. Seidel, B. Ruscic, A. Burcat, T. Zeuch: ” Prompt NO formation in flames: The influence of NCN thermochemistry”, *Proc. Comb. Inst.*, **34** (2013) 657-666.
- M. Schenk, L. Leon, K. Moshhammer, P. Oßwald, K. Kohse-Höinghaus, T. Zeuch, L. Seidel, F. Mauss: ” Detailed mass spectrometric and modeling study of isomeric butene flames”, *Combust. Flame.*, **160** (2013) 487-503.
- L. Seidel, K. Hoyer mann, F. Mauß, J. Nothdurft, T. Zeuch: ” Pressure dependent product formation in the photochemically initiated allyl + allyl reaction.”, *Molecules.*, **18** (2013), 13608-13622.
- U. Buck, C. C. Pradzysnki, T. Zeuch, J. Dieterich, B. Hartke: “A size resolved investigation of large water clusters“, *Phys. Chem. Chem. Phys.* **16** (2014) 6859-6871.
- A. Nawidiyal, N. Hansen, T. Zeuch, L. Seidel, F. Mauß: “Experimental and modelling study of speciation and benzene formation pathways in premixed 1-hexene flames”, *Proc. Combust. Inst.* **35** (2015) 325-332.
- F. Zurheide, C. W. Dierking, C. C. Pradzysnki, R. M. Forck, F. Flüggen, U. Buck, T. Zeuch: “Size-Resolved Infrared Spectroscopic Study of Structural Transitions in Sodium-Doped $(\text{H}_2\text{O})_{(n)}$ Clusters Containing 10-100 Water Molecules”, *J. Phys. Chem. A* **119** (2015) 2709-2720.
- L. Seidel, K. Moshhammer, X. X. Wang, T. Zeuch, K. Kohse-Höinghaus, F. Mauss: ” Comprehensive kinetic modeling and experimental study of a fuel-rich, premixed n-heptane flame”, *Combust. Flame.*, **162** (2015) 2045-2058.
- N. Giemelshein, S. Giemelshein, C. C. Pradzysnki, T. Zeuch, U. Buck: “The temperature and size distribution of large water clusters from a non-equilibrium model”, *J. Chem. Phys.* **132** (2015) 244305.
- C. W. Dierking, F. Zurheide, T. Zeuch, J. Med, S. Perez, P. Slavicek: “Revealing isomerism in sodium-water clusters: Photoionization spectra of $\text{Na}(\text{H}_2\text{O})_n$ ($n=2-90$)”, *J. Chem. Phys.* **146** (2017) 244303.
- P. T. M. Carlsson, T. Zeuch: “Investigation of nucleation kinetics in H_2SO_4 vapor through modeling of gas phase kinetics coupled with particle dynamics”, *J. Chem. Phys.* **148** (2018) 104303.
- K. P. Shrestha, L. Seidel, T. Zeuch, F. Mauß: “Detailed Kinetic Mechanism for the Oxidation of Ammonia Including the Formation and Reduction of Nitrogen Oxides”, *Energ. Fuel* (2018) doi:10.1021/acs.energyfuels.8b01056.