

Full Publication List of Dr. Patrick Hemberger

- [1] B. Noller, **P. Hemberger**, I. Fischer, C. Alcaraz, G. A. Garcia, and H. Soldi-Lose. The photoionisation of two phenylcarbenes and their diazirine precursors investigated using synchrotron radiation. *Phys. Chem. Chem. Phys.*, 2009, **11**, 5384–5391.
- [2] B. K. C. de Miranda, C. Alcaraz, M. Elhanine, B. Noller, **P. Hemberger**, I. Fischer, G. A. Garcia, H. Soldi-Lose, B. Gans, L. A. V. Mendes, S. Boye-Peronne, S. Douin, J. Zabka, and P. Botschwina. Threshold photoelectron spectroscopy of the methyl radical isotopomers, CH_3 , CH_2D , CHD_2 and CD_3 : Synergy between vuv synchrotron radiation experiments and explicitly correlated coupled cluster calculations. *J. Phys. Chem. A*, 2010, **114**, 4818–4830.
- [3] K. H. Fischer, **P. Hemberger**, I. Fischer, and A. M. Rijs. Infrared spectra of reactive species generated by flash pyrolysis in a free jet. *Chemphyschem*, 2010, **11**, 3228–3230.
- [4] M. Steinbauer, **P. Hemberger**, I. Fischer, M. Johnson, and A. Bodi. Photoionization of two substituted methyl radicals: Cyanomethyl and bromomethyl. *Chem. Phys. Lett.*, 2010, **500**, 232–236.
- [5] **P. Hemberger**, B. Noller, M. Steinbauer, I. Fischer, C. Alcaraz, B. K. C. de Miranda, G. A. Garcia, and H. Soldi-Lose. Threshold photoelectron spectroscopy of cyclopropenylidene, chlorocyclopropenylidene, and their deuterated isotopomers. *J. Phys. Chem. A*, 2010, **114**, 11269–11276.
- [6] **P. Hemberger**, B. Noller, M. Steinbauer, K. Fischer, and I. Fischer. The b^1b_1 state of cyclopropenylidene, $c\text{-C}_3\text{H}_2$. *J. Phys. Chem. Lett.*, 2010, **1**, 228–231.
- [7] **P. Hemberger**, M. Steinbauer, M. Schneider, I. Fischer, M. Johnson, A. Bodi, and T. Gerber. Photoionization of three isomers of the C_9H_7 radical. *J. Phys. Chem. A*, 2010, **114**, 4698–4703.
- [8] G. da Silva, A. J. Trevitt, M. Steinbauer, and **P. Hemberger**. Pyrolysis of fulvenallene (C_7H_6) and fulvenallenyl (C_7H_5): Theoretical kinetics and experimental product detection. *Chem. Phys. Lett.*, 2011, **517**, 144–148.
- [9] J. Kohler, **P. Hemberger**, I. Fischer, G. Piani, and L. Poisson. Ultrafast dynamics of isolated fluorone. *J. Phys. Chem. A*, 2011, **115**, 14249–14253.
- [10] M. Steinbauer, **P. Hemberger**, I. Fischer, and A. Bodi. Photoionization of C_7H_6 and C_7H_5 : Observation of the fulvenallenyl radical. *Chemphyschem*, 2011, **12**, 1795–1797.
- [11] **P. Hemberger**, M. Lang, B. Noller, I. Fischer, C. Alcaraz, B. K. C. de Miranda, G. A. Garcia, and H. Soldi-Lose. Photoionization of propargyl and bromopropargyl radicals: A threshold photoelectron spectroscopic study. *J. Phys. Chem. A*, 2011, **115**, 2225–2230.
- [12] A. Bodi, **P. Hemberger**, T. Gerber, and B. Sztaray. A new double imaging velocity focusing coincidence experiment: i(2)pepico. *Rev. Sci. Instrum.*, 2012, **83**, 083105.
- [13] **P. Hemberger***, A. Bodi, C. Schon, M. Steinbauer, K. H. Fischer, C. Kaiser, and I. Fischer. A pass too far: dissociation of internal energy selected paracyclophane cations, theory and experiment. *Phys. Chem. Chem. Phys.*, 2012, **14**, 11920–11929.
- [14] **P. Hemberger**, J. Kohler, I. Fischer, G. Piani, L. Poisson, and J. M. Mestdagh. Femtosecond dynamics of cyclopropenylidene, $c\text{-C}_3\text{H}_2$. *Phys. Chem. Chem. Phys.*, 2012, **14**, 6173–6178.
- [15] A. Bodi, **P. Hemberger**, and T. Gerber. A robust link between the thermochemistry of urea and isocyanic acid by dissociative photoionization. *J. Chem. Thermodyn.*, 2013, **58**, 292–299.
- [16] A. Bodi, **P. Hemberger**, D. L. Osborn, and B. Sztaray. Mass-resolved isomer-selective chemical analysis with imaging photoelectron photoion coincidence spectroscopy. *J. Phys. Chem. Lett.*, 2013, **4**, 2948–2952.
- [17] K. H. Fischer, **P. Hemberger***, A. Bodi, and I. Fischer. Photoionisation of the tropyli radical. *Beilstein J. Org. Chem.*, 2013, **9**, 681–688.
- [18] T. Gerber, Y. Z. Liu, G. Knopp, **P. Hemberger**, A. Bodi, P. Radi, and Y. Sych. Charged particle velocity map image reconstruction with one-dimensional projections of spherical functions. *Rev. Sci. Instrum.*, 2013, **84**, 033101.

- [19] J. Harvey, **P. Hemberger***, A. Bodi, and R. P. Tuckett. Vibrational and electronic excitations in fluorinated ethene cations from the ground up. *J. Chem. Phys.*, 2013, **138**, 124301.
- [20] F. Holzmeier, M. Lang, K. Hader, **P. Hemberger**, and I. Fischer. H_2cn^+ and h_2cnh^+ : New insight into the structure and dynamics from mass-selected threshold photoelectron spectra. *J. Chem. Phys.*, 2013, **138**, 214310.
- [21] M. Lang, F. Holzmeier, I. Fischer, and **P. Hemberger***. Threshold photoionization of fluorenyl, benzhydryl, diphenylmethylene, and their dimers. *J. Phys. Chem. A*, 2013, **117**, 5260–5268.
- [22] Y. Z. Liu, G. Knopp, **P. Hemberger**, Y. Sych, P. Radi, A. Bodi, and T. Gerber. Ultrafast imaging of electronic relaxation in o-xylene: a new competing intersystem crossing channel. *Phys. Chem. Chem. Phys.*, 2013, **15**, 18101–18107.
- [23] P. M. Mayer, D. Staedter, V. Blanchet, **P. Hemberger**, and A. Bodi. Comparing femtosecond multiphoton dissociative ionization of tetrathiafulvene with imaging photoelectron photoion coincidence spectroscopy. *J. Phys. Chem. A*, 2013, **117**, 2753–2759.
- [24] **P. Hemberger***, A. Bodi, T. Gerber, M. Wurtemberger, and U. Radius. Unimolecular reaction mechanism of an imidazolin-2-ylidene: An ipepico study on the complex dissociation of an arduengo-type carbene. *Chem. Eur. J.*, 2013, **19**, 7090–7099.
- [25] **P. Hemberger***, A. J. Trevitt, E. Ross, and G. da Silva. Direct observation of para-xylylene as the decomposition product of the meta-xylyl radical using vuv synchrotron radiation. *J. Phys. Chem. Lett.*, 2013, **4**, 2546–2550.
- [26] A. Bodi and **P. Hemberger**. Imaging breakdown diagrams for bromobutyne isomers with photoelectron-photoion coincidence. *Phys. Chem. Chem. Phys.*, 2014, **16**, 505–515.
- [27] V. B. F. Custodis, **P. Hemberger**, Z. Q. Ma, and J. A. van Bokhoven. Mechanism of fast pyrolysis of lignin: Studying model compounds. *J. Phys. Chem. B*, 2014, **118**, 8524–8531.
- [28] F. Holzmeier, M. Lang, **P. Hemberger**, A. Bodi, M. Schafer, R. D. Dewhurst, H. Braunschweig, and I. Fischer. Photoionization and pyrolysis of a 1,4-azaborinine: Retro-hydroboration in the cation and identification of novel organoboron ring systems. *Chem. Eur. J.*, 2014, **20**, 9683–9692.
- [29] F. Holzmeier, M. Lang, **P. Hemberger***, and I. Fischer. Improved ionization energies for the two isomers of phenylpropargyl radical. *Chemphyschem*, 2014, **15**, 3489–3492.
- [30] M. Lang, F. Holzmeier, I. Fischer, and **P. Hemberger***. Decomposition of diazomeldrum’s acid: A threshold photoelectron spectroscopy study. *J. Phys. Chem. A*, 2014, **118**, 11235–11243.
- [31] N. M. Neisius, M. Lutz, D. Rentsch, **P. Hemberger**, and S. Gaan. Synthesis of dolo-based phosphoramidates and their thermal properties. *Ind. Eng. Chem. Res.*, 2014, **53**, 2889–2896.
- [32] P. Osswald, **P. Hemberger**, T. Bierkandt, E. Akyildiz, M. Kohler, A. Bodi, T. Gerber, and T. Kasper. In situ flame chemistry tracing by imaging photoelectron photoion coincidence spectroscopy. *Rev. Sci. Instrum.*, 2014, **85**, 025101.
- [33] T. Schramm, G. Gantefor, A. Bodi, **P. Hemberger**, T. Gerber, and B. von Issendorff. Photoelectron spectroscopy of size-selected cluster ions using synchrotron radiation. *Appl. Phys. A: Mater. Sci. Process.*, 2014, **115**, 771–779.
- [34] **P. Hemberger***, A. J. Trevitt, T. Gerber, E. Ross, and G. da Silva. Isomer-specific product detection of gas-phase xylyl radical rearrangement and decomposition using vuv synchrotron photoionization. *J. Phys. Chem. A*, 2014, **118**, 3593–3604.
- [35] B. West, A. Sit, A. Bodi, **P. Hemberger**, and P. M. Mayer. Dissociative photoionization and threshold photoelectron spectra of polycyclic aromatic hydrocarbon fragments: An imaging photoelectron photoion coincidence (ipepico) study of four substituted benzene radical cations. *J. Phys. Chem. A*, 2014, **118**, 11226–11234.
- [36] T. Bierkandt, T. Kasper, E. Akyildiz, A. Lucassen, P. Osswald, M. Kohler, and **P. Hemberger**. Flame structure of a low-pressure laminar premixed and lightly sooting acetylene flame and the effect of ethanol addition. *Proc. Combust. Inst.*, 2015, **35**, 803–811.
- [37] J. Bouwman, A. Bodi, J. Oomens, and **P. Hemberger**. On the formation of cyclopentadiene in the $\text{c}_3\text{h}_5\cdot + \text{c}_2\text{h}_2$ reaction. *Phys. Chem. Chem. Phys.*, 2015, **17**, 20508–20514.
- [38] J. Bouwman, B. Sztaray, J. Oomens, **P. Hemberger**, and A. Bodi. Dissociative photoionization of quinoline and isoquinoline. *J. Phys. Chem. A*, 2015, **119**, 1127–1136.

- [39] G. T. Buckingham, T. K. Ormond, J. P. Porterfield, **P. Hemberger**, O. Kostko, M. Ahmed, D. J. Robichaud, M. R. Nimlos, J. W. Daily, and G. B. Ellison. The thermal decomposition of the benzyl radical in a heated micro-reactor. i. experimental findings. *J. Chem. Phys.*, 2015, **142**, 044307.
- [40] D. Felsmann, K. Moshhammer, J. Kruger, A. Lackner, A. Brockhinke, T. Kasper, T. Bierkandt, E. Akyildiz, N. Hansen, A. Lucassen, P. Osswald, M. Kohler, G. A. Garcia, L. Nahon, **P. Hemberger**, A. Bodi, T. Gerber, and K. Kohse-Hoinghaus. Electron ionization, photoionization and photoelectron/photoion coincidence spectroscopy in mass-spectrometric investigations of a low-pressure ethylene/oxygen flame. *Proc. Combust. Inst.*, 2015, **35**, 779–786.
- [41] F. Holzmeier, M. Lang, I. Fischer, X. Tang, B. C. de Miranda, C. Romanzin, C. Alcaraz, and **P. Hemberger**. Threshold photoelectron spectroscopy of unstable n-containing compounds: Resolution of δk subbands in hnco^+ and vibrational resolution in nco^+ . *J. Chem. Phys.*, 2015, **142**, 184306.
- [42] F. Holzmeier, M. Lang, I. Fischer, and **P. Hemberger***. The threshold photoelectron spectrum of cyanovinylacetylene leads to an upward revision of the ionization energy. *Chem. Phys. Lett.*, 2015, **638**, 201–204.
- [43] F. Holzmeier, M. Lang, I. Fischer, **P. Hemberger**, G. A. Garcia, X. Tang, and J. C. Loison. Assignment of high-lying bending mode levels in the threshold photoelectron spectrum of nh_2 : a comparison between pyrolysis and fluorine-atom abstraction radical sources. *Phys. Chem. Chem. Phys.*, 2015, **17**, 19507–19514.
- [44] M. Lang, F. Holzmeier, **P. Hemberger***, and I. Fischer. Threshold photoelectron spectra of combustion relevant c_4h_5 and c_4h_7 isomers. *J. Phys. Chem. A*, 2015, **119**, 3995–4000.
- [45] S. Y. Liang, **P. Hemberger***, N. M. Neisius, A. Bodi, H. Gruetzmacher, J. Levalois-Gruetzmacher, and S. Gaan. Elucidating the thermal decomposition of dimethyl methylphosphonate by vacuum ultraviolet (vuv) photoionization: Pathways to the po radical, a key species in flame-retardant mechanisms. *Chem. Eur. J.*, 2015, **21**, 1073–1080.
- [46] Z. Q. Ma, V. B. F. Custodis, **P. Hemberger**, C. Bahrle, F. Vogel, G. Jeschke, and J. A. van Bokhoven. Chemicals from lignin by catalytic fast pyrolysis, from product control to reaction mechanism. *Chimia*, 2015, **69**, 597–602.
- [47] T. K. Ormond, **P. Hemberger**, T. P. Troy, M. Ahmed, J. F. Stanton, and G. B. Ellison. The ionisation energy of cyclopentadienone: a photoelectron-photoion coincidence study. *Mol. Phys.*, 2015, **113**, 2350–2358.
- [48] J. D. Savee, J. Zador, **P. Hemberger**, B. Sztaray, A. Bodi, and D. L. Osborn. Threshold photoelectron spectrum of the benzyl radical. *Mol. Phys.*, 2015, **113**, 2217–2227.
- [49] **P. Hemberger***, A. Bodi, J. H. J. Berthel, and U. Radius. Intramolecular c-n bond activation and ring-expansion reactions of n-heterocyclic carbenes. *Chem. Eur. J.*, 2015, **21**, 1434–1438.
- [50] **P. Hemberger***, G. da Silva, A. J. Trevitt, T. Gerber, and A. Bodi. Are the three hydroxyphenyl radical isomers created equal? - the role of the phenoxy radical. *Phys. Chem. Chem. Phys.*, 2015, **17**, 30076–30083.
- [51] R. Tuckett, J. Harvey, **P. Hemberger**, and A. Bodi. The vacuum-ultraviolet photoelectron spectra of ch_2f_2 and ch_2cl_2 revisited. *J. Mol. Spectrosc.*, 2015, **315**, 172–183.
- [52] K. Voronova, C. M. M. Easter, K. J. Covert, A. Bodi, **P. Hemberger**, and B. Sztaray. Dissociative photoionization of diethyl ether. *J. Phys. Chem. A*, 2015, **119**, 10654–10663.
- [53] M. F. Heringa, J. G. Slowik, A. S. H. Prevot, U. Baltensperger, **P. Hemberger**, and A. Bodi. Dissociative ionization mechanism and appearance energies in adipic acid revealed by imaging photoelectron photoion coincidence, selective deuteration, and calculations. *J. Phys. Chem. A*, 2016, **120**, 3397–3405.
- [54] F. Holzmeier, I. Fischer, B. Kiendl, A. Krueger, A. Bodi, and **P. Hemberger***. On the absolute photoionization cross section and dissociative photoionization of cyclopropenylidene. *Phys. Chem. Chem. Phys.*, 2016, **18**, 9240–9247.
- [55] F. Holzmeier, I. Wagner, I. Fischer, A. Bodi, and **P. Hemberger***. Pyrolysis of 3-methoxypyridine. detection and characterization of the pyrrolyl radical by threshold photoelectron spectroscopy. *J. Phys. Chem. A*, 2016, **120**, 4702–4710.
- [56] D. L. Osborn, C. C. Hayden, **P. Hemberger**, A. Bodi, K. Voronova, and B. Sztaray. Breaking through the false coincidence barrier in electron-ion coincidence experiments. *J. Chem. Phys.*, 2016, **145**, 164202.

- [57] K. Voronova, C. M. M. Easter, K. G. Torma, A. Bodi, **P. Hemberger**, and B. Sztaray. Bifurcated dissociative photoionization mechanism of acetic acid anhydride revealed by imaging photoelectron photoion coincidence spectroscopy. *Phys. Chem. Chem. Phys.*, 2016, **18**, 25161–25168.
- [58] T. Bierkandt, **P. Hemberger**, P. Osswald, M. Kohler, and T. Kasper. Insights in m-xylene decomposition under fuel-rich conditions by imaging photoelectron photoion coincidence spectroscopy. *Proc. Combust. Inst.*, 2017, **36**, 1223–1232.
- [59] A. Bodi, **P. Hemberger**, and R.P. Tuckett. Coincident velocity map image reconstruction illustrated by the single-photon valence photoionisation of cf_3sf_5 . *Phys. Chem. Chem. Phys.*, 2017, **19**, 30173–30180.
- [60] V. B. F. Custodis, **P. Hemberger**, and J. A. van Bokhoven. How inter- and intramolecular reactions dominate formation of products in lignin pyrolysis. *Chem. Eur. J.*, 2017, **23**, 8658–8668.
- [61] M. F. Heringa, J. G. Slowik, M. Goldmann, R. Signorell, **P. Hemberger**, and A. Bodi. The distant double bond determines the fate of the carboxylic group in the dissociative photoionization of oleic acid. *Chem. Phys. Chem.*, 2017, **18**, 3595–3604.
- [62] F. Holzmeier, M.P. Herbert, I. Fischer, M. Steglich, A. Bodi, and **P. Hemberger***. A photoionization study of 2-propyl and t-butyl radicals. *J. Anal. Appl. Pyrolysis*, 2017, **124**, 454–460.
- [63] S. Liang, **P. Hemberger***, J. Levalois-Gruetzmacher, H. Gruetzmacher, and S. Gaan. Probing phosphorus nitride (pn) and other elusive species formed upon pyrolysis of dimethyl phosphoramidate. *Chem. Eur. J.*, 2017, **23**, 5595–5601.
- [64] K. Pachner, M. Steglich, **P. Hemberger**, and I. Fischer. Photodissociation dynamics of the ortho- and para-xylyl radicals. *J. Chem. Phys.*, 2017, **147**, 084303.
- [65] J. I. M. Pastoors, A. Bodi, **P. Hemberger**, and J. Bouwman. Dissociative ionization and thermal decomposition of cyclopentanone. *Chem. Eur. J.*, 2017, **23**, 13131–13140.
- [66] E. Reusch, F. Holzmeier, P. Constantinidis, **P. Hemberger***, and Ingo Fischer. Isomer-selective generation and spectroscopic characterization of picolyl radicals. *Angew. Chem. Int. Ed.*, 2017, **56**, 8000–8003.
- [67] M. Steglich, V. B. F. Custodis, A J. Trevitt, G. daSilva, Andras Bodi, and **P. Hemberger***. Photoelectron spectrum and energetics of the meta-xylylene diradical. *J. Am. Chem. Soc.*, 2017, **139**, 14348.
- [68] B. Sztaray, K. Voronova, K. Torma, K. Covert, A. Bodi, **P. Hemberger**, T. Gerber, and D. L. Osborn. Crf-pepico: Double velocity map imaging photoelectron photoion coincidence spectroscopy for reaction kinetics studies. *J. Chem. Phys.*, 2017, **147**, 013944.
- [69] **P. Hemberger***, V. B. F. Custodis, A. Bodi, T. Gerber, and J. A. van Bokhoven. Understanding the mechanism of catalytic fast pyrolysis by unveiling reactive intermediates in heterogeneous catalysis. *Nat. Commun.*, 2017, **8**, 15946.
- [70] X. Wu, X. Zhou, **P. Hemberger**, and A. Bodi. Dissociative photoionization of dimethyl carbonate: The more it is cut, the bigger the fragment ion. *J. Phys. Chem. A*, 2017, **121**, 2748–2759.
- [71] J. Bouwman, Andras Bodi, and **P. Hemberger**. Nitrogen matters: the difference between panh and pah formation. *Phys. Chem. Chem. Phys.*, 2018, **20**, 29910.
- [72] A. Candian, J. Bouwman, **P. Hemberger**, A. Bodi, and A. G. G. M. Tielens. Dissociative ionisation of adamantane: a combined theoretical and experimental study. *Phys. Chem. Chem. Phys.*, 2018, **20**, 5399–5406.
- [73] F. Hirsch, E. Reusch, P. Constantinidis, I. Fischer, S. Bakels, Rijs A. M., and **P. Hemberger***. Self-reaction of ortho-benzyne at high temperatures investigated by infrared and photoelectron spectroscopy. *J. Phys. Chem. A*, 2018, **122**, 9563.
- [74] D. Kaiser, E. Reusch, **P. Hemberger***, A. Bodi, E. Welz, B. Engels, and I. Fischer. The ortho-benzyne cation is not planar. *Phys. Chem. Chem. Phys.*, 2018, **20**, 3988–3966.
- [75] D. Kruger, P. Osswald, M. Kohler, **P. Hemberger**, T. Bierkandt, Y. Karakaya, and T. Kasper. Hydrogen abstraction ratios: A systematic ipepico spectroscopic investigation in laminar flames. *Combustion and Flam*, 2018, **191**, 343–352.
- [76] T. K. Ormond, J. H. Baraban, J. P. Porterfield, A. M. Scheer, **P. Hemberger**, T. P. Troy, M. Ahmed, M. R. Nimlos, D. J. Robichaud, J. W Daily, and G. B. Ellison. Thermal decompositions of the lignin model compounds: Salicylaldehyde and catechol. *J. Phys. Chem. A*, 2018, **122**, 5911–5924.
- [77] V. Paunovic, **P. Hemberger**, A. Bodi, N. Lopez, and J. Perez-Ramirez. Evidence of radical chemistry in catalytic methane oxybromination. *Nat. Catal.*, 2018, **1**, 363–370.

- [78] D. Schleier, P. Constantinidis, N. Faßheber, I. Fischer, G. Friedrichs, **P. Hemberger***, E. Reusch, B. Sztaray, and K. Voronova. Kinetics of the $\alpha\text{-C}_3\text{H}_5 + \text{O}_2$ reaction, investigated by photoionization using synchrotron radiation. *Phys. Chem. Chem. Phys.*, 2018, 20, 10721–10731.
- [79] M. Steglich, A. Bodi, J.P. Maier, and **P. Hemberger***. Probing different spin states in xylyl radicals and ions. *Phys. Chem. Chem. Phys.*, 2018, 20, 7180–7189.
- [80] **P. Hemberger*** and A. Bodi. Photoelectron photoion coincidence spectroscopy to unveil reaction mechanisms by isomer-selective detection of elusive molecules: From combustion to catalysis. *Chimia*, 2018, 72, 227–232.
- [81] K. Voronova, K.M. Ervin, K.G. Torma, **P. Hemberger**, A. Bodi, T. Gerber, D.L. Osborn, and B. Sztaray. Radical thermometers, thermochemistry, and photoelectron spectra: A photoelectron photoion coincidence spectroscopy study of the methyl peroxy radical. *J. Phys. Chem. Lett.*, 2018, 9, 534–539.
- [82] I. Antonov, K. Voronova, M.W. Chen, B. Sztaray, **P. Hemberger**, A. Bodi, D. L. Osborn, and L. Sheps. To boldly look where no one has looked before: Identifying the primary photoproducts of acetylacetone. *J. Phys. Chem. A*, 2019, 123, 5472–5490.
- [83] T. Bierkandt, **P. Hemberger**, P. Oßwald, D. Krüger, M. Köhler, and T. Kasper. Flame structure of laminar premixed anisole flames investigated by photoionization mass spectrometry and photoelectron spectroscopy. *Proc. Combust. Inst.*, 2019, 37, 1579–1587.
- [84] T. Bierkandt, **P. Hemberger**, P. Osswald, D. Kruger, M. Kohler, and T. Kasper. Flame structure of laminar premixed anisole flames investigated by photoionization mass spectrometry and photoelectron spectroscopy. *Proc. Combust. Inst.*, 2019, 37, 1579–1587.
- [85] A. Bodi and **P. Hemberger**. Low-energy photoelectron spectrum and dissociative photoionization of the smallest amides: Formamide and acetamide. *J. Phys. Chem. A*, 2019, 123, 272–283.
- [86] M. Gerlach, A. Bodi, and **P. Hemberger***. Metamorphic meta isomer: carbon dioxide and ketenes are formed via retro-diels-alder reactions in the decomposition of meta-benzenediol. *Phys. Chem. Chem. Phys.*, 2019, 21, 19480–19487.
- [87] D. Kruger, P. Osswald, M. Kohler, **P. Hemberger**, T. Bierkandt, and T. Kasper. The fate of the oh radical in molecular beam sampling experiments. *Proc. Combust. Inst.*, 2019, 37.
- [88] K. Majer, R. Signorell, M. F. Heringa, M. Goldmann, **P. Hemberger**, and A. Bodi. Valence photoionization of thymine: ionization energies, vibrational structure, and fragmentation pathways from the slow to the ultrafast. *Chem. Eur. J.*, 2019, 25, 14192–14204.
- [89] V. Paunovic, G. Zichittella, **P. Hemberger**, A. Bodi, and J. Perez-Ramirez. Selective methane functionalization via oxyhalogenation over supported noble metal nanoparticles. *ACS Catalysis*, 2019, 9, 1710–1725.
- [90] M.B. Prendergast, B. B. Kirk, J. D. Savee, D. L. Osborn, C.A. Taatjes, **P. Hemberger**, S.J. Blanksby, G. da Silva, and A.J. Trevitt. Product detection study of the gas-phase oxidation of methylphenyl radicals using synchrotron photoionisation mass spectrometry. *Phys. Chem. Chem. Phys.*, 2019, 21, 17939–17949.
- [91] E. Reusch, F. Holzmeier, M. Gerlach, I. Fischer, and **P. Hemberger***. Decomposition of picolyl radicals at high temperature: a mass selective threshold photoelectron spectroscopy study. *Chem. Eur. J.*, 2019, 25, 16652–16659.
- [92] E. Reusch, D. Kaiser, D. Schleier, R. Buschmann, A. Krueger, T. Hermann, B. Engels, I. Fischer, and **P. Hemberger***. Pentadiynylidene and its methyl-substituted derivatives: Threshold photoelectron spectroscopy of r1-c5-r2 triplet carbon chains. *J. Phys. Chem. A*, 2019, 123, 2008–2017.
- [93] G. Rouillé, M. Steglich, **P. Hemberger**, C. Jäger, and T. Henning. Threshold dissociation of the 1-ethynylpyrene cation at internal energies relevant to hi regions. *Astrophys. J.*, 2019, 885, 21 (10 pp.).
- [94] D. Schleier, E. Reusch, L. Lummel, **P. Hemberger**, and I. Fischer. Threshold photoelectron spectroscopy of io and hoi. *ChemPhysChem*, 2019, 20, 2413–2416.
- [95] M. Steglich, G. Knopp, and **P. Hemberger***. How the methyl group position influences the ultrafast deactivation in aromatic radicals. *Phys. Chem. Chem. Phys.*, 2019, 21, 581–588.
- [96] C. H. Strobel, G. Gantefoer, A. Bodi, and **P. Hemberger**. A magnetic bottle time-of-flight electron spectrometer suitable for continuous ionization sources. *Rev. Sci. Instrum.*, 2019, 90, 063105.
- [97] **P. Hemberger**, T. Gerber, and A. Bodi. Conference report ptpc2019: Photon tools for physical chemistry 2019. *Chimia*, 2019, 73, 210–211.

- [98] X. Wu, X. Zhou, **P. Hemberger**, and A Bodi. The ionization energy of the vinyl radical: a mexican standoff with a happy ending. *Phys. Chem. Chem. Phys.*, 2019, **21**, 22238–22247.
- [99] G. Zichittella, M. Scharfe, B. Puertolas, V. Paunovic, **P. Hemberger**, A. Bodi, L. Szentmiklosi, Nuria Lopez, and J. Perez-Ramirez. Halogen-dependent surface confinement governs selective alkane functionalization to olefins. *Angew. Chem. Int. Ed.*, 2019, **58**, 5877–5881.
- [100] S. Feng, X. Lin, X. Song, Y. Liu, Z. Jiang, **P. Hemberger**, A. Bodi, and Y. Ding. The role of h₂ on the stability of the single-metal-site ir₁/ac catalyst for heterogeneous methanol carbonylation. *J. Catal.*, 2020, **381**, 193–203.
- [101] S. Feng, **P. Hemberger**, A. Bodi, X. Song, T. Yu, Z. Jiang, Y. Liu, and Y. Ding. Preparation and regeneration of supported single-ir-site catalysts by nanoparticle dispersion via co and nascent i radicals. *J. Catal.*, 2020, **382**, 347–357.
- [102] M. Hoener, D. Kaczmarek, T. Bierkandt, A. Bodi, **P. Hemberger**, and T Kasper. A pressurized flow reactor combustion experiment interfaced with synchrotron double imaging photoelectron photoion coincidence spectroscopy. *Rev. Sci. Instrum.*, 2020, **91**, 045115.
- [103] S. Liang, **P. Hemberger***, M. Steglich, P. Simonetti, J. Levalois-Grützmacher, H. Grützmacher, and S. Gaan. The underlying chemistry to formation of po₂ radicals from organophosphorus compounds - a missing puzzle piece in the flame chemistry. *Chem. Eur. J.*, 2020, **26**, 10795–10800.
- [104] M. N. McCabe, **P. Hemberger**, E. Reusch, A. Bodi, and J. Bouwman. Off the beaten path: almost clean formation of indene from the ortho-benzyne + allyl reaction. *J. Phys. Chem. Lett.*, 2020, **11**, 2859–2863.
- [105] E. Mendez-Vega, W. Sander, and **P. Hemberger***. Isomer-selective threshold photoelectron spectra of phenylnitrene and its thermal rearrangement products. *J. Phys. Chem. A*, 2020, **124**, 3836–3843.
- [106] D. P. Mukhopadhyay, D. Schleier, S. Wirsing, J. Ramler, D. Kaiser, E. Reusch, **P. Hemberger**, T. Preitschopf, I. Krummenacher, B. Engels, I. Fischer, and C. Lichtenberg. Methylbismuth: an organometallic bismuthinidene biradical. *Chem. Sci*, 2020, **11**, 7562–7568.
- [107] C. Strobel, G. Gantfoer, A. Bodi, and **P. Hemberger**. Gridless electron trap for a high-duty cycle magnetic bottle time-of-flight spectrometer. *J. Electron Spectrosc. Relat. Phenom.*, 2020, **239**, 146900.
- [108] **P. Hemberger***, Z. Pan, A. Bodi, J. A van Bokhoven, T. K Ormond, G. B. Ellison, N. Genossar, and J. H. Baraban. On the threshold photoelectron spectrum of fulvenone, a reactive ketene derivative in lignin valorization. *Chem. Phys. Chem.*, 2020, **21**, 2217–2222.
- [109] **P. Hemberger***, J. A. van Bokhoven, J. Pérez-Ramírez, and A. Bodi. New analytical tools for advanced mechanistic studies in catalysis: photoionization and photoelectron photoion coincidence spectroscopy. *Catal. Sci. Technol.*, 2020, **10**, 1975–1990.
- [110] X. Wu, X. Zhou, **P. Hemberger**, and A. Bodi. Conformers, electronic states, and diabolical conical intersections in the valence photoelectron spectroscopy of halocyclohexanes. *J. Chem. Phys.*, 2020, **153**, 054305.
- [111] X. Wu, X. Zhou, **P. Hemberger**, and A. Bodi. A guinea pig for conformer selectivity and mechanistic insights into dissociative ionization by photoelectron photoion coincidence: fluorocyclohexane. *Phys. Chem. Chem. Phys.*, 2020, **22**, 2351–2360.
- [112] T. Yu, X. Wu, X. Zhou, A. Bodi, and **P. Hemberger***. Hydrogen migration as a potential driving force in the thermal decomposition of dimethoxymethane: New insights from pyrolysis imaging photoelectron photoion coincidence spectroscopy and computations. *Combust. Flame*, 2020, **222**, 123–132.
- [113] G. Zichittella, **P. Hemberger***, F. Holzmeier, A. Bodi, and J. Pérez-Ramírez. Operando photoelectron photoion coincidence spectroscopy unravels mechanistic fingerprints of propane activation by catalytic oxyhalogenation. *J. Phys. Chem. Lett.*, 2020, **11**, 856–863.
- [114] T. Bierkandt, P. Osswald, N. Gaiser, D. Kruger, M. Kohler, M. Hoener, S. Shaqiri, D. Kaczmarek, Y. Karakaya, **P. Hemberger**, and T. Kasper. Observation of low-temperature chemistry products in laminar premixed low-pressure flames by molecular-beam mass spectrometry. *Int. J. Chem. Kin.*, 2021, **53**, 1063–1081.
- [115] A. Bodi, **P. Hemberger**, and R.P. Tuckett. From energetics to intracluster chemistry: Valence photoionization of trifluoromethylsulfur pentafluoride (cf₃sf₅) by double velocity map imaging. *J. Phys Chem. A.*, 2021, **125**, 2601–2611.

- [116] L. Bosse, B. P. Mant, D. Schleier, M. Gerlach, I. Fischer, A. Krueger, **P. Hemberger**, and G. Worth. Threshold photoelectron spectrum of cyclobutadiene: Comparison with time-dependent wavepacket simulations. *J. Phys. Chem. Lett.*, 2021, **12**, 6901–6906.
- [117] J. Bouwman, H. R. Hrodmarsson, G. B. Ellisson, A. Bodi, and **P. Hemberger**. Five birds with one stone: Photoelectron photoion coincidence unveils rich phthalide pyrolysis chemistry. *J. Phys. Chem. A.*, 2021, **125**, 1738–1746.
- [118] G. A. Garcia, and F. Holzmeier J. C. Loison, B. Gans, L. Nahon C. Alcaraz, X. Wu, X. Zhou, A. Bodi, and **P. Hemberger***. Characterisation of the first electronically excited state of protonated acetylene c2h3+ by coincident imaging photoelectron spectroscopy. *Molec. Phys.*, 2021, **119**, 1–2.
- [119] M. Gerlach, S. Monninger, D. Schleier, **P. Hemberger**, J. T. Goettel, H. Braunschweig, and I. Fischer. Photoelectron photoion coincidence spectroscopy of ncl3 and ncl2. *Chem. Phys. Chem.*, 2021, **22**, 2164–2167.
- [120] S. Grimm, S. Baik, **P. Hemberger**, A. Bodi, A. M. Kempf, T. Kasper, and B Atakan. Gas-phase aluminium acetylacetonate decomposition: revision of the current mechanism by vuv synchrotron radiation. *Phys. Chem. Chem. Phys.*, 2021, **23**, 15059–15075.
- [121] M. Hoener, A. Bodi, **P. Hemberger**, T. Endres, and Tina Kasper. Threshold photoionization shows no sign of nitril hydride in methane oxidation with nitric oxide. *Phys. Chem. Chem. Phys.*, 2021, **23**, 1265–1272.
- [122] X. Li, S. Feng, **P. Hemberger**, A. Bodi, X. Song, Q. Yuan, J. Mu, B. Li, Z. Jiang, and Y. Ding. Iodide-coordinated single-site pd catalysts for alkyne dialkoxycarbonylation. *ACS Catal.*, 2021, **11**, 9242–9251.
- [123] Z. Pan, A. Puente-Urbina, A. Bodi, J. A van Bokhoven, and **P. Hemberger***. Isomer-dependent catalytic pyrolysis mechanism of the lignin model compounds catechol, resorcinol and hydroquinone. *Chem. Sci.*, 2021, **12**, 3161–3169.
- [124] A. Puente-Urbina, Z. Pan, V. Paunovic, P. Sot, **P. Hemberger**, and J. A van Bokhoven. Direct evidence on the mechanism of methane conversion under non-oxidative conditions over iron-modified silica: The role of propargyl radicals unveiled. *Angew. Chem. Int. Ed.*, 2021, **133**, 24204–24209.
- [125] D. Schleier, E. Reusch, M. Gerlach, T. Preitschopf, D. P. Mukhopadhyay, N. Faßheber, G. Friedrichs, **P. Hemberger***, and I. Fischer. Kinetics of 1- and 2-methylallyl + o2 reaction, investigated by photoionisation using synchrotron radiation. *Phys. Chem. Chem. Phys.*, 2021, **23**, 1539–1549.
- [126] M. Steglich, X. Wu, A. Bodi, and **P. Hemberger***. Double-imaging photoelectron photoion coincidence spectroscopy reveals the unimolecular thermal decomposition mechanism of dimethyl carbonate. *J. Phys Chem. A.*, 2021, **125**, 2895–2904.
- [127] **P. Hemberger***, A. Bodi, T. Bierkandt, M. Kohler, D. Kaczmarek, and T. Kasper. Photoelectron photoion coincidence spectroscopy provides mechanistic insights in fuel synthesis and conversion. *Energy Fuels*, 2021, **35**, 16265–26302.
- [128] X. Wu, X. Zhou, S. Bjelic, **P. Hemberger**, and A. Bodi. Valence photoionization and energetics of vanillin, a sustainable feedstock candidate. *J. Phys. Chem. A*, 2021, **125**, 3327–3340.
- [129] X. Wu, X. Zhou, **P. Hemberger**, and Andras Bodi. Dissociative photoionization of chloro-, bromo-, and iodocyclohexane: Thermochemistry and the weak c-br bond in the cation. *J. Phys Chem. A.*, 2021, **125**, 646–656.
- [130] A. Bodi, **P. Hemberger**, and Javier Pérez-Ramírez. Photoionization reveals catalytic mechanisms. *Nat. Catal.*, 2022, **5**, 850–851.
- [131] A. Cesarini, S. Mitchell, G. Zichittella, M. Agrachev, S. P. Schmid, G. Jeschke, Z. Pan, A. Bodi, **P. Hemberger***, and J. Pérez-Ramírez. Elucidation of radical- and oxygenate-driven paths in zeolite-catalysed conversion of methanol and methyl chloride to hydrocarbons. *Nat. Catal.*, 2022.
- [132] C. Fernholz, A. Bodi, and **P. Hemberger***. Threshold photoelectron spectrum of the phenoxy radical. *J. Phys Chem. A.*, 2022, **126**, 9022.
- [133] N. Gaiser, T. Bierkandt, P. Osswald, J. Zinsmeister, T. Kathrotia, S. Shaqiri, **P. Hemberger**, T. Kasper, M. Aigner, and M. Köhler. Oxidation of oxymethylene ether (ome0â5): An experimental systematic study by mass spectrometry and photoelectron photoion coincidence spectroscopy. *Fuel*, 2022, **313**, 122650.

- [134] N. Gaiser, T. Bierkandt, P. Osswald, J. Zinsmeister, **P. Hemberger**, S. Shaqiri, M. Aigner, T. Kasper, and M. Köhler. Oxidation of linear and branched ethers: A comparative flow reactor study of ome2 and trimethoxymethane. *Proc. Combust. Inst.*, 2022, <https://doi.org/10.1016/j.proci.2022.08.112>.
- [135] N. Gaiser, H. Zhang, T. Bierkandt, S. Schmitt, J. Zinsmeister, T. Kathrotia, **P. Hemberger**, S. Shaqiri, T. Kasper, M. Aigner, P. Oßwald, and M. Köhler. Investigation of the combustion chemistry in laminar, low-pressure oxymethylene ether flames (ome0–4). *Combust. Flame*, 2022, page 112060.
- [136] M. Gerlach, E. Karaev, D. Schaffner, **P. Hemberger***, and I. Fischer. Threshold photoelectron spectrum of m-benzyne. *J. Phys Chem. A.*, 2022, **13**, 11295.
- [137] S. Grimm, S. Baik, **P. Hemberger**, T. Kasper, Andreas M. Kempf, and B. Atakan. Insights into the decomposition of zirconium acetylacetonate using synchrotron radiation: Routes to the formation of volatile zr-intermediates. *J. Mater. Res.*, 2022, **37**, 1558–1575.
- [138] S. Grimm, **P. Hemberger**, T. Kasper, and B. Atakan. Mechanism and kinetics of the thermal decomposition of fe(c5h5)2 in inert and reductive atmosphere: A synchrotron-assisted investigation in a microreactor. *Adv. Mater. Interfaces*, 2022, **9**, 2200192.
- [139] M. N. McCabe, **P. Hemberger**, D. Campisi, J. C. Broxterman, E. Reusch, A. Bodi, and J. Bouwman. Formation of phenylacetylene and benzocyclobutadiene in the ortho-benzyne + acetylene reaction. *Phys. Chem. Chem. Phys.*, 2022, **24**, 1869–1876.
- [140] Z. Pan, A. Bodi, J. A. van Bokhoven, and **P. Hemberger***. On the absolute photoionization cross section and threshold photoelectron spectrum of two reactive ketenes in lignin valorization: fulvenone and 2-carbonyl cyclohexadienone. *Phys. Chem. Chem. Phys.*, 2022, **24**, 3655–3663.
- [141] Z. Pan, A. Bodi, J. A. van Bokhoven, and **P. Hemberger***. Operando pepico unveils the catalytic fast pyrolysis mechanism of the three methoxyphenol isomers. *Phys. Chem. Chem. Phys.*, 2022, **24**, 21786–21793.
- [142] V. Paunovic, **P. Hemberger**, A. Bodi, R. Hauert, and J. A. van Bokhoven. Impact of nonzeolite-catalyzed formation of formaldehyde on the methanol-to-hydrocarbons conversion. *ACS Catal.*, 2022, **12**, 13426–13434.
- [143] J. D. Savee, B. Sztaray, **P. Hemberger**, J. Zádor, A. Bodi, and D. L. Osborn. Unimolecular isomerisation of 1,5-hexadiyne observed by threshold photoelectron photoion coincidence spectroscopy. *Faraday Discuss.*, 2022, Doi: 10.1039/D2FD00028H.
- [144] D. Schleier, M. Gerlach, D. Schaffner and D. P. Mukhopadhyay an, **P. Hemberger***, and I. Fischer. Threshold photoelectron spectroscopy of trimethylborane and its pyrolysis products. *Phys. Chem. Chem. Phys.*, 2022, **25**, 4511.
- [145] D. Schleier, M. Gerlach, D. Mukhopadhyay, E. Karaev, D. Schaffner, **P. Hemberger***, and I. Fischer. Ammonia borane, nh3bh3: A threshold photoelectron–photoion coincidence study of a potential hydrogen-storage material. *Chem. Eur. J.*, 2022, **28**, e202201378.
- [146] D. Schleier, D. Schaffner, M. Gerlach, **P. Hemberger**, and I. Fischer. Threshold photoelectron spectroscopy of iminoborane, hbnh. *Phys. Chem. Chem. Phys.*, 2022, **24**, 20–24.
- [147] D. Schleier, **P. Hemberger**, A. Bodi, and J. Bouwman. Threshold photoelectron spectroscopy of quinoxaline, quinazoline, and cinnoline. *J. Phys Chem. A.*, 04 2022, **126**, 2211–2221.
- [148] **P. Hemberger***, X. Wu, Z. Pan, and A. Bodi. Continuous pyrolysis microreactors: Hot sources with little cooling? new insights utilizing cation velocity map imaging and threshold photoelectron spectroscopy. *J. Phys Chem. A.*, 04 2022, **126**, 2196–2210.
- [149] X. Wu, Z. Pan, S. Bjelic, **P. Hemberger**, and A. Bodi. Unimolecular thermal decarbonylation of vanillin stifled by the bimolecular reactivity of methyl-loss intermediate. *J. Anal. Appl. Pyrolysis*, 2022, **161**, 105410.
- [150] X. Wu, Z. Zhang, S. Pan, Z. nd Bjelić, A. Bodi, and **P. Hemberger***. Isomer-dependent selectivities in the pyrolysis of anisaldehyde. *Energy Fuels*, 07 2022, **36**, 7200–7205.
- [151] X. Wu, Z. Zhang, Z. Pan, X. Zhou, A. Bodi, and **P. Hemberger***. Ketenes in the induction of the methanol-to-olefins process. *Angew. Chem. Int. Ed.*, 2022, **61**, e2022077777.
- [152] X. Wu, X. Zhou, S. Bjelic, **P. Hemberger**, B. Sztáray, and A. Bodi. A plethora of isomerization processes and hydrogen scrambling in the fragmentation of the methanol dimer cation: a pepico study. *Phys. Chem. Chem. Phys.*, 2022, **24**, 1437–1446.

- [153] J. Zinsmeister, N. Gaiser, J. Melder, T. Bierkandt, **P. Hemberger**, T. Kasper, M. Aigner, M. Köhler, and P. Oßwald. On the diversity of fossil and alternative gasoline combustion chemistry: A comparative flow reactor study. *Combust. Flame*, 2022, page 111961.
- [154] J. Bouwman, M. N. McCabe, C. N. Shingledecker, J. Wandishin, V. Jarvis, E. Reusch, **P. Hemberger**, and A. Bodi. Five-membered ring compounds from the ortho-benzyne + methyl radical reaction under interstellar conditions. *Nat. Aston.*, 2023, 7, 423.
- [155] I. Fischer and **P. Hemberger***. Photoelectron photoion coincidence spectroscopy of biradicals. *Chem. Phys. Chem.*, 2023, 24, e202300334.
- [156] N. Genossar-Dan, S. Atlas, D. Fux, S. Har Lavan, U. Zamir, I. Rozenberg, T. Lam Nguyen, **P. Hemberger**, and J. H. Baraban. Direct observation of the ethyl radical in the pyrolysis of ethane. *Angew. Chem. Int. Ed.*, 2023, 62, e2023058.
- [157] M. Gerlach, B. Mant, T. Preitschopf, E. Karaev, D. Mayer, H. M. Quitián-Lara, **P. Hemberger**, J. Bozek, G. Worth, and I. Fischer. Photoelectron spectroscopy and dissociative photoionization of fulminic acid, hcnO. *J. Chem. Phys.*, 04 2023, **158**. 134303.
- [158] S. J. Goettl, L. B. Tuli, Y. Reyes A. M. Turner, A. H. Howlader, S. F. Wnuk, **P. Hemberger***, A. M. Mebel, and Ralf I. Kaiser. Gas-phase synthesis of coronene through stepwise directed ring annulation. *J. Am. Chem. Soc.*, 2023, 145, 15443–15455.
- [159] J. Kamer, D. Schleier, M. Donker, **P. Hemberger**, A. Bodi, and J. Bouwman. Threshold photoelectron spectrum and dissociative photoionization of benzonitrile. *Phys. Chem. Chem. Phys.*, 2023, 25, 29070.
- [160] K. Kanayama, C. Fernholz, H. Nakamura, K. Maruta, A. Bodi, and **P. Hemberger***. Lutidyl radical photoelectron spectra reveal additive substituent effects on benzyl derivatives' ionization energy. *Chem. Phys. Chem.*, 2023, 24, e202300359.
- [161] E. Karaev, M. Gerlach, L. Faschingbauer, J. Ramler, I. Krummenacher, C. Lichtenberg, **P. Hemberger***, and I. Fischer. Bonding in low-coordinated organoarsenic and organoantimony compounds: A threshold photoelectron spectroscopic investigation. *Chem. Eur. J.*, 2023, 29, e202300637.
- [162] N. Lokachari, G. Kukkadapu, B. D. Etz, G. M. Fioroni, S. Kim an M. Steglich, A. Bodi, **P. Hemberger**, S. S. Matveev, A. Thomas, H. Song, G. Vanhove, K. Zhang, G. Dayma, M. Lailliau, Z. Serinyel, A. A. Konnov, P. Dagaut, W. J. Pitz, and H. J. Curran. A comprehensive experimental and kinetic modeling study of di-isobutylene isomers: Part 2. *Combust. Flame*, 2023, 251, 112547.
- [163] N. Lokacharia, G. Kukkadapu, H. Song, G. Vanhove, M. Lailliau, G. Dayma, Z. Serinyel, K. Zhang, R. Dauphin, B. Etz, S. Kim, M. Steglich, A. Bodi, G. Fioroni, **P. Hemberger**, S. S. Matveev, A. A. Konnov, P. Dagaut, , S. Wagnon, W. J. Pitz, and H. J. Curran. A comprehensive experimental and kinetic modeling study of di-isobutylene isomers: Part 1. *Combust. Flame*, 2023, 251, 112301.
- [164] Z. Pan, A. Puente-Urbina, S. Rabia Batool, A. Bodi, X. Wu, Z. Zhang, J. A van Bokhoven, and **P. Hemberger***. Tuning the zeolite acidity enables selectivity control by suppressing ketene formation in lignin catalytic pyrolysis. *Nat. Commun.*, 2023, 14, 4512.
- [165] C. W. P. Pare, P. Rzepka, **P. Hemberger**, A. Bodi, R. Hauert, J. A. van Bokhoven, and V. Paunovic. Formaldehyde-induced deactivation of zsm5 catalysts during the methanol-to-hydrocarbons conversion. *ACS Catal.*, 2023, 14, 463.
- [166] M. Saraswat, A. Portela-Gonzalez, G. Karir, E. Mendez-Vega, W. Sander, and **P. Hemberger***. Photoelectron spectroscopic study of 2-naphthyl nitrene and its thermal rearrangement to cyanoidenes. *Phys. Chem. Chem. Phys.*, 2023, 25, 31146.
- [167] M. Saraswat, A. Portela-Gonzalez, G. Karir, E. Mendez-Vega, W. Sander, and **P. Hemberger***. Thermal decomposition of 2- and 4-iodobenzyl iodide yields fulvenallene and ethynylcyclopentadienes: A joint threshold photoelectron and matrix isolation spectroscopic study. *J. Phys Chem. A.*, 2023, 127, 8574.
- [168] **P. Hemberger***, Z. Pan, X. Wu, Z. Zhang, K. Kanayama, and A. Bodi. Photoion mass-selected threshold photoelectron spectroscopy to detect reactive intermediates in catalysis: From instrumentation and examples to peculiarities and a database. *J. Phys. Chem. C*, 2023, 127, 16751–16763.
- [169] L. B. Tuli, S. J. Goettl, A. M. Turner, A. H. Howlader, **P. Hemberger***, S. F. Wnuk, T. Guo, A. M. Mebel, and R. I. Kaiser. Gas phase synthesis of the c40 nano bowl c40h10. *Nat. Commun.*, 2023, 14, 1527.
- [170] X. Wu, S. Bjelić, **P. Hemberger**, and Andras Bodi. Isomer-dependent threshold photoelectron spec-

- troscopy and dissociative photoionization mechanism of anisaldehyde. *J. Phys Chem. A.*, 2023, **127**, 661.
- [171] X. Wu, Z. Pan, M. Steglich, P. Ascher, A. Bodi, S. Bjelić, and **P. Hemberger***. A direct liquid sampling interface for photoelectron photoion coincidence spectroscopy. *Rev. Sci. Instrum.*, 2023, **94**, 034103. 034103.
- [172] X. Wu, D. Salionov, **P. Hemberger**, F. Vogel, A. Bodi, and S. Bjelić. Beyond vanilla: The dissociation mechanism of vanillin in four charge states. *Comput. Theor. Chem.*, 2023, 1229, 114340.
- [173] X. Wu, **P. Hemberger**, and A. Bodi. Enlightening salt: enthalpy of formation of gaseous sodium chloride by photoelectron photoion coincidence spectroscopy. *Mol. Phys.*, 2023, 122, e2286308.
- [174] H. Yue, C. Zhang, X. Lin, Z. Wen, W. Zhang, S. Mostafa, P. Luo, Z. Zhang, **P. Hemberger**, C. Fittschen, and X. Tang. Dimeric product of peroxy radical self-reaction probed with vuv photoionization mass spectrometry and theoretical calculations: The case of c2h5ooc2h5. *Int. J. Mol. Sci.*, 2023, **24**, 3731.
- [175] Z. Zhang, J. Tian, X. Wu, I. Surin, J. Pérez-Ramírez, **P. Hemberger***, and A. Bodi. Unraveling radical and oxygenate routes in the oxidative dehydrogenation of propane over boron nitride. *J. Am. Chem. Soc.*, 2023, **145**, 7910.
- [176] A. Bodi, J. Knurr, P. Ascher, **P. Hemberger**, C. Bostedt, and A. Alhaddad. Publication preview source vuv absorption spectra of water and nitrous oxide by a double-duty differentially pumped gas filter. *J. Synchr. Rad.*, 2024, 31, 1257–1263.
- [177] S. J. Goettl, A. M. Turner, B.J. Sun, A. H. H. Chang, **P. Hemberger***, and R. I. Kaiser. Gas-phase preparation of the dibenzo[e,l]pyrene (c24h14) butterfly molecule via a phenyl radical-mediated ring annulation. *Chem. Comm.*, 2024, 60, 1404–1407.
- [178] N. Hansen, T. Bierkandt, N. Gaiser, P. Osswald, M. Kohler, and **P. Hemberger**. Formation of five-membered ring structures via reactions of o-benzyne. *Proc. Combust. Inst.*, 2024, 40, 105623.
- [179] K. Kanayama, H. Nakamura, K. Maruta, A. Bodi, and **P. Hemberger***. Conformer-specific photoelectron spectroscopy of carbonic acid: H₂CO₃. *J. Phys. Chem. Lett.*, 2024, 15, 2658–2664.
- [180] K. Kanayama, H. Nakamura, K. Maruta, A. Bodi, and **P. Hemberger***. The unimolecular decomposition mechanism of trimethyl phosphate. *Chem. Eur. J.*, 2024, 30, e202401750.
- [181] G. Karir, E. Mendez-Vega, A. Portela-Gonzalez, M. Saraswat, W. Sander, and **P. Hemberger***. The elusive phenylethynyl radical and its cation: synthesis, electronic structure, and reactivity. *Phys. Chem. Chem. Phys.*, 2024, 26, 18256–18265.
- [182] M. Muzika, N. Genossar-Dan, D. Fux, S. Har Lavan, U. Zamir, I. Rozenberg, **P. Hemberger**, and J. H. Baraban. Radical intermediates and stable products in acrolein pyrolysis. *Environ. Chem. Lett.*, 2024, 22, 491–497.
- [183] Z. Pan, X. Wu, A. Bodi, J. A van Bokhoven, and **P. Hemberger***. Catalytic pyrolysis mechanism of lignin moieties driven by aldehyde, hydroxyl, methoxy, and allyl functionalization: the role of reactive quinone methide and ketene intermediates. *Green Chemistry*, 2024, 26, 9899 – 9910.
- [184] V. Paunovic, X. Wu, L. Maggiulli, D. Ferri, **P. Hemberger**, A. Bodi, and J. A van Bokhoven. The formation, reactivity and transformation pathways of formaldehyde in the methanol-to-hydrocarbon conversion. *Catal. Sci. Technol.*, 2024, 14, 1216–1228.
- [185] M. Stuhr, S. Hesse, N. Faßheber, M. Wohler, M. Pal, Y. Sakai, **P. Hemberger**, and G. Friedrichs. Uv photolysis of oxalyl chloride: Clco radical decomposition and direct formation pathways. *Int. J. Chem. Kin.*, 2024, 56, 482–498.
- [186] M. S. Wagner, H. Peisert, T. Chassé, **P. Hemberger***, and H. F. Bettinger. Gas phase ionization energy of heptacene. *J. Phys. Chem. Lett.*, 2024, 15, 2332–2336.
- [187] Z. Zhang, Q. Li, X. Wu, C. Bourmaud, D. G. Vlachos, J. Lutterbacher, A. Bodi, and **P. Hemberger***. A solution for 4-propylguaiacol hydrodeoxygenation without ring saturation. *Nat. Commun.*, 2024, 15, 6330.
- [188] Z. Zhang, M. Vanni, X. Wu, **P. Hemberger***, A. Bodi, S. Mitchel, and J. Pérez-Ramírez. Co-feeding affects product distribution in CH₃Cl coupling over ZSM-5 zeolite: Pressure twists the plot. *Angew. Chem. Int. Ed.*, 2024, 63, e202401060.