# Chemical Dynamics Beamline Publications

**2015**

407. D. S. N. Parker, R. I. Kaiser, B. Bandyopadhyay, O. Kostko, T. P. Troy, and M. Ahmed, "Unexpected Chemistry from the Reaction of Naphthyl and Acetylene at Combustion-Like Temperatures," Angew. Chem. Int. Ed., DOI: 10.1002/anie.201411987 (2015, accepted)

406. T. P. Troy, and M. Ahmed, "Rings of fire: Carbon combustion from soot to stars," Phys. Today, **68**, 62, DOI: 10.1063/PT.3.2729 (2015)

405. L. G. Dodson, L. Shen, J. D. Savee, N. C. Eddingsaas, O. Welz, C. A. Taatjes, D. L. Osborn, S. P. Sander, and M. Okumura, "VUV Photoionization Cross Sections of $HO_2$, $H_2O_2$, and $H_2CO$," J. Phys. Chem. A, DOI: 10.1021/jp508942a (2015, accepted)

404. J. D. Savee, E. Papajak, B. Rotavera, H. Huang, A. J. Eskola, O. Welz, L. Sheps, , C. A. Taatjes, J. Zádor, and D. L. Osborn, "Direct observation and kinetics of a hydroperoxyalkyl radical (QOOH)," Science, **347**, 643, DOI: 10.1126/science.aaa1495 (2015)

403. D. S. N. Parker, R. I. Kaiser, O. Kostko, T. P. Troy, M. Ahmed, A. M. Mebel, and A. G. G. M. Tielens, "Gas Phase Synthesis of (Iso)Quinoline and Its Role in the Formation of Nucleobases in the Interstellar Medium," Astrophys. J., (2015, accepted)

402. E. C. Browne, J. P. Franklin, M. R. Canagaratna, P. Massoli, T. W. Kirchstetter, D. R. Worsnop, K. R. Wilson, and J. H. Kroll, "Changes to the Chemical Composition of Soot from Heterogeneous Oxidation Reactions," J. Phys. Chem. A, DOI: 10.1021/jp511507d (2015, accepted)

401. T. K. Ormond, A. M. Scheer, M. R. Nimlos, D. J. Robichaud, T. P. Troy, M. Ahmed, J. W. Daily, T. L. Nguyen, J. F. Stanton, and G. B. Ellison, "Pyrolysis of Cyclopentadienone: Mechanistic Insights From a Direct Measurement of Product Branching Ratios," J. Phys. Chem. A, DOI: 10.1021/jp511390f (2015, accepted)

400. P. T. Lynch, T. P. Troy, M. Ahmed, and R.S. Tranter, "Probing Combustion Chemistry in a Miniature Shock Tube with Synchrotron VUV Photo Ionization Mass Spectrometry," Anal. Chem., DOI: 10.1021/ac5041633 (2015, accepted)

399. M. R. Canagaratna, P. Massoli, E. C. Browne, J. P. Franklin, K. R. Wilson, T. B. Onasch, T. W. Kirchstetter, E. C. Fortner, C. E. Kolb, J. T. Jayne, J. H. Kroll, and D. R. Worsnop, "Chemical Compositions of Black Carbon Particle Cores and Coatings via Soot Particle Aerosol Mass Spectrometry with Photoionization and Electron Ionization," J. Phys. Chem. A., DOI: 10.1021/jp510711u (2015, accepted)

398. 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., **142**, 044307, DOI: 10.1063/1.4906156 (2015)

**2014**

397. J. F. Lockyear, M. Fournier, I. R. Sims, J.-C. Guillemin, C. A. Taatjes, D. L. Osborn, and S. R. Leone, "Formation of fulvene in the reaction of $C_2H$ with 1,3-butadiene," Int. J. Mass. Spectrom., **117**, 11013, DOI: 10.1016/j.ijms.2014.08.025 (2014, in press)

# Chemical Dynamics Beamline Publications

396. B. Rotavera, J. Zádor, O. Welz, L. Sheps, A. M. Scheer, J. D. Savee, M. A. Ali, T. S. Lee, B. A. Simmons, D. L. Osborn, A. Violi, and C. A. Taatjes, "Photoionization Mass Spectrometric Measurements of Initial Reaction Pathways in Low-Temperature Oxidation of 2,5-Dimethylhexane Low-Temperature Oxidation of 2,5-Dimethylhexane,"J. Phys. Chem. A, **118**, 10188, DOI: 10.1021/jp507811d (2014)

395. T. Nah, H. Zhang, D. R. Worton, C. Ruehl, B. B. Kirk, A. Goldstein, S. R. Leone, and K. R. Wilson, "Isomeric Product Detection in the Heterogeneous Reaction of Hydroxyl Radicals with Aerosol Composed of Branched and Linear Unsaturated Organic Molecules," J. Phys. Chem. A, **118**, 11555, DOI: 10.1021/jp508378z (2014)

394. D. M. Popolan-Vaida, S. R. Leone, and K. R. Wilson, "Reaction of Iodine Atoms with Submicrometer Squalane and Squalene Droplets: Mechanistic Insights into Heterogeneous Reactions," J. Phys. Chem. A, **118**, 10688, DOI: 10.1021/jp5085247 (2014)

393. M. R. Canagaratna, J. L. Jimenez, J. H. Kroll, Q. Chen, S. H. Kessler, P. Massoli, L. Hildebrandt Ruiz, E. Fortner, L. R. Williams, K. R. Wilson, J. D. Surratt, N. M. Donahue, J. T. Jayne, and D. R. Worsnop, "Elemental ratio measurements of organic compounds using aerosol mass spectrometry: characterization, improved calibration, and implications", Atmos. Chem. Phys. Discuss, **14**, 19791, DOI: 10.5194/acpd-14-19791-2014 (2014)

392. D. S. N. Parker, R. I. Kaiser, T. P. Troy, O. Kostko, M. Ahmed, and A. M. Mebel, "Toward the Oxidation of the Phenyl Radical and Prevention of PAH Formation in Combustion Systems," J. Phys. Chem. A., DOI: 10.1021/jp509170x (2014, accepted)

391**.** S. Chakraborty, B. H. Muskatel, T. L. Jackson, M. Ahmed, R. D. Levine, and M. H. Thiemens, "Massive isotopic effect in vacuum UV photodissociation of $N_2$ and implications for meteorite data," PNAS, **111**, 14704, DOI:10.1073/pnas.1410440111 (2014)

390. S. Y. Liu, M. Shawkey, D. Parkinson, T. Troy and M. Ahmed, "Elucidation of the chemical composition of avian melanin," RSC Advances, **4**, 40396, DOI: 10.1039/C4RA06606E (2014)

389. T. Bierkandt, T.Kasper, E. Akyildiz, A. Lucassen, P. Oßwald, M. Köhler, 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., DOI: 10.1016/j.proci.2014.05.094 (2014, in press)

388. N. Hansen, B. Yang, and T. Kasper, edited by X. Zhang, "Synchrotron-Based VUV Photoionization Mass Spectrometry in Combustion Chemistry Research," Synchrotron Radiation Application, World Scientific Press (2014, in press)

387. K. O. Johansson, J. Y. W. Lai, S. A. Skeen, K. R. Wilson, N. Hansen, A. Violi, and H. A. Michelsen, "Soot Precursor Formation and Limitations of the Stabilomer Grid," Proc. Combust. Inst., DOI: 10.1016/j.proci.2014.05.033 (2014, in press)

386. A. Lucassen, S. Park, N. Hansen, and S. M. Sarathy, "Combustion Chemistry of Alcohols: Experimental and Modeled Structure of a Premixed 2-Methylbutanol Flame," Proc. Combust. Inst., DOI: 10.1016/j.proci.2014.05.008 (2014, in press)

385. N. Hansen, M. Braun-Unkhoff, T. Kathrotia, A. Lucassen, and B. Yang, "Understanding the Reaction Pathways in Premixed Flames Fueled by Blends of 1,3-Butadiene and n-Butanol," Proc. Combust. Inst., DOI: 10.1016/j.proci.2014.05.005 (2014, in press)

# Chemical Dynamics Beamline Publications

384. F. N. Egolfopoulos, N. Hansen, Y. Ju, K. Kohse-Höinghaus, C. K. Law, and F. Qi, "Advances and challenges in laminar flame experiments and implications for combustion chemistry," Prog. Energy Combust. Sci., **43**, 36, DOI: 10.1016/j.pecs.2014.04.004 (2014)

383. D. S. N. Parker, R. I. Kaiser, T. P. Troy, and M. Ahmed, "Hydrogen Abstraction-Acetylene Addition Revealed," Angew. Chem. Int. Ed., **53**, 7740, DOI: 10.1002/anie.201404537 (2014)

382. T. Nah, S. H. Kessler, K. E. Daumit, J. H. Kroll, S. R. Leone, and K. R. Wilson, "The influence of molecular structure and chemical functionality on the heterogeneous OH-initiated oxidation of unsaturated organic particles," J. Phys. Chem. A, **118**, 4106, DOI: 10.1021/jp502666g (2014)

381. D. R. Worton, G. Isaacman, D. R. Gentner, T. R. Dallmann, A. W. H. Chan, C. Ruehl, T. W. Kirchstetter, K. R. Wilson, R. A. Harley, and A. H. Goldstein, "Lubricating oil dominates primary organic aerosol emissions from motor vehicles," Environ. Sci. Technol., **48**, 3698, DOI: 10.1021/es405375j (2014)

380. A. M. Scheer, O. Welz, J. Zádor, D. L. Osborn and C. A. Taatjes, *"*Low-temperature combustion chemistry of novel biofuels: resonance-stabilized QOOH in the oxidation of diethyl ketone*"* Phys. Chem. Chem. Phys.**, 16**, 13027, DOI: 10.1039/C3CP55468F (2014)

379. M. Y. Ng, J. Nelson, C. A. Taatjes, D. L. Osborn, and G. Meloni, *"*Synchrotron Photoionization Study of Mesitylene Oxidation Initiated by Reaction with Cl($^2$P) or O($^3$P) Radicals*,"* J. Phys. Chem. A, **118**, 3735, DOI**:** 10.1021/jp500260f (2014)

378. O. Welz, A. J. Eskola, L. Sheps, B. Rotavera, J. D. Savee, A. M. Scheer, D. L. Osborn, D. Lowe, A. M. Booth, P. Xiao, M. A. H. Khan, C. J. Percival, D. E. Shallcross, and C. A. Taatjes, *"*Rate Coefficients of C1 and C2 Criegee Intermediate Reactions with Formic and Acetic Acid Near the Collision Limit: Direct Kinetics Measurements and Atmospheric Implications*,"* Angew. Chem. Int. Ed., **53**, 4547 (2014)

377. C. A. Taatjes, D. E. Shallcross, and C. J. Percival, "*Research frontiers in the chemistry of Criegee intermediates and tropospheric ozonolysis*," Phys. Chem. Chem. Phys., **16**, 1704 (2014)

376. J.W. Allen, A. M. Scheer, C. W. Gao, S. S. Merchant, S. S. Vasu, O. Welz, J. D. Savee, D. L. Osborn, C. Lee, S. Vranckx, Z. Wang, F. Qi, R. X. Fernandes, W. H. Green, M. Z. Hadi, and C. A. Taatjes, "A coordinated investigation of the combustion chemistry of diisopropyl ketone, a prototype for biofuels produced by endophytic fungi," Combustion and Flame, **161**, 711 (2014)

375. J. B. Randazzo, P. Croteau, O. Kostko, M. Ahmed and K. A. Boering, "Isotope effects and spectroscopic assignments in the non-dissociative photoionization spectrum of $N_2$," J. Chem. Phys. **140**, 194303 (2014)

374. N. Hansen, S. A. Skeen, H. A. Michelsen, K. R. Wilson, and K. Kohse-Höinghaus, "Flame Experiments at the Advanced Light Source: New Insights into Soot Formation Processes," J. Vis. Exp. **87**, doi:10.3791/51369 (2014)

373. K. R. Kolesar, G. Buffaloe, K. R. Wilson, and C. D. Cappa, "OH-Initiated Heterogeneous Oxidation of Internally-Mixed Squalane and Secondary Organic Aerosol," Environ. Sci. Technol., **48**, 3196 (2014)

372. M. Perera, K. M. Roenitz, R. B. Metz, O. Kostko, and M. Ahmed, "VUV photoionization measurements and electronic structure calculations of the ionization energies of gas-phase tantalum oxides TaOx (x=3-6)," J. Spectrosc. Dyn., **4**, 21 (2014)

# Chemical Dynamics Beamline Publications

**2013**

371. A. J. Eskola, O. Welz, J. D. Savee, D. L. Osborn, and C. A. Taatjes, "Synchrotron Photoionization Mass Spectrometry Measurements of Product Formation in Low-Temperature n-Butane Oxidation: Toward a Fundamental Understanding of Autoignition Chemistry and *n*-$C_4H_9$ + $O_2$/s-$C_4H_9$ + $O_2$ Reactions," J. Phys. Chem. A, **117**, 12216, DOI: dx.doi.org/10.1021/jp408467g (2013)

370. N. Hansen, S. S. Merchant, M. R. Harper, and W. H. Green, "The predictive capability of an automatically generated combustion chemistry mechanism: Chemical structures of premixed iso-butanol flames," Combust. Flame, **160**, 2343, DOI: 10.1016/j.combustflame.2013.05.013 (2013)

369. K. Moshammer, S. Vranckx, H. K. Chakravarty, P. Parab, R. X. Fernandes, and K. Kohse-Höinghaus, "An experimental and kinetic modeling study of 2-methyltetrahydrofuran flames," Combust. Flame **160**, 2729, DOI: 10.1016/j.combustflame.2013.07.006 (2013)

368. K. R. Kolesar, "Effects of the Heterogeneous OH Oxidation of Squalane Organic Aerosol on Particle Evaporation Kinetics," masters thesis, University of California, Davis, Davis, California, USA, (2013), advisor Christopher Cappa. (9.0.2)

367. J. H. Kim, "Mechanistic Studies of the Pyrolysis of Methylated Furans," doctoral dissertation, Univ. Colorado, Boulder, CO, (2013), advisor G. Barney Ellison. (9.0.2)

366. S. H. Kessler, "The Aging of Organic Aerosol in the Atmosphere: Chemical Transformations by Heterogeneous Oxidation," doctoral dissertation, Massachusetts Institute of Technology, Cambridge, MA, (2013), advisor PhD. (9.0.2)

365. M. Keiluweit, "Assessing the Role of Reactive Metal Species in Soil Organic Matter Cycling using Chemical Imaging," doctoral dissertation, Oregon State University, Corvallis, Oregon, (2013), advisor Markus Kleber (5.3.2.2,11.0.2,1.4,9.0.2,10.3.2)

364. O. Welz, J. Zador, J. D. Savee, L. Sheps, D. L. Osborn, and C. A. Taatjes, "Low-Temperature Combustion Chemistry of n-Butanol: Principal Oxidation Pathways of Hydroxybutyl Radicals," J. Phys. Chem. A., **117**, 11983, DOI: 10.1021/jp403792t (2013)

363. H. Zhang, C. R. Ruehl, A. W. H. Chan, T. Nah, D. Worton, G. Isaacman, A. H. Goldstein, and K. R. Wilson, "OH- Initiated Heterogeneous Oxidation of Cholestane: A Model System for Understanding the Photochemical Aging of Cyclic Alkane Aerosols," J. Phys. Chem. A., **117**, 12449, DOI: 10.1021/jp407994m (2013)

362. J. Czekner, C. A. Taatjes, D. Osborn, and G. Meloni, "Absolute photoionization cross-sections of selected furanic and lactonic potential biofuels," Int. J. Mass Spectrom., **348**, 39, DOI: 10.1016/j.ijms.2013.04.020 (2013)

361. A. J. Eskola, O. Welz, J. D. Savee, D. L. Osborn, and C. A. Taatjes, "Synchrotron photoionization measurements of fundamental autoignition reactions: Product formation in low-temperature isobutane oxidation," Proc. Comb. Inst., **34**, 385, DOI: 10.1016/j.proci.2012.06.116 (2013)

360. F. Goulay, A. Derakhshan, E. Maher, A. J. Trevitt, J. D. Savee, A. M. Scheer, D. L. Osborn, and C. A. Taatjes, "Formation of dimethylketene and methacrolein by reaction of the CH radical with acetone," Phys. Chem. Chem. Phys., **15**, 4049, DOI: 10.1039/C3CP43829E (2013)

# Chemical Dynamics Beamline Publications

359. R. S. Tranter, and P. T. Lynch, "A miniature high repetition rate shock tube," Rev. Sci. Instrum., **84**, 094102, DOI: 10.1063/1.4820917 (2013)

358. A. J. Trevitt, M. B. Prendergast, F. Goulay, J. D. Savee, D. L. Osborn, C. A. Taatjes , and S. R. Leone, "Product Branching Fractions of the CH + Propene Reaction from Synchrotron Photoionization Mass Spectrometry," J. Phys. Chem. A., **117**, 6450, DOI: 10.1021/jp404965k (2013)

357. J. F. Lockyear, O. Welz, J. D. Savee, F. Goulay, A. J. Trevitt, C. A. Taatjes, D. L. Osborn, and S. R. Leone, "Isomer Specific Product Detection in the Reaction of CH with Acrolein," J. Phys. Chem. A., **117**, 11013, DOI: 10.1021/jp407428v (2013)

356. S. Chakraborty, T. L. Jackson, M. Ahmed, and M. H. Thiemens, "Sulfur isotopic fractionation in vacuum UV photodissociation of hydrogen sulfide and its potential relevance to meteorite analysis," PNAS., **110***,* 17650, DOI: 10.1073/pnas.1213150110, (2013) LBNL- 5802E

355. T. Nah, S. H. Kessler, K. E. Daumit, J. H. Kroll, S. R. Leone and K. R. Wilson, "OH- initiated oxidation of sub-micron unsaturated fatty acid particles," Phys. Chem. Chem. Phys., **15**, 18649, DOI: 10.1039/c3cp52655k (2013)

354. C. Bhardwaj, Y. Cui, T. Hofstetter, S-Y. Liu, H. C. Bernstein, R. P. Carlson, M. Ahmed and L. Hanley, "Differentiation of microbial species and strains in coculture biofilms by multivariate analysis of laser desorption postionization mass spectra," Analyst, **138,** 6844, DOI: 10.1039/C3AN01389H (2013)

353. K. N. Urness, Q. Guan, A. Golan, J. W. Daily, M. R. Nimlos, J. F. Stanton, M. Ahmed, and G. B. Ellison, "Pyrolysis of Furan in a Microreactor," J. Chem. Phys., **139**, 124305, DOI: 10.1063/1.4821600 (2013)

352. F. Bell, Q. N. Ruan, A. Golan, P. R. Horn, M. Ahmed, S. R. Leone, and M. Head-Gordon, "Dissociative Photoionization of Glycerol and its Dimer Occurs Predominantly via a Ternary Hydrogen-Bridged Ion-Molecule Complex," J. Am. Chem. Soc., **135,** 14229, 10.1021/ja405511v (2013)

351. K. Khistyaev, A. Golan, K. B. Bravaya, N. Orms, A. I. Krylov, and M. Ahmed, "Proton Transfer in Nucleobases is Mediated by Water," J. Phys. Chem. A., **117**, 6789, DOI: 10.1021/jp406029p (2013)

350. A. W. H. Chan, G. Isaacman, K. R. Wilson, D. R. Worton, C. R. Ruehl, T. Nah, D. R. Gentner, T. R. Dallman, T. W. Kirchstetter, R. A. Harley, J. B. Gilman, W. C. Kuster, J. A. de Gouw, J. H. Offenberg, T. E. Kleindienst, Y. H. Lin, C. L. Rubitschun, J. D. Surratt, P. L. Hayes, J. L. Jimenez, and A. H. Goldstein, "Detailed chemical characterization of unresolved complex mixtures in atmospheric organics: Insights into emission sources, atmospheric processing and secondary organic aerosol formation," J. Geophys. Res., [Atmos.] **118**, 6783, DOI: 10.1002/jgrd.50533 (2013)

349. J. Bouwman, M. Fournier, I. R. Sims, S. R. Leone, and K. R. Wilson, "Reaction Rate and Isomer-Specific Product Branching Ratios of $C_2H$ + $C_4H_8$: 1-Butene, *cis*-2-Butene, *trans*-2-Butene and Isobutene at 79K," J. Phys. Chem. A., **117**, 5093, DOI: 10.1021/jp403637t (2013)

348. S-Y. Liu, M. Kleber, L. K. Takahashi, P. Nico, M. Keiluweit, M. Ahmed, "Synchrotron-Based Mass Spectrometry to Investigate the Molecular Properties of Mineral-Organic Associations," Anal. Chem., **85**, 6100, DOI: 10.1021/ac400976z (2013)

347. C. R. Ruehl, T. Nah, G. Isaacman, D. R. Worton, A. W. H. Chan, K. R. Kolesar, C. D. Cappa, A. H. Goldstein, and K. R. Wilson, "The Influence of Molecular Structure and Aerosol Phase on the Heterogeneous Oxidation of Normal and Branched Alkanes by OH," J. Phys. Chem. A., **117**, 3990, DOI: 10.1021/jp401888q (2013)

# Chemical Dynamics Beamline Publications

346. C. A. Taatjes, O. Welz, A. J. Eskola, J. D. Savee, A. M. Scheer, D. E. Shallcross, B. Rotavera, E. P. F. Lee, J. M. Dyke, D. K. W. Mok, D. L. Osborn, and C. J. Percival, "Direct Measurements of Conformer-Dependent Reactivity of the Criegee Intermediate $CH_3CHOO$," Science, **340,** 177, DOI: 10.1126/science.1234689 (2013)

345. S. A. Skeen, H. A. Michelsen, K. R. Wilson, D. M. Popolan, A. Violi, and N. Hansen, "Near-threshold photoionization mass spectra of combustion-generated high-molecular-weight soot precursors," J. Aerosol Sci., **58,** 86, DOI: 10.1016/j.jaerosci.2012.12.008 (2013)

344. M. Perera, R. B. Metz, O. Kostko, and M. Ahmed, "Vacuum Ultraviolet Photoionization Studies of $PtCH_2$ and H-Pt-$CH_3$: A Potential Energy Surface for the Pt + $CH_4$ Reaction," Agnew. Chem. Int. Ed. **125**, 922, DOI: 10.1002/ange.201207931 (2013)

343. L. Lee, P. Wooldridge, T. Nah, K. R. Wilson, and R. Cohen, "Observation of rates and products in the reaction of $NO_3$ with submicron squalane and squalene aerosol," Phys. Chem. Chem. Phys., **15**, 882, DOI: 10.1039/c2cp42500a (2013)

342. A. Golan, M. Ahmed, A. M. Mebel, and R. I. Kaiser, "A VUV photoionization study of the multichannel reaction of phenyl radicals with 1,3-butadiene under combustion relevant conditions," Phys. Chem. Chem. Phys., **15**, 341, DOI: 10.1039/c2cp42848b, (2013) **LBNL# 5510E**

341. B. Yang, C. K. Westbrook, T. A. Cool, N. Hansen, K. Kohse-Höinghaus, "Photoionization mass spectrometry and modeling study of premixed flames of three unsaturated $C_5H_8O_2$ esters," Proc. Combust. Inst., **34**, 443, DOI: 10.1016/j.proci.2012.05.034 (2013)

340. A. W. Jasper and N. Hansen, "Hydrogen-assisted isomerizations of fulvene to benzene and of larger cyclic aromatic hydrocarbons," Proc. Combust. Inst., **34**, 279, 10.1016/j.proci.2012.06.165 (2013)

339. S. A. Skeen, B. Yang, H. A. Michelsen, J. A. Miller, A. Violi, N. Hansen, "Studies of laminar opposed-flow diffusion flames of acetylene at low-pressures with photoionization mass spectrometry," Proc. Combust. Inst., **34**, 1067, DOI: 10.1016/j.proci.2012.06.075 (2013)

338. N. J. Labbe, V. Seshadri, T. Kasper, N. Hansen, P. Oßwald, K. Kohse-Höinghaus, and P. R. Westmoreland, "Flame chemistry of tetrahydropyran as a model heteroatomic biofuel," Proc. Combust. Inst., **34**, 259, DOI: 10.1016/j.proci.2012.07.027 (2013)

337. O. Welz, J. Zador, J.D. Savee, A. J. Eskola, L. Sheps, D. L. Osborn, and C. A. Taatjes, "Low-temperature combustion chemistry of biofuels: pathways in the initial low-temperature (550 – 750K) oxidation chemistry of isopentanol and tert-butanol," Proc. Combust. Inst., **34**, 493, DOI: 10.1016/j.proci.2012.05.058 (2013)

**2012**

336. S. Soorkia, S. R. Leone, and K. R. Wilson, "Radical-neutral chemical reactions studied at low temperature with VUV synchrotron photoionization mass spectrometry," AIP. Conf. Proc., **1501**, 1365, DOI: 10.1063/1.4769699 (2012)

335. D. Gentner, G. Isaacman, D. R. Worton, A. W. H. Chan, T. R. Dallmann, L. Davis, S. Liu, D. A. Day, L. M. Russell, K. R. Wilson, R. Weber, A. Guha, R. A. Harley, and A. H. Goldstein, "Elucidating secondary organic aerosol from diesel and gasoline vehicles through detailed characterization of organic carbon emissions," PNAS., **109***,* 18318, DOI: 10.1073/pnas.1212272109 *(*2012)

# Chemical Dynamics Beamline Publications

334. C. A. Taatjes, O. Welz, A. J. Eskola, J. D. Savee, D. L. Osborn, E. P. F. Lee, J. M. Dyke, D. W. K. Mok, D. E. Shallcross, and C. J. Percival, "Direct measurement of Criegee intermediate ($CH_2OO$) reactions with acetone, acetaldehyde, and hexafluoroacetone," Phys. Chem. Chem. Phys., **14***,* 10391, DOI: 10.1039/C2CP40294G *(*2012)

333. S. D. Chambreau, J. A. Boatz, G. L. Vaghjiani, C. Koh, O. Kostko, A. Golan, and S. R. Leone, "Thermal Decomposition Mechanism of 1-Ethyl-3-methylimidazolium Bromide Ionic Liquid," J. Phys. Chem. A. **116***,* 5867, DOI: 10.1021/jp209389d *(*2012)

332. S. D. Chambreau, G. L. Vaghjiani, C. J. Koh, A. Golan, and S. R. Leone, "Ultraviolet Photoionization Efficiency of the Vaporized Ionic Liquid 1-Butyl-3-methylimidazolium Tricyanomethanide: Direct Detection of the Intact Ion Pair," J. Phys. Chem. Lett., **3***,* 2910, DOI: 10.1021/jz301242w (2012)

331. R. I. Kaiser, S. P. Krishtal, A. M. Mebel, O. Kostko, and M. Ahmed, "An Experimental and Theoretical Study of the Ionization Energies of SiC2Hx (x = 0, 1, 2) Isomers," Astrophys. J., **761**, 178, DOI: 10.1088/0004-637X/761/2/178, (2012) **LBNL# 5641E**

330. A. Golan and M. Ahmed, "Molecular beam mass spectrometry with tunable vacuum ultraviolet (VUV) synchrotron radiation," J. Vis. Exp., **68**, e50164, DOI: 10.3791/50164 (2012)

329. A. K. Vasiliou, K. M. Piech, B. Reed, X. Zhang, M. R. Nimlos, M. Ahmed, A. Golan, O. Kostko, D. L. Osborn, D. E. David, K. N. Urness, J. W. Daily, J. F. Stanton, and G. B. Ellison, "Thermal decomposition of $CH_3CHO$ studied by matrix infrared spectroscopy and photoionization mass spectroscopy," J. Chem. Phys., **137**, 164308, DOI: 10.1063/1.4759050 (2012)

328. G. Isaacman, A. W. H. Chan, T. Nah, D. R. Worton, C. R. Ruehl, K. R. Wilson, and A. H. Goldstein, "Heterogeneous OH Oxidation of Motor Oil Particles Causes Selective Depletion of Branched and Less Cyclic Hydrocarbons," Environ. Sci. Technol., **46**, 10632, DOI: 10.1021/es302768a (2012)

327. N. Hansen, J. A. Miller, S. J. Klippenstein, P. R. Westmoreland, and K. Kohse-Höinghaus, "Exploring formation pathways of aromatic compounds in laboratory-based model flames of aliphatic fuels," Combust. Expl. Shock Waves, **48**, 508, DOI: 10.1134/S0010508212050024 (2012)

326. J. H. Kroll, J. D. Smith, D. R. Worsnop, and K. R. Wilson, "Characterisation of lightly oxidised organic aerosol formed from the photochemical aging of diesel exhaust particles," Environ. Chem., **9**, 211, DOI: 10.1071/EN11162 (2012)

325. K. S. Kalogerakis, C. Romanescu, M. Ahmed, K. R. Wilson, and T. G. Slanger, "CO prompt emission as a $CO_2$ marker in comets and planetary atmospheres," Icarus, **220**, 205, DOI: 10.1016/j.icarus.2012.04.028 (2012) **LBNL# 5509E**

324. A. W. Ray, C. A. Taatjes, O. Welz, D. L. Osborn and G. Meloni, "Synchrotron Photoionization Measurements of OH-Initiated Cyclohexene Oxidation: Ring-Preserving Products in OH + Cyclohexene and Hydroxycyclohexyl + $O_2$ Reactions," J. Phys. Chem. A., **116**, 6720, DOI: 10.1021/jp3022437 (2012)

323. J. Bouwman, F. Goulay, S. R. Leone, and K. R. Wilson, "Bimolecular Rate Constant and Product Branching Ratio Measurements For the Reaction of $C_2H$ with Ethene and Propene at 79 K," J. Phys. Chem. A., **116**, 3907, DOI: 10.1021/jp301015b (2012)

# Chemical Dynamics Beamline Publications

322. F. Zhang, R.I. Kaiser, A. Golan, M. Ahmed and N. Hansen, "A VUV Photoionization Study of the Combustion-Relevant Reaction of the Phenyl Radical ($C_6H_5$) with Propylene ($C_3H_6$) in a High Temperature Chemical Reactor," J. Phys. Chem. A., **116**, 3541, DOI: 10.1021/jp300875s (2012), **LBNL# 5354E**

321. S. Chakraborty, R. D. Davis, M. Ahmed, T. L. Jackson, and M. H. Thiemens, "Oxygen isotope fractionation in the vacuum ultraviolet photodissociation of carbon monoxide: Wavelength, pressure and temperature dependency," J. Chem. Phys., **137**, 024309, DOI: /10.1063/1.4730911 (2012), **LBNL# 5258E**

320. S. H. Kessler, T. Nah, K. E. Daumit, J. D. Smith, S. R. Leone, C. E. Kolb, D. R. Worsnop, K. R. Wilson, and J. H. Kroll, "OH-Initiated Heterogeneous Aging of Highly Oxidized Organic Aerosol," J. Phys. Chem. A., **116**, 6358, DOI: 10.1021/jp212131m (2012), **LBNL# 5256E**

319. G. Isaacman, K. R. Wilson, A. W. H. Chan, D. R. Worton, J. R. Kimmel, T. Nah, T. Hohaus, M. Gonin, J. H. Kroll, D. R. Worsnop, and A. H. Goldstein, "Improved Resolution of Hydrocarbon Structures and Constitutional Isomers in Complex Mixtures Using Gas Chromatography-Vacuum Ultraviolet-Mass Spectrometry," Anal. Chem., **84**, 2335, DOI: 10.1021/ac2030464 (2012), **LBNL# 5281E Pt. 2**

318. A. Golan, K. B. Bravaya, R. Kudirka, O. Kostko, S. R. Leone, A. I. Krylov, and M. Ahmed, "Ionization of dimethyluracil dimers leads to facile proton transfer in the absence of H-bonds," Nat. Chem., **4**, 323, DOI: 10.1038/nchem.1298 (2012), **LBNL# 5205E**

317. B. Yang, J. Wang, T. A. Cool, N. Hansen, S. Skeen, and D. L. Osborn, "Absolute photoionization cross-sections of some combustion intermediates," Int. J. Mass Spectrom., **309**, 118, DOI: 10.1016/j.ijms.2011.09.006 (2012)

316. A. Golan and M. Ahmed, "Ionization of Water Clusters Mediated by Exciton Energy Transfer from Argon Clusters," J. Phys. Chem. Lett., **3**, 458, DOI: 10.1021/jz2016654 (2012), **LBNL# 5374E**

315. F. Goulay, A. J. Trevitt, J. D. Savee, J. Bowman, D. L. Osborn, C. A. Taatjes, K. R. Wilson, and S. R. Leone, "Product Detection of the CH Radical Reaction with Acetaldehyde," J. Phys. Chem. A., **116**, 6091, DOI: 10.1021/jp2113126 (2012)

314. J. D. Savee, O. Welz, C. A. Taatjes, and D. L. Osborn, "New mechanistic insights to the O(3P)+ propene reaction from multiplexed photoionization mass spectrometry," Phys. Chem. Chem. Phys., **14**, 10410, DOI: 10.1039/C2CP41200D (2012)

313. K. R. Wilson, J. D. Smith, S. H. Kessler, and J. H. Kroll, "The statistical evolution of multiple generations of oxidation products in the photochemical aging of chemically reduced organic aerosol," Phys. Chem. Chem. Phys., **14**, 1468, DOI: 10.1039/C1CP22716E (2012), **LBNL# 5224E**

312. M. J. Berg, K. R. Wilson, C. Sorensen, A. Chakrabarti, and M. Ahmed, "Discrete dipole approximation for low-energy photoelectron emission from NaCl nanoparticles," J. Quant. Spectrosc. Ra., **113**, 259, DOI: 10.1016/j.jqsrt.2011.10.007, (2012) **LBNL# 5236E**

311. O. Welz, J. D. Savee, D. L. Osborn, S. S. Vasu, C. J. Percival, D. E. Shallcross, and C. A. Taatjes, "Direct Kinetic Measurements of Criegee Intermediate ($CH_2OO$) Formed by Reaction of $CH_2I$ with $O_2$," Science, **335**, 204, DOI: 10.1126/science.1213229 (2012)

# Chemical Dynamics Beamline Publications

310. O. Welz, J. Zador, J.D. Savee, M. Y. Ng, G. Meloni, R.X. Fernandes, L. Sheps, B. A. Simmons, T. S. Lee, D. L. Osborn, and C. A. Taatjes, "Low-temperature combustion chemistry of biofuels: pathways in the initial low-temperature (550 – 750K) oxidation chemistry of isopentanol," Phys. Chem. Chem. Phys., **14,** 3112, DOI: 10.1039/C2CP23248K (2012)

309. K. Kohse-Höinghaus, P. Oßwald, F. Herrmann, A. Lucassen, "Biokraftstoffe als saubere Alternative? Moderne Analysemethoden verraten Details der Verbrennungschemie," GIT Labor-Fachzeitschrift, **6,** 453 (2012)

308. E. P. F. Lee, D. K. W. Mok, D. E. Shallcross, C. J. Percival, D. L. Osborn, C. A. Taatjes, and J. M. Dyke, "Spectroscopy of the Simplest Criegee Intermediate $CH_2OO$: Simulation of the First Bands in Its Electronic and Photoelectron Spectra ," Chem. Eur. J. **18**, 12411, DOI: 10.1002/chem.201200848 (2012)

307. D. Ghosh, A. Golan, L. K. Takahashi, A. I. Krylov, and M. Ahmed, "A VUV Photoionization and Ab Initio Determination of the Ionization Energy of a Gas-Phase Sugar (Deoxyribose)," J. Phys. Chem. Lett., **3,** 97, DOI: 10.1021/jz201446r, (2012) **LBNL# 5204E**

306. A. Lucassen, K. Zhang, J. Warkentin, K. Moshammer, P. Glarborg, P. Marshall, and K. Kohse-Höinghaus, "Fuel-nitrogen conversion in the combustion of small amines using dimethylamine and ethylamine as biomass-related model fuels," Combust. Flame, **159,** 2254, DOI: 10.1016/j.combustflame.2012.02.024 (2012)

305. J. D. Savee, S. Soorkia, O. Welz, T. M. Selby, C. A. Taatjes, and D. L. Osborn, "Absolute photoionization cross-section of the propargyl radical," J. Chem. Phys., **136,** 134307, DOI: 10.1063/1.3698282 (2012)

304. K. R. Wilson, H. Bluhm, and M. Ahmed "Aerosol Photoemission," Fundamentals and Applications in Aerosol Spectroscopy, eds. Ruth Signorell and Jonathan P. Reid, Boca Raton, CRC Taylor and Francis Books, Inc. 367 (2012)

**2011**

303. A. K. Vasiliou, "Thermochemical conversion of biomass: a molecular viewpoint," doctoral dissertation, University of Colorado at Boulder, Boulder, CO, United States (2011) advisor Barney Ellison (9.0.2)

302. A. Lucassen, "Systematische Analyse von Flammen Stickstoffhaltiger Modellsubstanzen mittels Molekularstrahlmassenspektrometrie," doctoral dissertation, Bielefeld University, Bielefeld, Germany (2011) advisor Katharina Kohse-Höinghaus (9.0.2)

301. G. Gaspar, "Ms imaging of antibiotics within staph, epidermidis bacterial biofilms by laser desorption postionization," doctoral dissertation, University of Illinois at Chicago, Chicago, IL, United States (2011) advisor Luke Hanley (9.0.2)

300. L. K. Takahashi, "Synchrotron vacuum-ultraviolet postionization mass spectrometry with laser and ion probes for intact molecular spatial mapping of lignin," doctoral dissertation, University of California, Berkeley, Berkeley, CA, United States (2011) advisor Stephen R. Leone (9.0.2)

299. F. Goulay, S. Soorkia, G. Meloni, D. L. Osborn, C. A. Taatjes, and S. R. Leone, "Detection of pentatetraene by reaction of the ethynyl radical ($C_2H$) with allene ($CH_2=C=CH_2$) at room temperature," Phys. Chem. Chem. Phys., **13,** 20820, DOI: 10.1039/C1CP22609F (2011)

# Chemical Dynamics Beamline Publications

298. A. J. Trevitt, S. Soorkia, J. D. Savee, T. S. Selby, D. L. Osborn, C. A. Taatjes, and S. R. Leone, "Branching Fractions of the CN + $C_3H_6$ Reaction Using Synchrotron Photoionization Mass Spectrometry: Evidence for the 3-Cyanopropene Product," J. Phys. Chem. A., **115,** 13467, DOI: 10.1021/jp208496r (2011)

297. 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,** 1029, DOI: 10.1524/zpch.2011.0148 (2011)

296. A. Lucassen, N. Labbe, P.R. Westmoreland, K. Kohse-Höinghaus, "Combustion chemistry and fuel-nitrogen conversion in a laminar premixed flame of morpholine as a model biofuel," Combust. Flame, **158,** 1647, DOI: 10.1016/j.combustflame.2011.02.010 (2011)

295. B. Yang, C. K. Westbrook, T. A. Cool, N. Hansen**,** and K. Kohse-Höinghaus, "The Effect of Carbon-Carbon Double Bonds on the Combustion Chemistry of Small Fatty Acid Esters," Z. Phys. Chem., **225,** 1293, DOI: 10.1524/zpch.2011.0167 (2011)

294. T. Kasper, A. Lucassen, A. W. Jasper, W. Li, P. R. Westmoreland, K. Kohse-Höinghaus, B. Yang, J. Wang, T. A. Cool, and N. Hansen, "Identification of Tetrahydrofuran Reaction Pathways in Premixed Flames," Z. Phys. Chem., **225,** 1237, DOI: 10.1524/zpch.2011.0163 (2011)

293. S. A. Skeen, B. Yang, A. W. Jasper, W. J. Pitz, and N. Hansen, "Chemical Structures of Low-Pressure Premixed Methylcyclohexane Flames as Benchmarks for the Development of a Predictive Combustion Chemistry Model," Energy Fuels, **25,** 5611, DOI: 10.1021/ef201507x (2011)

292. F. Zhang, R. I. Kaiser, V. V. Kislov, A. M. Mebel, A. Golan and M. Ahmed, "A VUV Photoionization Study of the Formation of the Indene Molecule and Its Isomers," J. Phys. Chem. Lett., **2**, 1731, DOI: 10.1021/jz200715u, (2011) **LBNL# 5299E**

291. S. Soorkia, C-L. Liu, J. D. Savee, S. J. Ferrell, S. R. Leone and K. R. Wilson, "Airfoil sampling of a pulsed Laval beam with tunable vacuum ultraviolet synchrotron ionization quadrupole mass spectrometry: Application to low-temperature kinetics and product detection," Rev. Sci. Instrum., **82**, 124102, DOI: 10.1063/1.3669537 (2011), **LBNL# 5228E**

290. N. Hansen, M. R. Harper, and W. H. Green, "High-temperature oxidation chemistry of n-butanol – experiments in low-pressure premixed flames and detailed kinetic modeling," Phys. Chem. Chem. Phys., **13**, 20262, DOI: 10.1039/C1CP21663E (2011)

289. S. H. Kessler, T. Nah, A. Carrasquillo, J. T. Wayne, D. R. Worsnop, K. R. Wilson, and J. H. Kroll, "Formation of Secondary Organic Aerosol from the Direct Photolytic Generation of Organic Radicals," J. Phys. Chem. Lett., **2**, 1295, DOI: 10.1021/jz200432n (2011)

288. E. R. Mysak, J. D. Smith, P. D. Ashby, J. T. Newberg, K. R. Wilson, and H. Bluhm, "Competitive reaction pathways for functionalization and volatilization in the heterogeneous oxidation of coronene thin films by hydroxyl radicals and ozone," Phys. Chem. Chem. Phys., **13**, 7554, DOI: 10.1039/C0CP02323J (2011)

287. C. D. Cappa, D. L. Che, S. H. Kessler, J. H. Kroll, and K. R. Wilson, "Variations in organic aerosol optical and hygroscopic properties upon heterogeneous OH oxidation," J. Geophys. Res., [Atmos.], **116**, D1520, DOI: 10.1029/2011JD015918 (2011)

286. W. Li, M. E. Law, P. R. Westmoreland, T. Kasper, N. Hansen, K. Kohse-Höinghaus, "Multiple benzene-formation paths in a fuel-rich cyclohexane flame," Combust. Flame, **158**, 2077, DOI: 10.1016/j.combustflame.2011.03.014 (2011)

# Chemical Dynamics Beamline Publications

285. O. Kostko, L. K. Takahashi, and M. Ahmed, "Desorption Dynamics, Internal Energies and Imaging of Organic Molecules from Surfaces with Laser Desorption and Vacuum Ultraviolet (VUV) Photoionization," Chem. Asian Journal, **6**, 3066, DOI: 10.1002/asia.201100419, (2011) 9.0.2.1 **LBNL# 4658E**

284. A. G. Vasiliou, K. M. Piech, X. Zhang, M. R. Nimlos, M. Ahmed, A. Golan, O. Kostko, D. L. Osborn, J. W. Daily, J. F. Stanton, and G. B. Ellison, "The products of the thermal decomposition of $CH_3CHO$," J. Chem. Phys., **135**, 014306, DOI: 10.1063/1.3604005, (2011) 9.0.2.1 **LBNL# 4493E**

283. L. Lee, P. Wooldridge, T. Nah, K. Wilson, and R. Cohen, "Reactive uptake coefficients for $NO_3$ on squalane and squalene aerosol," Abstracts of Papers of the American Chemical Society, 242nd National Meeting, **242**, 36-ENVR. (August 2011)

282. M. Blaze M. T., L. K. Takahashi, J. Zhou, M. Ahmed, G. L. Gaspar, F. D. Pleticha, and L. Hanley, "Brominated Tyrosine and Polyelectrolyte Multilayer Analysis by Laser Desorption VUV Postionization and Secondary Ion Mass Spectrometry," Anal. Chem., **83**, 4962, DOI: 10.1021/ac200693h (2011) 9.0.2. **LBNL# 4436E**

281. N. Hansen, T. Kasper, B. Yang, T. A. Cool, W. Li, P. R. Westmoreland, P. Oßwald, and K. Kohse-Höinghaus, "Fuel-structure dependence of benzene formation of processes in premixed flames fueled by $C_6H_{12}$," Proceedings of the Combustion Institute, **33,** 585, DOI: 10.1016/j.proci.2010.05.056, (2011)

280. C. J. Koh, C-L. Liu, C. W. Harmon, D. Strasser, A. Golan, O. Kostko, S. D. Chambreau, G. L.Vaghjiani, and S. R. Leone, "Soft Ionization of Thermally Evaporated Hypergolic Ionic Liquid Aerosols" J. Phys. Chem. A., **115,** 4630, DOI: 10.1021/jp200633b, (2011) **LBNL# 5424E**

279. S. Dooley, F. L. Dryer, B. Yang, J. Wang, T. A. Cool, T. Kasper and N. Hansen, "An experimental and kinetic modeling study of methyl formate low-pressure flames," Combustion and Flame, **158,** 732, DOI: 10.1016/j.combustflame.2010.11.003, (2011)

278. B. Yang, C. K. Westbrook, T. A. Cool, N. Hansen, and K. Kohse-Höinghaus, "Fuel-specific influences on the composition of reaction intermediates in premixed flames of three $C_5H_{10}O_2$ ester isomers," Phys. Chem. Chem. Phys., **13**, 6901, DOI: 10.1039/C0CP02065F (2011)

277. K. Khistyev, K. B. Bravaya, E. Kamarchik, O. Kostko, M. Ahmed, and A. I. Krylov, "The effect of microhydration on ionization energies of thymine," Faraday Discussions**, 150,** 313, DOI: 10.1039/C0FD00002G, (2011) 9.0.2.1 **LBNL# 4251E**

276. C-L. Liu, J.D. Smith, D.L. Che, M. Ahmed, S.R. Leone, and K.R. Wilson, "The Direct Observation of Secondary Radical Chain Chemistry in the Heterogeneous Reaction of Chlorine Atoms with Submicron Squalane Droplets," Phys. Chem. Chem. Phys., **13**, 8993, DOI: 10.1039/C1CP20236G, (2011) 9.0.2.1 **LBNL# 5245E**

275. L. K. Takahashi, J. Zhou, O. Kostko, A. Golan, S.R. Leone, and M. Ahmed, "Vacuum-Ultraviolet Photoionization and Mass Spectrometric Characterization of Lignin Monomers Coniferyl and Sinapyl Alchohols," J. Phys. Chem. A, **115**, 3279, DOI: 10.1021/jp111437e, (2011) 9.0.2.1 **LBNL# 4654E**

274. P. Croteau, J. B. Randazzo, O. Kostko, M. Ahmed, M.C. Liang, Y. L. Yung, and K. A. Boering, "Measurements of isotope effects in the photoionization of $N_2$ and implications for Titan's atmosphere," Astrophys. J. Lett., **728**, L32, DOI:10.1088/2041-8205/728/2/L32, (2011) 9.0.2.1 **LBNL# 4202E**

# Chemical Dynamics Beamline Publications

273. G. L. Gasper, L. K. Takahashi, J. Zhou, M. Ahmed, J. F. Moore, and L. Hanley, "Comparing Vacuum and Extreme Ultraviolet Radiation for Postionization of Laser Desorbed Neutrals from Bacterial Biofilms and Organic Fullerene," Nuclear Instruments and Methods in Physics Research Section A, **649**, 222, DOI: 10.1016/j.nima.2010.12.024, (2011) 9.0.2.1 **LBNL# 4263E**

272. C. D. Cappa, K. R. Wilson, "Evolution of organic aerosol mass spectra upon heating: implications for OA phase and partitioning behavior," Atmos. Chem. Phys., **11**, 1895, DOI: 10.5194/acp-11-1895-2011, (2011) 9.0.2.1 **LBNL# 4204E**

271. J. H. Kroll, N. M. Donahue, J. L. Jimenez, S. H. Kessler, M. R. Canagaratna, K. R. Wilson, K. E. Altieri, L. R. Mazzoleni, A. S. Wozniak, H. Bluhm, E. R. Mysak, J. D. Smith, C. E. Kolb, D. R. Worsnop, "Carbon oxidation state as a metric for describing the chemistry of atmospheric organic aerosol," Nature Chem., **3**, 133, DOI: 10.1038/nchem.948, (2011) 9.0.2.1 **LBNL# 4394E**

270. W. K. S. Chiu, C. P. Grigoropoulos, and B. Q. Li., "Special Issue on Advanced Thermal Processing," J. Heat Transfer, **133**, 030301, DOI:10.1115/1.4002442, (2011)

269. L. Lee, P. Wooldridge, T. Nah, K. R. Wilson, R. Cohen, "Reactive uptake coefficients for NO(3) on squalane and squalene aerosol," Abstracts of Papers of the 242nd National Meeting of the American Chemical Society, 306-ENVR, Denver, CO, August (2011)

**2010**

268. P. Croteau, "Nitrous oxide and molecular nitrogen isotopic compositions and aerosol optical properties: Experiments and observations relevant to planetary atmospheres," doctoral dissertation, University of California, Berkeley, Berkeley, CA, United States (2010) advisor Kristie A. Boering (9.0.2)

267. E. R. Mysak, D. E. Starr, K. R. Wilson, and H. Bluhm, "Note: A combined aerodynamic lens/ambient pressure x-ray photoelectron spectroscopy experiment for the on-stream investigation of aerosol surfaces," Review of Sci. Inst., **81**, 016106, DOI: 10.1063/1.3276714, (2010)

266. S. H. Kessler, J. D. Smith, C. L. Dung, D. R. Worsnop, K. R. Wilson, and J. H. Kroll, "Chemical Sinks of Organic Aerosol: Kinetics and Products of the Heterogeneous Oxidation of Erythritol and Levoglucosan," Environ. Sci. Technol., **44**, 7005, DOI: 10.1021/es101465m (2010)

265. N. Hansen, W. Li, M. E. Law, T. Kasper, P. R. Westmoreland, B. Yang, T. A. Cool, A. Lucassen, "The importance of fuel dissociation and propargyl + allyl association for the formation of benzene in a fuel-rich 1-hexene flame," Phys. Chem. Chem. Phys., **12**, 12112, DOI: 10.1039/C0CP00241K, (2010) 9.02.3

264. K. B. Bravaya, O. Kostko, S. Dolgikh, A. Landau, M. Ahmed, A. I. Krylov, "Electronic Structure and Spectroscopy of Nucleic Acid Bases: Ionization Energies, Ionization-Induced Structural Changes, and Photoelectron Spectra," J. Chem. Phys. A., **114**, 12305, DOI: 10.1021/jp1063726, (2010) 9.02.3 **LBNL# 4111E**

263. A. W. Rollins, J. D. Smith, K. R. Wilson, R. C. Cohen, "Real Time In Situ Detection of Organic Nitrates in Atmospheric Aerosols," Environ. Sci. Technol., **44**, 5540, DOI: 10.1021/es100926x, (2010) 9.0.2.1 **LBNL# 4352E**

262. W. G. Rellergert, D. DeMille, R. R. Greco, M. P. Hehlen, J. R. Torgerson, E. R. Hudson, "Constraining the Evolution of the Fundamental Constants with a Solid-State Optical Frequency Reference Based on the $229^{Th}$ Nucleus," Phys. Rev. Lett., **104**, 200802, DOI: http://dx.doi.org/10.1103/PhysRevLett.104.200802, (2010) 9.0.2.1

# Chemical Dynamics Beamline Publications

261. G. L. Gasper, L. K. Takahashi, J. Zhou, J. Moore, M. Ahmed, and L. Hanley, "Laser Desorption Postionization Mass Spectrometry of Antibiotic-Treated Bacterial Biofilms Using Tunable Vacuum Ultraviolet Radiation," Anal. Chem., **82**, 7472, DOI: 10.1021/ac101667q, (2010) 9.0.2.2 **LBNL# 3963E**

260. M. Sleiman, H. Destaillats, J.D. Smith, Chen-Lin Liu, M. Ahmed, K.R. Wilson, and L.A. Gundel, "Secondary organic aerosol formation from ozone-Initiated reactions with nicotine and secondhand smoke," Atmos. Environ., **44**, 4191, DOI: 10.1016/j.atmosenv.2010.07.023, (2010) 9.0.2.1

259. R. I. Kaiser, B. J. Sun, H. M. Lin, A. H. H. Chang, A. Mebel, O. Kostko and M. Ahmed, "An Experimental and Theoretical Study on the Ionization Energies of Polyynes (H-(C≡C)$_n$-H; n = 1 - 9)," Astrophys. J., **719**, 1884, DOI: 10.1088/0004-637X/719/2/1884, (2010) 9.0.2.3 **LBNL# 3962E**

258. H. Imanaka, M. A. Smith, "Formation of nitrogenated organic aerosols in the Titan upper atmosphere," PNAS, **107**, 12423, DOI: 10.1073/pnas.0913353107, (2010) 9.0.2.1

257. S. Soorkia, C. A. Taatjes, D. L. Osborn, T. M. Selby, A. J. Trevitt, K. R. Wilson, and S. R. Leone, "Direct detection of pyridine formation by the reaction of CH (CD) with pyrrole: a ring expansion reaction," Phys. Chem. Chem. Phys., **12**, 8750, DOI: 10.1039/c002135k, (2010) 9.02.3 **LBNL# 3290E**

256. J. Wang, B. Yang, T. A. Cool, and N. Hansen, "Absolute Cross-Sections for Dissociative Photoionization of Some Small Esters," Int. J. Mass Spectrom., **292**, 14, DOI: 10.1016/j.ijms.2010.02.010, (2010) 9.02.3

255. O. Kostko, J. Zhou, B. J. Sun, J. S. Lie, A. H. H. Chang, R. I. Kaiser, and M. Ahmed, "Determination of ionization energies of $C_nN$ (n=3-14) clusters: Vacuum-ultraviolet (VUV) photoionization experiments and theoretical calculations," Astrophys. J., **717**, 674, DOI: 10.1088/0004-637x/717/2/674, (2010) 9.02.3 **LBNL# 3964E**

254. E. Kamarchik, O. Kostko, J. M. Bowman, M. Ahmed, and A. I. Krylov, "Spectroscopic signatures of proton transfer dynamics in the water dimer cation," J. Chem. Phys., **132**, 194311, DOI: 10.1063/1.3432198, (2010) 9.02.3 **LBNL# 3334E**

253. K. Kohse-Höinghaus, P. Oßwald, T. A. Cool, T. Kasper, N. Hansen, F. Qi, C. K. Westbrook, P. R. Westmoreland, "Biofuel Combustion Chemistry: From Ethanol to Biodiesel," Angew. Chem., **49**, 3572, DOI: 10.1002/anie.200905335, (2010)

252. R. I. Kaiser, P. Maksyutenko, C. Ennis, F. Zhang, X. Gu, A. Mebel, O. Kostko, M. Ahmed, **"**Untangling the chemical evolution of Titan's atmosphere and surface: from homogeneous to heterogeneous chemistry," Faraday. Disc., **147,** 429, DOI: 10.1039/c003599h, (2010) 9.0.2.3 **LBNL# 3295E**

251. S. R. Leone, M. Ahmed, K. R. Wilson, "Chemical Dynamics, Molecular Energetics, and Kinetics at the Synchrotron," Phys. Chem. Chem. Phys., **12**, 6564 (2010) 9.0.2.1, 9.0.2.2, 9.0.2.3 **LBNL# 3288E**

250. J. Zhou, L. K. Takahashi, K. R. Wilson, S. R. Leone, M. Ahmed, "Internal Energies of Ion-Sputtered Neutral Tryptophan and Thymine Molecues determined by Vacuum Ultraviolet Photoionization," Anal. Chem., **82**, 3905, DOI: 10.1021/ac1004629, (2010) 9.0.2.2 **LBNL# 3287E**

249. O. Kostko, K. B. Bravaya, A. I. Krylov and M. Ahmed, "Ionization of cytosine monomer and dimer studied by VUV photoionization and electronic structure calculations," Phys. Chem. Chem. Phys., **12,** 2860, DOI: 10.1039/B921498D, (2010) 9.0.2.3 **LBNL# 2986E**

# Chemical Dynamics Beamline Publications

248. C. A. Taatjes, D. L. Osborn, T. Selby, G. Meloni, A. J. Trevitt, E. Epifanovsky, A. I. Krylov, B. Sirjean, E. Dames, and H. Wang, "Products of the Benzene + O(3P) Reaction," J. Phys. Chem. A., **114,** 3355, DOI: 10.1021/jp9114145, (2010) 9.02.3 **LBNL# 2985E**

247. S. Soorkia, A. J. Trevitt, T. Selby, D. L. Osborn, C. A. Taatjes, K. R. Wilson, S. R. Leone, "Reaction of the C2H radical with 1-butyne ($C_4H_6$): Low Temperature Kinetics and Isomer-Specific Product Detection," J. Phys. Chem. A., **114**, 3340, DOI: 10.1021/jp911132r, (2010) 9.02.3 **LBNL# 3312E**

246. K. B. Bravaya, O. Kostko, M. Ahmed, and A. I. Krylov, "The effect of π-stacking, h-bonding, and electrostatic interactions on the ionization energies of nucleic acid bases: adenine-adenine, thymine-thymine and adenine-thymine dimers," Phys. Chem. Chem. Phys., **12,** 2292, DOI: 10.1039/B919930F, (2010) 9.02.3 **LBNL# 2653E**

245. S. D. Chambreau, G. L.Vaghjiani, A. To, C. Koh, D. Strasser, O. Kostko, and S. R. Leone, "Heats of vaporization of room temperature ionic liquids by tunable vacuum ultraviolet photoionization," J. Phys. Chem. B., **114,** 1361, DOI: 10.1021/jp909423m, (2010) 9.02.3 **LBNL# 3289E**

244. D. Strasser, F. Goulay, L. Belau, O. Kostko, C. Koh, S. D. Chambreau, G. L.Vaghjiani, M. Ahmed, and S. R. Leone, "Tunable Wavelength Soft Photionization of Ionic Liquid Vapors," J. Phys. Chem. A., **114,** 879, DOI: 10.1021/jp909727f, (2010) 9.02.3 **LBNL# 3160E**

243. O. Kostko, S. R. Leone, M. A. Duncan, and M. Ahmed, "Determination of Ionization Energies of Small Silicon Clusters with Vacuum-Ultraviolet (VUV) Radiation," J. Phys. Chem. A., **114,** 3176, DOI: 10.1021/jp9091688, (2010) 9.02.3 **LBNL# 2867E**

242. R. I. Kaiser, A. M. Mebel, O. Kostko, and M. Ahmed, "On the Ionization Energies of $C_4H_3$ Isomers," Chem. Phys. Lett., **485**, 281, DOI: 10.1016/j.cplett.2009.12.027, (2010) 9.02.3 **LBNL# 2652E**

241. A. J. Trevitt, F. Goulay, C. A. Taatjes, D. L. Osborn, and S. R. Leone, "Reactions of the CN Radical with Benzene and Toluene: Product Detection and Low-Temperature Kinetics," J. Phys. Chem. A., **114,** 1749, DOI: 10.1021/jp909633a, (2010) 9.02.3 **LBNL# 3333E**

240. E. E. Greenwald, B. Ghosh, K. C. Anderson, K. S. Dooley, P. Zou, T. Selby, D. L. Osborn, G. Meloni, C. A. Taatjes, F. Goulay, and S. W. North, "Isomer-selective study of the OH initiated oxidation of isoprene in the presence of $O_2$ and NO. I. the minor inner OH-addition channel," J. Phys. Chem. A., **114,** 904, DOI: 10.1021/jp908543a, (2010)

**2009**

239. A. C. Noell, "Laboratory studies of the self and cross reactions of atmospheric peroxy radicals," doctoral dissertation, California Institute of Technology, Pasadena, CA, United States, (2009) advisor Mitchio Okumura (9.0.2)

238. K. M. Perra, "Electronic spectroscopy and dissociation dynamics of gas-phase transition metal containing cations and dications," doctoral dissertation, University of Massachusetts Amherst, Amherst, MA (2009) Ricardo B. Metz (9.0.2)

237. J. Zádor, R. X. Fernandes, Y. Georgievskii, G. Meloni, C. A. Taatjes, and J. A. Miller, "The reaction of hydroxyethyl radicals with $O_2$: a theoretical analysis and experimental product study," Proc. Combust. Inst., **32,** 271, DOI: 10.1016/j.proci.2008.05.020, (2009)

# Chemical Dynamics Beamline Publications

236. N. Hansen, J. A. Miller, P. R. Westmoreland, T. Kasper, K. Kohse-Höinghaus, J. Wang, and T. A. Cool, "Isomer-specific combustion chemistry in allene and propyne flames," Combustion and Flame, **156,** DOI: 2153, 10.1016/j.combustflame.2009.07.014, (2009)

235. J. H. Kroll, J. D. Smith, D. L. Che, S.H. Kessler, D. R. Worsnop, and K. R. Wilson, "Measurement of fragmentation and functionalization pathways in the heterogeneous oxidation of organic aerosol," Phys. Chem. Chem. Phys., **11**, 8005, DOI: 10.1039/b905289e, (2009), 9.02.1 **LBNL# 1700E**

234. H. Imanaka and M. A. Smith, "EUV Photochemical Production of Unsaturated Hydrocarbons: Implications to EUV Photochemistry in Titan and Jovian Planets," J. Phys. Chem. A., **113**, 11187, DOI: 10.1021/jp9041952, (2009) 9.0.2.1

233. O. Kostko, S. K. Kim, S. R. Leone, and M. Ahmed, "Mass-Analyzed Threshold Ionization (MATI) Spectroscopy of Atoms and Molecules using VUV Synchrotron Radiation," J. Phys. Chem. A., **113**, 14206, DOI: 10.1021/jp9008338, (2009) 9.02.3 **LBNL# 1646E**

232. D. L. Che, J. D. Smith, S. R. Leone, M. Ahmed, and K. R. Wilson, "Quantifying the reactive uptake of OH by organic aerosols in a continuous flow stirred tank reactor," Phys. Chem. Chem. Phys., **11**, 7885, DOI: 10.1039/B904418C, (2009) 9.02.1 **LBNL# 2575E**

231. T. Kasper, P. Oßwald, U. Struckmeier, K. Kohse-Höinghaus, C.A. Taatjes, J. Wang, T.A. Cool, M.E. Law, A. Morel, and P.R. Westmoreland, "Combustion chemistry of the propanol isomers — investigated by electron ionization and VUV-photoionization molecular-beam mass spectrometry," Combustion and Flame, **156,** 1181, DOI: 10.1016/j.combustflame.2009.01.023, (2009)

230. S. Chakraborty, M. Ahmed, T. L. Jackson, and M. H. Thiemens, "Reply to comment on Experimental Test of Self-Shielding in Vacuum Ultraviolet Photodissociation of CO," Science, **324**, 1516, DOI: 10.1126/science.1167919, (2009) 9.02.1

229. M. T. Timko, Z. Yu, J. Kroll, J. T. Jayne, D. R. Worsnop, R. C. Miake-Lye, T. B. Onasch, D. Liscinsky, T. W. Kirchstetter, H. Destaillats, A. L. Holder, J. D. Smith, and K. R.Wilson, "Sampling Artifacts from Conductive Silicone Tubing," Aerosol Science and Technology, **43**, 855, DOI: 10.1080/02786820902984811, (2009) 9.02.1 **LBNL# 2150E**

228. H. Ismail, P. R. Abel, W. H. Green, A. Fahr, L. E. Jusinski, A. M. Knepp, J. Zádor, G. Meloni, T. M. Selby, D. L. Osborn and C. Taatjes "Temperature-Dependent Kinetics of the Vinyl Radical ($C_2H_3$) Self-Reaction," J. Phys. Chem. A., **113**, 1278**,** DOI: 10.1021/jp8096132, (2009) 9.02.3

227. J. D. Smith, J. H. Kroll, C. D. Cappa, D. L. Che, C.L. Liu, M. Ahmed, S. R. Leone, D. R. Worsnop, and K. R. Wilson, "The heterogeneous reaction of squalane particles with OH radicals," Atmos. Chem. Phys., **9**, 3209, DOI: 10.5194/acp-9-3209-2009, (2009) 9.02.1

226. J. Wang, M. Chaos, B. Yang, T. A. Cool, F. L. Dryer, T. Kasper, N. Hansen, P. Oßwald, K. Kohse-Höinghaus, and P. R. Westmoreland, "Composition of reaction intermediates for stoichiometric and fuel-rich dimethyl ether flames: flame-sampling mass spectrometry and modeling studies," Phys. Chem. Chem. Phys., **11**, 1328, DOI: 10.1039/B815988B, (2009) 9.02.3

225. C. K. Westbrook, W. J. Pitz, P. R. Westmoreland, F. L. Dryer, M. Chaos, P. Oßwald, K. Kohse-Höinghaus, T. A. Cool, J. Wang, B. Yang, N. Hansen, and T. Kasper, "A detailed chemical kinetic mechanism for oxidation of four small alkyl esters in laminar premixed flames," Proc. Combust. Inst., **32**, 221, DOI: 10.1016/j.proci.2008.06.106, (2009) 9.02.3

# Chemical Dynamics Beamline Publications

224. A. Lucassen, P. Oßwald, U. Struckmeier, K. Kohse-Höinghaus, T. Kasper, N. Hansen, T. A. Cool, and P. R. Westmoreland, "Species identification in a laminar premixed low-pressure flame of morpholine as a model substance for oxygenated nitrogen-containing fuels," Proc. Combust. Inst., **32**, 1269, DOI: 10.1016/j.proci.2008.06.053, (2009) 9.02.3

223. N. Hansen, J. A. Miller, T. Kasper, K. Kohse-Höinghaus, P. R. Westmoreland, J. Wang, T. A. Cool, "Benzene Formation in Premixed Fuel-Rich 1,3-Butadiene Flames," Proc. Combust. Inst., **32**, 623, DOI: 10.1016/j.proci.2008.06.050, (2009) 9.02.3

222. N. Hansen, T.A. Cool, P.R. Westmoreland, and K. Kohse-Höinghaus, "Recent contributions of flame-sampling molecular-beam mass spectrometry to a fundamental understanding of combustion chemistry," Progress in Energy and Combustion Science, **35**, 169, DOI: 10.1016/j.pecs.2008.10.001, (2009) 9.02.3

221. F. Goulay, A. J. Trevitt, G. Meloni, T. M. Selby, D. L. Osborn, C. A. Taatjes, L. Vereecken, and S. R. Leone, "Cyclic Versus Linear Isomers Produced by Reaction of the Methylidyne Radical (CH) with Small Unsaturated Hydrocarbons," J. Am. Chem. Soc., **131,** 993, DOI: 10.1021/ja804200v, (2009) 9.02.3 **LBNL# 2480E**

220. J. Zhou, O. Kostko, C. Nicolas, X. N. Tang, L. Belau, M. S. de Vries, and M. Ahmed "Experimental observation of guanine tautomers with VUV photoionization," J. Phys. Chem. A., **113**, 4829, DOI: 10.1021/jp811107x, (2009) 9.02.3 **LBNL# 1330E**

219. L. K. Takahashi, J. Zhou, K. R. Wilson, S. R. Leone, and M. Ahmed "Imaging with Mass Spectrometry: A Secondary Ion and VUV-Photoionization Study of Ion-Sputtered Atoms and Clusters from GaAs and Au," J. Phys. Chem. A., **113**, 4035, DOI: 10.1021/jp810408v, (2009) 9.02.2 **LBNL# 1743E**

218. O. Kostko, M. Ahmed, and R. B. Metz, "A VUV photoionization measurement and *ab-initio* calculation of the ionization energy of gas phase $SiO_2$," J. Phys. Chem. A., **113**, 1225, DOI: 10.1021/jp8091495, (2009) 9.02.3 **LBNL# 2471E**

217. A. J. Trevitt, F. Goulay, G. Meloni, D. L. Osborn, C.A. Taatjes, and S. R. Leone, "Isomer-specific product detection of CN radical reactions with ethene and propene by tunable VUV photoionization mass spectrometry," Int. J. Mass. Spectrom. **280**, 113, DOI: 10.1016/j.ijms.2008.07.033, (2009) 9.02.3

216. J. L. Jimenez, M. R. Canagaratna, N. M. Donahue, A. H. Prevot, Q. Zhang, J. H. Kroll, P. F. DeCarlo, J. D. Allan, H. Coe, N. L. Ng, A. C. Aiken, K. S. Docherty, I. M. Ulbrich, A. P. Grieshop, A. L. Robinson, J. Duplissy, J. D. Smith, K. R. Wilson, V. A. Lanz, C. Hueglin, Y. L. Sun, J. Tian, A. Laaksonen, T. Raatikainen, J. Rautiainen, P. Vaattovaara, M. Ehn, M. Kulmala, J. M. Tomlinson, D. R. Collins, M. J. Cubison, E. J. Dunlea, J. A. Huffman, T. B. Onasch, M. R. Alfarra, P. I. Williams, K. Bower, Y. Kondo, J. Schneider, F. Drewnick, S. Borrmann, S. Weimer, K. Demerjian, D. Salcedo, L. Cottrell, R. Griffin, A. Takami, T. Miyoshi, S. Hatakeyama, A. Shimono, J. Y. Sun, Y. M. Zhang, K. Dzepina, J. R. Kimmel, D. Sueper, J. T. Jayne, S. C. Herndon, A. M. Trimborn, L. R. Williams, E. C. Wood, A. M. Middlebrook, C. E. Kolb, U. Baltensperger, and D. R. Worsnop, "Evolution of organic aerosols in the atmosphere," Science, **326**(5959), 1525, DOI: 10.1126/science.1180353, (2009)

**2008**

215. G. Meloni, T. M. Selby, C. A. Taatjes, and D. L. Osborn, "Enol Formation and Ring-Opening in OH-Initiated Oxidation of Cycloalkenes," J. Phys. Chem. A, **112**, 13444, DOI: 10.1021/jp808015f, (2008) 9.02.3

# Chemical Dynamics Beamline Publications

214. D. L. Osborn, P. Zou, H. Johnsen, C. C. Hayden, C. A. Taatjes, V. D. Knyazev, S. W. North, D. S. Peterka, M. Ahmed, and S. R. Leone, "The multiplexed chemical kinetic photoionization mass spectrometer: a new approach to isomer-resolved chemical kinetics," Rev. Sci. Instrum., **79,** 104103, DOI: 10.1063/1.3000004, (2008) 9.02.3 **LBNL# 1809E**

213. T. M. Selby, G. Meloni, F. Goulay, S. R. Leone, A. Fahr, C. A. Taatjes, and D. L. Osborn, "Synchrotron Photoionization Mass Spectrometry Measurements of Kinetics and Product Formation in the Allyl Radical ($H_2CCHCH_2$) Self-Reaction," J. Phys. Chem. A, **112**, 9366, DOI: 10.1021/jp802330k, (2008) 9.02.3

212. C. C. Wang, O. Kornilov, O. Gessner, J. H. Kim, D. S. Peterka, and D. Neumark, "Photoelectron Imaging of Helium Droplets Doped with Xe and Kr Atoms," J. Phys. Chem. A, **112,** (39), 9356, DOI: 10.1021/jp802332f, (2008) 9.02.3

211. C. A. Taatjes, G. Meloni, T. M. Selby, A. J. Trevitt, D. L. Osborn, C. J. Percival, and D. E. Shallcross, "Direct Observation of the Gas-Phase Criegee Intermediate ($CH_2OO$)," J. Am. Chem. Soc., **130,** (36); 11883-11885, DOI: 10.1021/ja804165q, (2008) 9.02.3

210. S. Chakraborty, M. Ahmed, T. L. Jackson, and M. H. Thiemens, "Experimental Test of Self-Shielding in Vacuum Ultraviolet photodissociation of CO," Science **321,** 1328, DOI: 10.1126/science.1159178, (2008) 9.02.1

209. M. Citir, R. B. Metz, L. Belau and M. Ahmed, "Direct Determination of the Ionization Energies of PtC, PtO and $PtO_2$ with VUV Radiation," J. Phys. Chem. A., **112,** (39); 9584, DOI: 10.1021/jp8024733, (2008) 9.02.3 **LBNL# 1231E**

208. O. Kostko, L. Belau, K. R. Wilson, and M. Ahmed, "Vacuum-Ultraviolet (VUV) Photoionization of Small Methanol and Methanol-Water Clusters,", J. Phys. Chem. A., **112,** (39); 9555, DOI: 10.1021/jp8020479, (2008), 9.02.3 **LBNL# 1230E**

207. J. Wang, U. Struckmeier, B. Yang, T. A. Cool, P. Oßwald, K. Kohse-Höinghaus, T. Kasper, N. Hansen, and P. R. Westmoreland, "Isomer-Specific Influences on the Composition of Reaction Intermediates in Dimethyl Ether/Propene and Ethanol/Propene Flame," J. Phys. Chem. A., **112,** (39); 9255-9265, DOI: 10.1021/jp8011188, (2008) 9.02.3

206. C. A. Taatjes, D. L. Osborn, T. M. Selby, G. Meloni, H. Fan, and S. T. Pratt. "Absolute Photoionization Cross-Section of the Methyl Radical," J. Phys. Chem. A., **112,** (39); 9336-9343, DOI: 10.1021/jp8022937, (2008) 9.02.3

205. J. Wang, B. Yang, T. A. Cool, N. Hansen and T. Kasper "Near-threshold absolute photoionization cross-sections of some reaction intermediates in combustion," Int. J. Mass Spectrom.**, 269**, (3); 210, DOI: 10.1016/j.ijms.2007.10.013, (2008) 9.02.3

204. N. Hansen, S. J. Klippenstein, P. R. Westmoreland, T. Kasper, K. Kohse-Höinghaus, J. Wang and T. A. Cool, "A combined ab initio and photoionization mass spectrometric study of polyynes in fuel-rich flames," Phys. Chem. Chem. Phys., **10,** 366, DOI: 10.1039/B711578D, (2008) 9.02.3

203. C. A. Taatjes, N. Hansen, D. L. Osborn, K. Kohse-Höinghaus, T. A. Cool and P. R. Westmoreland, "'Imaging' combustion chemistry via multiplexed synchrotron-photoionization mass spectrometry," Phys. Chem. Chem. Phys., **10,** 20, DOI: 10.1039/B713460F, (2008) 9.02.3

# Chemical Dynamics Beamline Publications

202. D. E. Starr, E. K. Wong, D. R. Worsnop, K. R., Wilson, and H. Bluhm, "A combined droplet train and ambient pressure photoemission spectrometer for the investigation of liquid/vapor interfaces," Phys. Chem. Chem. Phys., **10,** 3093, DOI: 10.1039/b800717a, (2008) 9.02.3

201. R. C. Maher, L. F. Cohen, P. Lohsoontorn, D.J. L. Brett, and N. P. Brandon, "Raman Spectroscopy as a Probe of Temperature and Oxidation State for Gadolinium-Doped Ceria Used in Solid Oxide Fuel Cells**", J. Phys. Chem. A.,** 112, **7**; 1497-1501, DOI: 10.1021/jp076361j, (2008)

**2007**

200. G. Meloni, T. M. Selby, F. Goulay, S. R. Leone, D. L. Osborn, and C. A. Taatjes, "Photoionization of 1-Alkenylperoxy and Alkylperoxy Radicals and a General Rule for the Stability of Their Cations," J. Am. Chem. Soc., **129,** (45), 14019, DOI: 10.1021/ja075130n, (2007) 9.023

199. C. R. Howle, A. N. Arrowsmith, V. Chikan, and S. R. Leone, "State-Resolved Dynamics of the CN($B^{2+}$) and CH($A^2$) Excited Products Resulting from the VUV Photodissociation of $CH_3CN$," J. Phys. Chem. A., **111,** (29), 6637, DOI: 10.1021/jp068544w, (2007). 9.02.3

198. M.J. Northway, J.T. Jayne, D.W. Toohey, M.R. Canagaratna, A. Trimborn, K-I. Akiyama, A. Shimono, J. L. Jimenez, P. F. DeCarlo, K. R. Wilson, and D. R. Worsnop. "Demonstration of a VUV Lamp Photoionization Source for Improved Organic Speciation in an Aerosol Mass Spectrometer," Aerosol Science & Technology, **41**, 828, DOI: 10.1080/02786820701496587, (2007) 9.02.1

197. L. Belau, K. R. Wilson, S. R. Leone, and M. Ahmed, "Vacuum Ultraviolet (VUV) photoionization of small water clusters," J. Phys. Chem A., **111**, 10075, DOI: 10.1021/jp075263v, (2007) LBNL-62671 9.02.3

196. L. Belau, S. E. Wheeler, B. W. Ticknor, M. Ahmed, S. R. Leone, W. D. Allen, H. F. Schaefer III, and M. A. Duncan, "Ionization Thresholds of Small Carbon Clusters: Tunable VUV Experiments and Theory," J. Am. Chem. Soc., **129**, 10229, DOI: 10.1021/ja072526q, (2007) LBNL-62670 9.02.3

195. K. R. Wilson, S. Zou, J. Shu, E. Rühl, S. R. Leone, G. C. Schatz and M. Ahmed, "Size-Dependent Angular Distributions of Low Energy Photoelectrons emitted from NaCl Nanoparticles," Nano Letters **7**, 2014, DOI: 10.1021/nl070834g, (2007) LBNL-62649 9.02.3

194. D. S. Peterka, J. H. Kim, C. C. Wang, L. Poisson, and D. M. Neumark, "Photoionization dynamics in pure helium droplets," J. Phys. Chem A., **111,** 7449, DOI: 10.1021/jp0710032, (2007) LBNL-62405 9.02.3

193. L. Belau, K. R. Wilson, S. R. Leone, and M. Ahmed, "Vacuum-Ultraviolet Photoionization Studies of the Micro-Hydration of DNA Bases (Guanine, Cytosine, Adenine and Thymine)," J. Phys. Chem. A., **111**, 7562, DOI: 10.1021/jp0705929, (2007) LBNL-62328 9.02.3

192. J. Li, J. Yang, Y. X. Mo, K. C. Lau, X. M. Qian, Y. Song, J. Liu, and C. Y. Ng, "Combined vacuum ultraviolet laser and synchrotron pulsed field ionization study of CH2BrCl," J. Chem. Phys., **126**, 184304, DOI: 10.1063/1.2730829, (2007) 9.02.2

191. R. I. Kaiser, L. Belau, S. R. Leone, M. Ahmed, Y. Wang, B. J. Braams, and J. M. Bowman, "A Combined Experimental and Computational Study on the Ionization Energies of the Cyclic and Linear C3H Isomers," Chem. Phys. Chem. **8**, 1236, DOI: 10.1002/cphc.200700109, (2007) LBNL-62329 9.02.3

# Chemical Dynamics Beamline Publications

190. P. Oßwald, U. Struckmeier, T. Kasper, K. Kohse-Höinghaus, J. Wang, T. A. Cool, N. Hansen, P.R. Westmoreland, "Isomer-Specific Fuel Destruction Pathways in Rich Flames of Methyl Acetate and Ethyl Formate and Consequences for the Combustion Chemistry of Esters," J. Phys. Chem. A. **111**, 4093, DOI: 10.1021/jp068337w, (2007) LBNL-62478 9.02.3

189. F. Goulay, D. L. Osborn, C. A. Taatjes, P. Zou, G. Meloni, and S. R. Leone, "Direct detection of polynes formation from the reaction of ethynyl radical (C2H) with propyne (CH3-CCH) and allene (CH2=C=CH2)," Phys. Chem. Chem. Phys. **9,** 4291, DOI: 10.1039/B614502G, (2007) LBNL-61760 9.02.3

188. N. Hansen, T. Kasper, S. J. Klippenstein, P. R. Westmoreland, M. E. Law, C. A. Taatjes, K. Kohse-Höinghaus, J. Wang, T. A. Cool, "Initial steps of aromatic ring formation in a laminar premixed fuel-rich cyclopentene flame," J. Phys. Chem. A., **111**, 4081, DOI: 10.1021/jp0683317, (2007) LBNL-62385 9.02.3

187. S. Stimson, M. Evans, C. -W. Hsu and C. Y. Ng, "Rotationally resolved vacuum ultraviolet pulsed field ionization-photoelectron vibrational bands for $HD^+$," J. Chem. Phys., **126**, 164303, DOI: 10.1063/1.2720843, (2007), 9.02.2

186. H. Imanaka, and M. A. Smith, "Role of photoionization in the formation of complex organic molecules in Titan's upper atmosphere," Geophys. Res. Lett., **34,** L02204, DOI: 10.1029/2006GL028317, (2007) LBNL-61808 9.02.1

185. M.E. Law, P.R. Westmoreland, T.A. Cool, J. Wang, N. Hansen, C.A. Taatjes, T. Kasper, K. Kohse-Höinghaus, "Benzene precursors and formation routes in a stoichiometric cyclohexane flame," Proc. Combust. Inst., **31,** 565-573, DOI: 10.1016/j.proci.2006.07.259, (2007), LBNL- 59297 9.02.3

184. K. Kohse-Höinghaus, P. Oßwald, U. Struckmeier, T. Kasper, N. Hansen, C. A. Taatjes, J. Wang, T. A. Cool, S. Gon, and P. R. Westmoreland, "The influence of ethanol addition on a premixed fuel-rich propene-oxygen flame," Proc. Combust. Inst., **31, (1)**, 1119-1127, DOI: 10.1016/j.proci.2006.07.007, (2007) LBNL-59295 9.02.3

183. N. Hansen, J. A. Miller, C.A. Taatjes, J. Wang, T. A. Cool, M. E. Law, and P.R. Westmoreland, "Photoionization mass spectrometric studies and modeling of fuel-rich allene and propyne flames," Proc. Combust. Inst., **31 (1)**, 1157-1164, DOI:10.1016/j.proci.2006.07.045, (2007) LBNL-59296 9.02.3

182. T. A. Cool, J. Wang, N. Hansen, P. R. Westmoreland, F. L. Dryer, Z. Zhou, A. Kazakov, T. Kasper and K. K.-Höinghaus, "Photoionization mass spectrometry and modeling studies of the chemistry of fuel-rich dimethyl ether flames," Proc. Combust. Inst., **31 (1)**, 285-293, DOI: 10.1016/j.proci.2006.08.044, (2007) LBNL-59290 9.02.3

**2006**

181. M. Ahmed, "Photoionization of desorbed neutrals from surfaces," Encyclopedia of Mass Spectrometry, Vol. 6, Elseiver (2006) LBNL-60001 9.02.1

180. A. Das, E. D. Poliakoff, R. R. Lucchese, J. D. Bozek, "Launching a particle on a ring: b2u_ke2g ionization of C6F6," J. Chem. Phys., **125**, 164316, DOI: 10.1063/1.2360532 (2006) LBNL-61875.

179. R. A. Dressler, Y. Chiu, D. J. Levandier, X. N. Tang, Y. Hou, C. Chang, C. Houchins, H. Xu, and C-Y. Ng, "The study of state-selected ion-molecule reactions using the vacuum ultraviolet pulsed field ionization-photoion technique," J. Chem. Phys., **125**, 132306, DOI: 10.1063/1.2207609 (2006). LBNL-61737

# Chemical Dynamics Beamline Publications

178. G. Meloni, P. Zou, S.J. Klippenstein, M. Ahmed, S. R. Leone, C. A. Taatjes, and D. L. Osborn, "Energy-resolved photoionization of alkyl peroxy radicals and the stability of their cations," J. Am. Chem. Soc., **128,** 13559, DOI: 10.1021/ja064556j (2006). LBNL-60848

177. E. Gloaguen, E. R. Mysak, S. R. Leone, M. Ahmed, and K. R. Wilson "Investigating the chemical composition of mixed organic-inorganic particles by "soft" VUV photoionization: the reaction of ozone with anthracene on sodium chloride particles," Int. J. Mass Spectrom., **258**, 74, DOI: 10.1016/j.ijms.2006.07.019 (2006) LBNL-60212

176. D. S. Peterka, J. H. Kim, C. C. Wang, and D. M. Neumark, "Photoionization and Photofragmentation of $SF_6$ in Helium Nanodroplets." J. Phys Chem. B., **110,** 19945, DOI: 10.1021/jp062195o (2006) LBNL-60028

175. J. Plenge, C. Nicolas, A. G. Caster, M. Ahmed, and S. R. Leone, "Two-Color Visible/Vacuum Ultraviolet Photoelectron Imaging Dynamics of Br2," J. Chem. Phys., **125**, 133315, DOI: 10.1063/1.2217375 (2006) LBNL-59988

174. J. H. Kim, D. S. Peterka, C. C. Wang and D. M. Neumark, "Photoionization of helium nanodroplets doped with rare gas atoms," J. Chem. Phys., **124**, 214301, DOI: 10.1063/1.2202313 (2006) LBNL-59959

173. J. Shu, K. R. Wilson, M. Ahmed, and S. R. Leone, "Coupling a versatile aerosol apparatus to a synchrotron: vacuum ultraviolet light scattering, photoelectron imaging, and fragment free mass spectrometry," Rev. Sci. Instrum., **77**, 043106, DOI: 10.1063/1.2194474 (2006) LBNL-59987

172. K. R. Wilson, D. S. Peterka, M. Jimenez-Cruz, S.R. Leone, and M. Ahmed, "VUV photoelectron imaging of biological nanoparticles – Ionization energy determination of nano-phase glycine and phenylalanine-glycine-glycine," Phys. Chem. Chem. Phys. **8**, 1884, DOI: 10.1039/B517487B (2006) LBNL-59291

171. N. E. Sveum, S. J. Goncher, and D. M. Neumark, "Determination of absolute photoionization cross sections of the phenyl radical," Phys. Chem. Chem. Phys. **8**, 592, DOI: 10.1039/B513960K (2006) LBNL-58957

170. N. Hansen, S. J. Klippenstein, J. A. Miller, J. Wang, T. A. Cool, M. E. Law, P. R. Westmoreland, T. Kasper, and K. Kohse-Höinghaus, "Identification of $C_5Hx$ Isomers in Fuel-Rich Flames by Photoionization Mass Spectrometry and Electronic Structure Calculations," J. Phys. Chem. A, **110**, 4376, DOI: 10.1021/jp0569685 (2006) LBNL-59298

169. T. Zhang, X. N. Tang, C. Y. Ng, C. Nicolas, D. S. Peterka, M. Ahmed, M. L. Morton, B. Ruscic, R. Yang, L. X. Wei, C. Q. Huang, B. Yang, J. Wang, L. S. Sheng, Y. W. Zhang, and F. Qi, "Direct identification of propargyl radical in combustion flames by VUV photoionization mass spectrometry," J. Chem. Phys., **124**, 074302, DOI: 10.1063/1.2168448 (2006) LBNL-59109

168. N. Hansen, S. J. Klippenstein, C. A. Taatjes, J. A. Miller, J. Wang, T. A. Cool, B. Yang, R. Yang, L. Wei, C. Huang, J. Wang, F. Qi, M. E. Law, P. R. Westmoreland, "Identification and Chemistry of C4H3 and C4H5 Isomers in Fuel-Rich Flames," J. Phys. Chem. A., **110**, 3670, DOI: 10.1021/jp056769l (2006) LBNL-59110

167. P. R. Westmoreland, M.E. Law, T.A. Cool, J. Wang, C.A. Taatjes, N. Hansen, T. Kasper. "Analysis of Flame Structure by Molecular-Beam Mass Spectrometry Using Electron-Impact and Synchrotron-Photon Ionization," Combustion, Explosion and Shock Waves, **42(6),** 672-677, DOI: 10.1007/s10573-006-0100-0 (2006). LBNL59292

# Chemical Dynamics Beamline Publications

166. K. R. Wilson, L. Belau, C. Nicolas, M. Jimenez-Cruz, S. R. Leone, and M. Ahmed, "Direct determination of the ionization energy of histidine with VUV synchrotron radiation" Int. J. Mass Spectrom. **249-250**, 155, DOI: 10.1016/j.ijms.2005.12.044 (2006) LBNL-58989

165. K. R. Wilson, M. Jimenez-Cruz, C. Nicolas, L. Belau, S. R. Leone, and M. Ahmed, "Thermal Vaporization of Biological Nanoparticles: Fragment-Free VUV Photoionization Mass Spectra of Tryptophan, Phenylalanine-Glycine-Glycine and β-carotene**,"** J. Phys. Chem. A.,**110**, 2106, DOI: 10.1021/jp0543734 (2006) LBNL58668

164. J. Shu, K. R. Wilson, M. Ahmed, S. R. Leone, C. E. Graf, and E. Ruhl, "Elastic light scattering from nanoparticles by monochromatic vacuum-ultraviolet radiation," J. Chem. Phys., **124**, 034707, DOI: 10.1063/1.2159485 (2006) LBNL-58667

163. C. Nicolas, J. Shu, D. S. Peterka, M. Hochlaf, L. Poisson, S. R. Leone, and M. Ahmed, "Vacuum ultraviolet photoionization of C3," J. Am. Chem. Soc. **128**, 220 (2006) LBNL-58669

**2005**

162. M.-K. Bahng, X. Xing, S. J. Baek, X.-M. Qian, and C. Y. Ng, "A combined VUV synchrotron pulsed field ionization-photoelectron and IR-VUV laser photoion depletion study of ammonia", J. Phys. Chem. A. **110,** 8488 (2006). LBNL-58988

161. V. Chikan, F. Fournier, S. R. Leone, and B. Nizamov, "State-resolved Dynamics of the CH($A^2\Delta$) Channels from Single and Multiple Photon Dissociation of Bromoform in the 10-20 eV Energy Range." J. Phys. Chem. A.,**110**, 2850 (2005) LBNL-58984

160. C. A. Taatjes, N. Hansen, J. A. Miller, T. A. Cool, J. Wang, P. R. Westmoreland, M. E. Law, T. Kasper, K. Kohse-Höinghaus, "Combustion Chemistry of Enols: Possible Ethenol Precursors in Flames," J. Phys. Chem. A.**110**, 3254 (2005) LBNL-59111

159. A. Morel, "Molecular-Beam Mass Spectrometer Measurements and Modeling of Propene and Related Flames," masters thesis, University of Massachusetts Amherst, Amherst, Massachusetts, 2005, Advisor Phillip R. Westmoreland.

158. M. E. Law, "Molecular-Beam Mass Spectrometry of Ethylene and Cyclohexane Flames," doctoral dissertation, University of Massachusetts Amherst, Amherst, Massachusetts, 2005, Advisor Phillip R. Westmoreland.

157. D. S. Peterka, "Imaging Chemical Dynamics with the Vacuum Ultraviolet". Doctoral dissertation, University of California, Berkeley, 2005. Advisor; Daniel Neumark, LBNL-59209

156. L. R. McCunn, M. J. Krisch, Y. Liu, L. J. Butler, and J. Shu, "A Study of the Unimolecular Dissociation of the 2-Buten-2-yl Radical via the 193 nm Photodissociation of 2-Chloro-2-butene," J. Phys. Chem. A. **109**, 6430 (2005) LBNL-59112

155. T. Zhang, C. Y. Ng, F. Qi, C-S. Lam, and W-K. Li, "A 193 nm Laser Photofragmentation Timeof-Flight Mass Spectrometric Study of CH2ICl", J. Chem. Phys., **123**, 174316 (2005) LBNL-58987

154. M. Hochlaf, T. Baer, X. M. Qian, and C. Y. Ng, "A vacuum ultraviolet pulsed field ionization-photoelectron study of cyanogen cation in the energy range of 13.2-15.9 eV," J. Chem. Phys., **123**, 144302 (2005). LBNL-58986

# Chemical Dynamics Beamline Publications

153. X. N. Tang, Y. Hou, C. Y. Ng, and B. Ruscic, "Pulsed field ionization photoelectron-photoion coincidence study of the process N2 + hν → $N^+$ + N + $e^-$: Bond Dissociation Energies of N2 and $N2^+$," J. Chem. Phys., **123**, 074330 (2005). LBNL-58985

152. J. C. Robinson, N. E. Sveum, S. J. Goncher, and D. M. Neumark, "Photofragment translational spectroscopy of allene, propyne, and propyne-d3 at 193 nm." Mol. Phys. **103**, 1765 (2005). LBNL-56845

151. R. B. Metz, C. Nicolas, M. Ahmed, and S. R. Leone, "Direct determination of the ionization energies of FeO and CuO with VUV radiation," J. Chem. Phys., **123,** 114313 (2005). LBNL-58665

150. T. A. Cool, J. Wang, K. Nakajima, C. A. Taatjes, and A. McIlroy, "Photoionization cross sections for reaction intermediates in hydrocarbon combustion," Int. J. Mass Spectrom., **247**, 18 (2005)

149. T. A. Cool, A. McIlroy, F. Qi, P. R. Westmoreland, L. Poisson, D. S. Peterka, and M. Ahmed, "A photoionization mass spectrometer for studies of flame chemistry with a synchrotron light source," Rev. Sci. Instrum. **76,** 094102 (2005). LBNL-57979

148. X. N. Tang, H. Xu, T. Zhang, Y. Hou, C. Chang, C. Y. Ng, Y. Chiu, R. A. Dressler, and D. J. Lavandier, "A pulsed-field ionization photoelectron secondary ion coincidence study of the $H^+2(X,v^+=O\downarrow 15,N^+=1)$ + He proton transfer reaction," J. Chem. Phys., **122,** 164301 (2005). LBNL-57996

147. E. R. Mysak, K. R. Wilson, M. Jimenez-Cruz, M. Ahmed, and T. Baer. "Synchrotron Radiation Based Aerosol Time-of-Flight Mass Spectrometry for Organic Constituents," Anal. Chem. **77**, 5953 (2005). LBNL-57998

146. C. A. Taatjes, N. Hansen, A. McIlroy, J. A. Miller, J. P. Senosiaian, S. J. Klippenstein, F. Qi, L. Sheng, Y. Zhang, T. A. Cool, J. Wang, P. R. Westmoreland, M. E. Law, T. Kasper, and K. Kohse-Höinghaus, "Enols are common intermediates in hydrocarbon oxidation," Science **308**, 1887 (2005). LBNL-57997

145. J. L. Miller, M. J. Krisch, L. J. Butler, and J. Shu, "Dissociation channels of the 1-buten-2yl radical and its photolytic precursor 2-bromo-1-butene," J. Phys. Chem. A, **109**, 4038 (2005). LBNL-57563

144. C. A. Taatjes, S. J. Klippenstein, N. Hansen, J. A. Miller, T. A. Cool, J. Wang, M. E. Law, and P. R. Westermoreland, "Synchrotron photoionization measurements of combustion intermediates: Photoionization efficiency of $C_3H_2$ isomers," Phys. Chem. Chem. Phys. **7,** 806 (2005). LBNL-56986

143. J. Yang, Y. Mo, K. C. Lau, Y. Song, X. M. Qian, and C. Y. Ng, "A combined vacuum ultraviolet laser and synchrotron pulsed field ionization study of $BCl_3$," Phys. Chem. Chem. Phys. **7**, 1518 (2005). LBNL-57507

142. C.Y. Ng, "Two-color photoionization and photoelectron studies by combining infrared and vacuum ultraviolet," J. Electron Spectrom. Rel.Phenom., **142**, 179 (2005). LBNL-57510

141. D. S. Peterka and M. Ahmed, "Atoms to Aerosols – The Chemical Dynamics Beamline," Synchron. Rad. News., **18**, 35 (2005). LBNL-57509

140. J. Shu, K. R. Wilson, A. N. Arrowsmith, M. Ahmed, and S. R. Leone, "Light scattering of ultrafine silica particles by VUV synchrotron radiation," Nano Lett. **6,** 1009 (2005) LBNL-57433

139. M. E. Law, T. Carrière, P. R. Westmoreland, "Allene Addition to a Fuel-Lean Ethylene Flat Flame," Proc. Comb. Inst. **30**, 1353 (2005) LBNL-56989

# Chemical Dynamics Beamline Publications

138. T. A. Cool, K. Nakajima, C. A. Taatjes, A. McIlroy, P. R. Westmoreland, M. E. Law, and A. Morel, “Studies of a fuel-rich propane flame with photoionization mass spectrometry,” Proc. Comb. Inst. **30**, 1681 (2005). LBNL-56990

**2004**

137. J. Miller, "Unimolecular Reacton Channels of Organic Radicals," doctoral dissertation, University of Chicago, Chicago, IL, 2004, Advisor Laurie Butler.

136. M. J. Krisch, M. C. Reid, L. R. McCunn, L. J. Butler, and J. Shu, “Photofragment translational spectroscopy of nitric acid at 248 nm with UV photoionization detection of products,” Chem. Phys. Lett. **397**, 21 (2004). LBNL-57508

135. H. F. Davis, J. Shu, D. S. Peterka, and M. Ahmed, “Crossed beams study of the reaction (CH2)-C-1+C2H2→C3H3+H,” J. Chem. Phys., **121**, 6254, (2004). LBNL-56521

134. J. Shu, D. S. Peterka, S. R. Leone, and M. Ahmed, “Tunable Synchrotron Vacuum Ultraviolet Ionization, Time-of-Flight Investigation of the Photodissociation of Trans-Crotonaldehyde at 193 nm,“ J. Phys. Chem. A.,**108,** 7895 (2004). LBNL-55475

133. L. R. McCunn, M. J. Krisch, K. Takematsu, L. J. Butler, & J. Shu, “Competing Pathways in the 248 nm Photodissociation of Propionyl Chloride and the Barrier to Dissociation of the Propionyl Radical,” J. Phys. Chem. **108**, 7889 (2004). LBNL-56519

132. J. L. Miller, L. R. McCunn, M. J. Krisch, L. J. Butler & J. Shu, “Dissociation of the ground state vinoxy radical and its photolytic precursor chloroacetaldehyde: Electronic nonadiabaticity and the suppression of the H+ketene channel,” J. Chem. Phys., **121**, 1830 (2004). LBNL-56518

131. C. A. Taatjes, D. L. Osborn, T. A. Cool, and K. Nakajima, “Synchrotron photoionization measurements of combustion intermediates: the photoionization efficiency of HONO,” Chem. Phys. Lett. **394**, 19 (2004). LBNL-56517

130. X. M. Qian, K. C. Lau, and C. Y. Ng, “A high-resolution pulsed field ionization-photoelectronphotoion coincidence study of vinyl bromide,” J. Chem. Phys., **120**, 11031, (2004). LBNL-56516

129. X.-M. Qian, K.-C. Lau, G. Z. He, and C. Y. Ng, and M. Hochlaf, “Vacuum ultraviolet pulsed field ionization study of ND3: Accurate thermochemistry for the ND2-$ND_2^+$ and ND3-$ND_3^+$ system,” J. Chem. Phys., **120**, 8476, (2004). LBNL-56515

128. M. Hochlaf, K.-M. Weitzel, and C. Y. Ng, “Vacuum ultaviolet pulsed-field ionization-photoelectron study of H2S in the energy range of 10-17 eV,” J. Chem. Phys., **120**, 6944, (2004). LBNL56514

127. M. J. Krisch, L. R. McCunn, K. Takematsu, L. J. Butler, F. R. Blasé, and J. Shu “Photodissociation of $CH_3OCl$ to $CH_3O$ + C1 at 248 nm,” J. Phys. Chem. A.,**108**, 1650, (2004). LBNL56511

126. P. Zou, J. Shu, T. J. Sears, G. E. Hall, and S. W. North, “Photodissociation of Bromoform at 248 nm: Single and Multiphoton Processes,” J. Phys. Chem. A., **108,** 1482, (2004). LBNL-56512

125. D.E. Szpunar, J. L. Miller, and L. J. Butler and F. Qi, “193-nm photodissociation of acryloyl chloride to probe the unimolecular dissocatin of $CH_2CHCO$ radicals and $CH_2CCO$,” J. Chem. Phys., **120**, 4223, (2004). LBNL-56513

# Chemical Dynamics Beamline Publications

124. J. C. Robinson, N. E. Sveum, D. M. Neumark, “Determination of absolute photoionization cross sections for isomers of C3H5: allyl and 2-propenyl radicals,” Chem. Phys. Lett. **383**, 601, (2004). LBNL-54327

**2003**

123. T. Zhang, "State-selected study of ion-molecule reaction dynamics, photodissociation dynamics, and free radical studies using synchrotron radiation," doctoral dissertation, UC Davis, Sacramento, CA, 2003, Advisor Professor Cheuk Ng.

122. X.-M., Qian, "Applications of third generation synchrotron radiation in vacuum ultraviolet (VUV) photoionization spectroscopy and dynamics," doctoral dissertation, UC Davis, Sacramento, CA, 2003, Advisor Professor Cheuk Ng.

121. X.-M. Qian, A. H. Kung, Tao Zhang, K. C. Lau, and C. Y. Ng, “Rovibrational-State-Selected Photoionization of Acetylene by the Two-Color IR + VUV Scheme: Observation of Rotationally Resolved Rydbery Transitions,” Phys. Rev. Lett. **91**, 233001, (2003). LBNL-54308

120. T. Zhang, X.-M. Qian, X. N. Tang, C. Y. Ng, Y. Chiu, D. J. Levandier, J. S. Miller, and R. A. Dressler, “A state-selected study of the $H_2^+$ (X,$v^+$=0-17,$N^+$=1)+Ne proton transfer reaction using the pulsed-field ionization-photoelectron-secondary ion coincidence scheme,” J. Chem. Phys., **119**, 10175, (2003). LBNL-54307

119. J. C. Robinson, N. E. Sveum, and D. M. Neumark, “Determination of absolute photoionization cross sections for vinyl and propargyl radicals,” J. Chem. Phys., **119**, 5311, (2003). LBNL-54304

118. D. E. Szpunar, Y. Liu, M. J. McCullagh, and L. J. Butler, “Photodissociation of allyl-dd iodide excited at 193 nm: Stability of highly rationally excited H2CDCH2 radicals to C-D fission,” J. Chem. Phys., **119**, 5078, (2003). LBNL-54306

117. T. A. Cool, K. Nakajima, T. A. Mostefaoui, F. Qi, A. McIlroy, P. R. Westmoreland, M. E. Law, L. Poisson, D. S. Peterka, and M. Ahmed, “Selective detection of isomers with photoionization mass spectrometry for studies of hydrocarbon flame,” J. Chem. Phys.,, **119**, 8356, (2003). LBNL-54303

116. X.-M. Qian, T. Zhang, C. Chang, P. Wang, C. Y. Ng, Y-H Chiu, D. J. Levandier J. S. Miller, R. A. Dressler, T. Baer, D. S. Peterka. “High-Resolution State-Selected Ion-Molecule Reaction Studies Using Pulsed Field Ionization Photoelectron-Secondary Ion Coincidence Method,” Rev. Sci. Instrum., **74**, 4096, (2003) LBNL-54305

115. X.-M. Qian, T. Zhang, C. Y. Ng, A. Kung, and M. Ahmed. “Two-Color Photoionization Spectroscopy Using Vacuum Ultraviolet Synchrotron Radiation and Infrared Optical Parametric Oscillator Laser Source,” Rev. Sci. Instrum., **74**, 2784, (2003) LBNL- 52347

114. M. J. Krisch, J. L. Miller, L. J. Butler, H. Su, R. Bersohn, and J. Shu, “Photodissociation Dynamics of Ethyl Ethynyl Ether: A new ketenyl radical precursor,” J. Chem. Phys.,**119**, 176 (2003) LBNL-52348

113. W.Li, L. Poisson, D.S. Peterka, M. Ahmed, R. Lucchese and A. G. Suits, “Dissociative Photoionization Dynamics in Ethane Studied by Velocity Map Imaging,” Chem. Phys. Lett. **374**, 334, (2003) LBNL-52019

112. D. S. Peterka, A. Lindinger, L. Poisson, M. Ahmed, D. M. Neumark, “Photoelectron imaging of helium droplets,” Phys. Rev. Lett. 91, 043401, (2003) LBNL-52017

# Chemical Dynamics Beamline Publications

111. J. Liu, M. Hochlaf, and C. Y. Ng, “Pulsed Field Ionization-Photoelectron Bands for $CS2^+$ in the Energy Range of 13.2 –17.6 eV: An Experimental and Theoretical Study,” J. Chem. Phys., **118**, 4487 (2003) LBNL-52350

110. X. M. Qian, T. Zhang, Y. Chiu, D. J. Levandier, J. S, Miller, R. A. Dressler, and C. Y. Ng, “Rovibrational State-Selected Study of $H2^+$(X, $v^+$=0-17, $N^+$=1)+Ar Using the Pulsed Field IonizationPhotoelectron-Secondary Ion Coincidence Scheme,” J. Chem. Phys., **118**, 2455 (2003) LBNL-523549

109. W. Chen, J. Liu, and C. Y. Ng, “Vacuum Ultraviolet Pulsed Field Ionization-Photoelectron Study for $N2O^+$ in the Energy Range of 16.3 - 21.0 eV,” J. Phys. Chem. A., **107**, 8086 (2003) LBNL- 52026

108. J. Liu, W. Chen, M. Hochlaf, X. Qian, C. Chang and C.-Y. Ng, “Unimolecular decay pathways of state selected $CO2^+$ in the internal energy range of 5.2-6.2 eV’: An experimental and theoretical study,” J. Chem. Phys., **118**, 149 (2003). LBNL-52039.

**2002**

107. J. C. Robinson, "Photofragment translational spectroscopy studies of unsaturated hydrocarbons," doctoral dissertation, UC Berkeley, Berkeley, CA, 2002, Advisor Professor Daniel Neumark.

106. Morton, M.L., "Molecular beam studies of selected radical isomers and photolytic precursors," doctoral dissertation, University of Chicago, Chicago, IL, 2002, Advisor Laurie Butler.

105. J. C. Robinson, S. A. Harris, W. Sun, N. E. Sveum, and D. M. Neumark, “Photofragment translational spectroscopy of 1,3-butadiene and 1,3-butadiene-1,1,4,4-d4 at 193 nm,” J. Am. Chem. Soc. **124**, 10211 (2002). LBNL-49510.

104. J. L. Miller, M. L. Morton, L. J. Butler, F. Qi, M. J. Krisch, and J. Shu, “Dissociation Channels of the 1-Propenyl Radical and its Photolytic Precursor cis-1-Bromopropene ” J. Phys. Chem. A.,**106**, 10965-10967 (2002). LBNL-52028.

103. C.Y. Ng, “State-Selected and State to State Ion-Molecule Reaction Dynamics,” J. Phys. Chem. A.,**106** , 5953-5966 (2002) LBNL-52033

102. F. Qi and A.G. Suits, " Photodissociation of propylene sulfide 193 nm: a photofragment translational spectroscopy study with VUV synchrotron radiation**,**" J. Chem. Phys., A., **106** 11017-11024 (2002) LBNL-47976.

101. J. K. C. Lau, W. K. Li, F. Qi and A. G. Suits. “A Gaussian-3 study of the photodissociation channels of propylene sulfide. J. Phys. Chem. A., **106** 11025 (2002). LBNL-52027

100. M.L. Morton, J. L. Miller, L. J. Butler, and F. Qi, “Dissociation Channels of the 1-Propenyl Radical and its Photolytic Precursor cis-1-Bromopropene,” J. Phys. Chem. A., **106**, 10831-10842 (2002) LBNL-52028

99. D. E. Szpunar, M. L. Morton, L. J. Butler, and P. M. Regan, “Primary and Secondary Dissociation of Allyl Iodide Excited at 193 nm: Centrifugal Effects in the Unimolecular Dissociation of the Allyl Radical,” J. Phys. Chem. B., **106,** 8086-8095 (2002) LBNL-52030

98. M. L. Morton, L. J. Butler, T. A. Stephenson, F. Qi, “C-Cl bond fission, HCl elimination and secondary radical decomposition in the 193 nm photodissociation of allyl chloride,” J. Chem. Phys., **116**, 2763-2775, (2002). LBNL-52031

# Chemical Dynamics Beamline Publications

97**.** C. Y. Ng, “Vacuum Ultraviolet Spectroscopy and Chemistry by Photoionization and Photoelectron Methods,” Ann. Rev. Phys. Chem., **53**, 101, (2002). LBNL-52032

96. W. Chen, M. Hochlaf, P. Rosmus, G.-Z. He, and C. Y. Ng, “Vacuum Ultraviolet Pulsed Field Ionization Photoelectron Study of OCS in the Energy range of 15.0-19.0 eV,” J. Chem. Phys., **116**, 5612-5621, (2002). LBNL-52026

95. X-M. Qian, Y. Song, K.-C. Lau, C. Y. Ng, J. Liu, W. Chen, and G. Z. He, “A pulsed field ionization photoelectron-photoion coincidence study of the dissociative photoionization process D2O+hv > $OD^+$ + D +$e^-$,” Chem. Phys. Lett., **353** 19-26 (2002). LBNL-52034

94. B. Ruscic, A. F. Wagner, L. B. Harding, R. L. Asher, D. Feller, K. A. Peterson, Y. Song, X.M. Qian, C.Y. Ng, J. Liu, and W. Chen, “On the Enthalpy of Formation of Hydroxyl Radical and Gas-Phase Dissociation energies of Water and Hydroxyl,” J. Phys. Chem. A, **106**, 2727, (2002) LBNL-52023

93. F. Qi, L. Sheng, M. Ahmed, D.S. Peterka, and T. Baer, "Exclusive production of excited state sulfur ($^1$D) from 193 nm photolysis of thietane," Chem.Phys. Lett., **357**, 204-208, (2002). LBNL-48178.

**2001**

92. J.C. Robinson, W. Sun, S.A. Harris, F. Qi and D.M. Nuemark, “Photofragment Translational spectroscopy of 1, 2 Butadiene at 193 nm,” J. Chem Phys., **115**, 8359-8365 (2001). LBNL-48934.

91. D. G. Fedorov, M. S. Gordon, Y. Song, and C. Y. Ng, “A Theoretical Study of the Spin-orbit coupling in $O2^+$($A^2$Π3/2,1/2u, $v^+$=0-15; $a^4$Π5/2,3/2,1/2,-1/2u, $v^+$=0-18),” J. Chem. Phys., **115**, 7393-7400 (2001) LBNL49534

90. Y. Song, X-M. Qian, K.-C. Lau, and C.Y. Ng, "A pulsed field ionization study of the dissociative photoionization reaction CD4 + hv $CD3^+$ + D + $e^-$," Chem. Phys. Lett., **347**, 51-58 (2001) LBNL-48188

*89. M. Ahmed, D.S. Peterka, P. Regan, X. Liu, and A.G. Suits, "Ion pair imaging spectroscopy: CH3Cl → $CH3^+$ + Cl,” Chem. Phys. Lett., **339**, 203-208, (2001) LBNL-47082

88. Y. Song, X.-M. Qian, K.-C. Lau, and C.Y. Ng, J.B. Liu and W.W. Chen "High-resolution energy-selected study of the reaction $CH3X^+$ → $CH3^+$ +X: accurate thermochemistry for the CH3X/$CH3X^+$ (X=Br,I) system," J. Chem. Phys., **115**, 4095-4104 (2001) LBNL-48340

87. Y. Song, X.-M. Qian, K.-C. Lau, C.Y. Ng, J. Liu, and W. Chen, "High-resolution energy-selected study of the reaction $NH3^+$ → $NH2^+$ + H: accurate thermochemistry for the NH2/$NH2^+$ and NH3/$NH3^+$ systems," J. Chem. Phys., **115**, 2582-2589, (2001) LBNL-48265

86. Y. Song, C.Y. Ng, G.K. Jarvis, and R.A. Dressler, "Rotational-resolved pulsed field ionization-photoelectron study of $NO^+$ (A' $^1$Σ, $v^+$=0-17) in the energy range of 17.20-20.10 eV," J. Chem. Phys., **115**, 2101-2108, (2001) LBNL-48267

85. K-M. Weitzel, G.K. Jarvis, M. Malow, T. Baer, Y. Song, and C.Y. Ng, "Observation of accurate ion dissociation thresholds in pulsed field ionization-photoelectron studies," Phys. Rev. Lett, **86**, 3526-3529, (2001). LBNL-46802

# Chemical Dynamics Beamline Publications

84. A.G. Suits and F. Qi, "The photodissociation dynamics of cyclic sulfides probed with tunable undulator radiation," (invited), J. Electron Spectroscopy & Related Phenomena, **119**,127-145, (2001). LBNL-47177

83. J.A. Mueller, B.F. Parsons, L.J. Butler, F. Qi, O. Sorkhabi, and A.G. Suits, "Competing isomeric product channels in the 193 nm photolysis of 2-chloropropene and in the unimolecular dissociation of the 2-propenyl radical," J. Chem. Phys.,, **114**, 4505-4521, (2001). LBNL-46730

82. O. Sorkhabi, F. Qi, A.H. Rizvi, and A.G. Suits, "The ultraviolet photochemistry of phenylacetylene and the enthalpy of formation of 1,3,5-hexatriyne," J. Am. Chem. Soc., **123**, 671-676, (2001). LBNL-45822

*81. M. Ahmed, D.S. Peterka, and A.G. Suits, "Photodissociation of $NO_2$ near 225 nm by velocity map imaging," in Atomic and molecular beams: the state of the art 2000, R. Campargue, ed., (Springer-Verlag, Berlin, 2001), 343-352. LBNL-42491

80. M. Ahmed, D.S. Peterka, and A. G. Suits, "New directions in reaction dynamics using velocity map imaging," in Imaging in chemical dynamics, A. G. Suits and R. E. Continetti, eds., ACS Symposium Series, **770** (American Chemical Society, Washington DC, 2001), Chapt. 11. LBNL-45395

*79. E.R. Wouters, M. Ahmed, D.S. Peterka, A.S. Bracker, A.G. Suits, and O.S. Vasyutinskii, "Imaging the atomic orientation and alignment in photodissociation," in Imaging in chemical dynamics, A.G. Suits and R.E. Continetti, eds., ACS Symposium Series: **770**, (American Chemical Society, Washington DC, 2001), Chapt. 15. LBNL-45397

**2000**

78. F. Qi, O. Sorkhabi, A.G. Suits, S.-H. Chien, and W.-K. Li, "Photodissociation of ethylene sulfide at 193 nm: a photofragment translational spectroscopy study with VUV synchrotron radiation and ab initio calculations," J. Am. Chem. Soc., **123**, 148-161, (2000) LBNL-46800

77. J. Liu, M. Hochlaf, G. Chambaud, P. Rosmus, and C.Y. Ng, "High resolution pulsed field ionization-photoelectron bands for $CS2^{+}(A^{2}\Pi u)$: an experimental and theoretical study," J. Phys. Chem., **105**, 2183-2191, (2000) LBNL-45909

*76. A.G. Suits and R.E. Continetti, "Imaging in chemical dynamics: the state of the art," in Imaging in chemical dynamics, A.G. Suits and R.E. Continetti, eds., ACS Symposium Series: **770**, (American Chemical Society, Washington DC, 2000), Chapt. 1. LBNL-45396

75. C.Y. Ng, "Vacuum ultraviolet photoionization and photoelectron studies in the new millennium: recent developments and applications," Int. J. Mass. Spectrom., **200**, 357-386, (2000) LBNL- 46731

74. J. Liu, M. Hochlaf, and C.Y. Ng, "Pulsed field ionization-photoelectron bands of $CO2^{+}(A^{2}\Pi u$ and $B^{2}\Sigma u^{+})$: an experimental and theoretical study," J. Chem. Phys.,, **113**, 7988-7999, (2000) LBNL-45908

73. H. Lefebvre-Brion and C.Y. Ng, "Pulsed field ionization photoelectron spectrum for $CO^{+}(A^{2}\Pi u, v^{+}=1)$," Chem. Phys. Lett., **327**, 404-408, (2000). LBNL-45882.

72. C.Y. Ng, "Pulsed field ionization photoelectron-photoion spectroscopy: determination of accurate bond dissociation energies for neutrals and cations," J. Electron Spectroscopy & Related Phenomena, **112**, 31-46 (2000). LBNL-45883.

# Chemical Dynamics Beamline Publications

71. A.Yencha, M.C.A. Lopes, G.C. King, M. Hochlaf, Y. Song, and C.Y. Ng, "Ion-pair formation observed in a pulsed-field ionization photoelectron spectroscopic study of HF," Faraday Discussion, **115**, 355-362, (2000). LBNL-45887.

70. C.Y. Ng, "Advances in photoionization and photoelectron studies using third generation synchrotron radiation," J. Electron Spectroscopy & Related Phenomena, **108**, 41-45, (2000). LBNL-45885.

69. J.A. Mueller, J.L. Miller, L.J. Butler, F. Qi, O. Sorkhabi, and A.G. Suits, "Internal energy dependence of the H + allene/H + propyne product branching from the unimolecular dissociation of 2-propenyl radicals," J. Phys. Chem. A., **104**, 11261-11264, (2000) LBNL-46729.

68. W.S. McGivern, O. Sorkhabi, A.G. Suits, A. Derecskei-Kovacs, and S.W. North, "Primary and secondary processes in the photodissociation of $CHBr_3$" J. Phys. Chem. A., **104**, 10085-10091, (2000) LBNL-45435.

67. P. Zou, W.S. McGivern, O. Sorkhabi, A.G. Suits, and S.W. North, "Quantum yields and energy partitioning in the ultraviolet photodissociation of 1,2 dibromo-tetrafluorethane (Halon-2402)," J. Chem. Phys., **113**, 7149-7157, LBNL-47083.

66. N. R. Forde, L. J. Butler, B. Ruscic, O. Sorkhabi, F. Qi, and A. G. Suits, "Characterization of nitrogen-containing products from the photodissociation of trimethylamine at 193 nm using photoionization detection," J. Chem. Phys., **113,** 3088-3097, (2000). LBNL-45219.

65. T. Baer, Y. Song, C.Y. Ng, J. Liu, and W. Chen, "Pulsed field ionization - photoelectron photoion coincidence spectroscopy with synchrotron radiation: the heat of formation of the $C2H5^+$ ion," Faraday Discussion, **115**, 137-145, (2000) LBNL-45886

64. C.Y. Ng, "Advances in photoionization and photoelectron studies using third generation synchrotron radiation and UV/VUV lasers," in Photoionization and photodetachment, edited by C.Y. Ng (World Scientific, Singapore, 2000), Adv. Ser Phys. Chem., Vol. 10, Chapt. 9, 394-538 LBNL-45888

63. J. Liu, W. Chen, C.-W. Hsu, M. Hochlaf, M. Evans, S. Stimson, and C.Y. Ng, "High resolution pulsed field ionization-photoelectron study of $CO2^+$ ($X^2$ IIg) in the energy range of 13.6-14.7 eV," J. Chem. Phys., **112**, 10767, (2000). LBNL-45884

62. F. Qi, O. Sorkhabi, and A.G. Suits, "Evidence of triplet ethylene produced from photodissociation of ethylene sulfide," J. Chem. Phys., **112**, 10707, (2000). LBNL-45562

*61. M. Ahmed, D.S. Peterka, and A.G. Suits, "H abstraction dynamics by crossed-beam velocity map imaging: Cl + CH3OH → CH2OH + HCl," Chem. Phys. Lett., **317**, 264, (2000) LBNL-44126

*60. M. Ahmed, D.S. Peterka, and A.G. Suits, "Imaging H abstraction dynamics in crossed molecular beams: Cl + ROH reactions," Phys. Chem. Chem. Phys., **2**, 861, (2000) LBNL-44340

59. G.K. Jarvis, R.C. Shiell, J.W. Hepburn, Y. Song, and C.Y. Ng, "Pulsed field ionization-photoion spectroscopy using two-bunch synchrotron radiation: time-of-flight selection scheme," Rev. Sci. Instrum., **71**, 1325, (2000) LBNL-44290

58. T. Baer, Y.Song, C.Y. Ng, J. Liu, and W. Chen "The heat of formation of $C3H7^+$ and proton affinity of C3H6 determined by pulsed field ionization -photoelectron photoion coincidence spectroscopy," J. Phys. Chem., **104**, 1959, (2000) LBNL-44291

# Chemical Dynamics Beamline Publications

57. Y. Song, M. Evans, C.Y. Ng, C.-W. Hsu, and G.K. Jarvis, "Rotationally resolved pulsed field ionization photoelectron bands for $O2^+(A^2\Pi u, v^+=0\text{-}12)$in the energy range of 17.0-18.2 eV," J. Chem. Phys., **112**, 1271, (2000). LBNL-44113

56. Y. Song, M. Evans, C.Y. Ng, C.-W. Hsu, and G.K. Jarvis, "Rotationally resolved pulsed field ionization photoelectron bands for $O2^+(a^4\Pi u, v^+=0\text{-}18)$ in the energy range of 16.0-18.2 eV," J. Chem. Phys., **112**, 1306-1315, (2000). LBNL-45218

55. W.S. McGivern, O. Sorkhabi, A.H. Rizvi, A.G. Suits, and S.W. North, "Photofragment translational spectroscopy with state-selective 'universal detection': the ultraviolet photodissociation of CS2," J. Chem. Phys., **112**, 5301, (2000). LBNL-44681

**1999**

54. N. R. Forde, "Intramolecular vibrations and electronically nonadiabatic dynamics in photodissocation reactions," doctoral dissertation, University of Chicago, Chicago, IL, 1999, Advisor Laurie Butler.

53. M. Evans and C.Y. Ng, "Rotationally resolved pulsed field ionization photoelectron bands for $CO^+(X, v^+=0\text{-}42)$ in the energy range of 13.98-21.92 eV," J. Chem. Phys., **111,** 8879, (1999) LBNL-44116

52. M Ahmed, E.R. Wouters, D.S. Peterka, O.S. Vasyutinskii, and A.G. Suits, "Atomic orbital alignment and coherence in N2O photodissociation at 193.3 nm," Faraday Discussion, **113**, 425-436, (1999). LBNL-43097

51. M. Ahmed, D.S. Peterka, and A.G. Suits, "The photodissociation of the vinyl radical (C2H3) at 243 nm studied by velocity map imaging," J. Chem. Phys., **110**, 4248, (1999) LBNL-42490

50. M. Ahmed, D.S. Peterka, and A.G. Suits, "Crossed beam reaction of $O(^1D) + D2 \rightarrow OD + D$ by velocity map imaging," Chem. Phys. Lett., **301**, 372, (1999) LBNL-42488

49. M. Ahmed, D.S. Peterka, A.S. Bracker, O.S. Vasyutinskii, and A.G. Suits, "Coherence in polyatomic photodissociation: Aligned $O(^3P)$ from photodissociation of NO2 at 212.8 nm," J. Chem. Phys., **110**, 4115, (1999) LBNL-42489

48. D.S. Peterka, M. Ahmed, and A.G. Suits, "Erratum: Unraveling the mysteries of metastable O4," J. Chem. Phys., **111**, 5279, (1999) LBNL-42662

47. D.S. Peterka, M. Ahmed, and A.G. Suits, "Unraveling the mysteries of metastable O4," J. Chem. Phys., **110**, 6095, (1999) LBNL-42662

46. D.S. Peterka, M. Ahmed, C.Y. Ng, and A.G. Suits, "Dissociative photoionization dynamics of SF6 by ion imaging with synchrotron undulator radiation," Chem. Phys. Lett., **312**, 108, (1999) LBNL-43243

45. F. Qi, O. Sorkhabi, A.H. Rizvi, and A.G. Suits, "193 nm photodissociation of thiophene probed using synchrotron radiation," J. Phys. Chem. A, **103**, 8351, (1999) LBNL-43495

44. G.K. Jarvis, K.-M. Weitzel, M. Malow, T. Baer, Y. Song, and C.Y. Ng. "High-resolution pulsed field ionization photoelectron-photoion coincidence study of C2H2: accurate 0 K dissociation threshold for $C2H^+$," Phys. Chem. Chem. Phys., (Communication) **1**, 5259, (1999) LBNL-44292

# Chemical Dynamics Beamline Publications

43. G.K. Jarvis, Y. Song, C.Y. Ng, and E.R. Grant, "A characterization of vibrationally and electronically excited $NO2^+$ by high-resolution threshold photo-ionization spectroscopy," J. Chem Phys., **111**, 9568, (1999) LBNL-44293
42. G.K. Jarvis, M. Evans, C.Y. Ng, and K. Mitsuke, "Rotational-resolved pulsed field ionization photoelectron study of $NO^+$ ($X^1\Sigma^+$, $v^+$=0-32) in the energy range of 9.24-16.80 eV," J. Chem. Phys., **111**, 3058, (1999) LBNL-44118

41. G.K. Jarvis, Y. Song, and C.Y. Ng, "Rotational-resolved pulsed field ionization photoelectron study of $NO^+$ ($a^3\Sigma^+$, $v^+$=0-16) in the energy range of 15.6-18.2 eV," J. Chem. Phys., **111,** 1937, (1999) LBNL-45891

40. G.K. Jarvis, K.-M. Weitzel, M. Malow, T, Baer, Y. Song, and C.Y. Ng, "High resolution pulsed field ionization photoelectron-photon coincidence spectroscopy using synchrotron radiation," Rev. Sci. Instrum., **70**, 3892, (1999) LBNL-44115

39. G.K. Jarvis, Y. Song, and C.Y. Ng, "High resolution pulsed field ionization photoelectron spectroscopy using multi-bunch synchrotron radiation: time-of-flight selection scheme," Rev. Sci. Instrum., **70**, 2615, (1999) LBNL-45894

38. R.C. Shiell, M. Evans, S. Stimson, C-W Hsu, C.Y. Ng, and J.W. Hepburn, "A ZEKE study of the $D^2\Pi$ and $3^2\Sigma^+$ satellite states of $CO^+$," Chem. Phys. Lett., **315**, 390-396, DOI: 10.1016/S0009-2614(99)01261-0, (1999) LBNL-45889

37. R.C. Shiell, M. Evans, S. Stimson, C-W Hsu, C.Y. Ng, and J.W. Hepburn, "Characteristics of correlation satellites below 25 eV in xenon probed by pulsed-field-ionization zero kinetic energy photoelectron spectroscopy," Phys. Rev. A, **59**, 2903, DOI: 10.1103/PhysRevA.59.2903, (1999) LBNL-45895

36. K.-M. Weitzel, M. Malow, G.K. Jarvis, T. Baer, Y. Song, and C.Y. Ng, "High-resolution pulsed field ionization photoelectron-photoion coincidence study of CH4: Accurate 0 K dissociation threshold for $CH3^+$," J. Chem. Phys., (Communication), **111**, 8267, DOI: 10.1063/1.480169, (1999) LBNL-44114

35. M.D. Evans, "High-resolution photoionization studies performed utilizing third-generation synchrotron radiation at the Advanced Light Source," Ph.D. thesis, Iowa State University of Science and Technology, (1999) LBNL-45890

34. D.G. Fedorov, M. Evans, Y. Song, M.S. Gordon, and C.Y. Ng, "An experimental and theoretical study of the spin-orbit interaction for $CO^+$ ($A^2\Pi$3/2,1/2, $v^+$=0-42) and $O2^+$ ($X^2\Pi$3/2,1/2, $v^+$=0-38)," J. Chem. Phys., **111**, 6413, DOI: 10.1063/1.479941, (1999) LBNL-44117

33. Y. Song, M. Evans, C.Y. Ng, C.-W. Hsu, and G.K. Jarvis, "Rotationally-resolved pulsed field ionization photoelectron bands of $O2^+$ ($X^2\Pi$1/2, 3/2,$v^+$=0-38) in the energy range of 12.05-18.15 eV," J. Chem. Phys., **111**, 1905, DOI: 10.1063/1.479459, (1999) LBNL-45892

32. O. Sorkhabi, F. Qi, A.H. Rizvi, and A.G. Suits, "Ultraviolet photodissociation of furan probed by tunable synchrotron radiation," J. Chem. Phys., **111**, 100, DOI: 10.1063/1.479257, (1999) LBNL-42892

31. A.S. Bracker, E.R. Wouters, A.G. Suits, and O.S. Vasyutinskii, "Imaging the alignment angular distribution: State symmetries, coherence, and nonadiabatic dynamics in photodissociation," J. Chem. Phys., **110**, 6749, DOI: 10.1063/1.478668, (1999) LBNL-42486

# Chemical Dynamics Beamline Publications

30. W. Sun, K. Yokoyama, J. Robinson, A.G. Suits, and D.M. Neumark, "Discrimination of product isomers in the photodissociation of propyne and allene at 193 nm," J. Chem. Phys., **110**, 4363, DOI: 10.1063/1.478318, (1999) LBNL-42855

**1998**

29. A.S. Bracker, S.W. North, A.G. Suits, and Y.T. Lee, "The near ultraviolet dissociation dynamics of azomethane: Correlated V-T energy disposal and product appearance times," J. Chem Phys., **109,** 7238, DOI: 10.1063/1.477402, (1998) LBNL-42021

28. N. Hemmi and A.G. Suits, "The dynamics of hydrogen abstraction reactions: Crossed-beam reaction Cl + n-C5H12 → C5H12 + HCl," J. Chem Phys., **109,** 5338, DOI: 10.1063/1.476523, (1998) LBNL-42023

27. W.M. Jackson, R.J. Price, D.D. Xu, J.D. Wrobel, M. Ahmed, D.S. Peterka, and A.G. Suits, "Velocity map imaging studies of the Lyman α photodissociation mechanism for H atom production from hydrocarbons," J. Chem. Phys., **109**, 4703, DOI: 10.1063/1.477082, (1998) LBNL-42029

26. M. Evans, S. Stimson, C.Y. Ng, and C.-W. Hsu, "High resolution pulsed field ionization photoelectron study of O2: Predissociation lifetimes and high-n Rydberg lifetimes converging to $O2^+(c^4\Sigma u, v^+=0,1)$," J. Chem. Phys., **109**, 1285, DOI: 10.1063/1.476678, (1998) LBNL-45896

25. D.A. Blank, N. Hemmi, A.G. Suits, and Y.T. Lee, "A crossed molecular beam investigation of the reaction Cl + propane → HCl + $C_3H_7$ using VUV synchrotron radiation as a product probe," Chem. Phys. **231**, 261, DOI: 10.1016/S0301-0104(98)00021-4, (1998) LBNL-40947

24. D.A. Blank, W. Sun, A.G. Suits, Y.T. Lee, S.W. North, and G.E. Hall, "Primary and secondary processes in the 193 nm photodissociation of vinyl chloride," J. Chem. Phys., **108**, 5414, DOI: 10.1063/1.475930, (1998) LBNL-41168

23. D.A. Blank, A.G. Suits, Y.T. Lee, S.W. North, and G.E. Hall, "Photodissociation of acrylonitrile at 193 nm: A photofragment translational spectroscopy study using synchrotron radiation for product photoionization," J. Chem. Phys., **108**, 5784, DOI: 10.1063/1.475989, (1998) LBNL-40942

22. D. Stranges, M. Stemmler, X. Yang, J.D. Chesko, A.G. Suits, and Y.T. Lee, "UV photodissociation dynamics of allyl radical by photofragment translational spectroscopy," J. Chem. Phys., **109**, 5372, DOI: 10.1063/1.477156, (1998) LBNL-41439R1

21. C.-W. Hsu, M. Evans, S. Stimson, and C.Y. Ng "Rotationally resolved photoelectron study of O2: identification of the vibrational progressions for $O2^+(2^2\Pi u, {}^2\Sigma u^-)$ at 19.6-21.0 eV," J. Chem. Phys., **108**, 4701, DOI: 10.1063/1.475920, (1998) LBNL-45897

20. C.-W. Hsu, M. Evans, S. Stimson, C.Y. Ng, and P. Heimann "High resolution photoelectron spectroscopy using multibunch synchrotron radiation: rotational-resolved photoelectron bands of $O2^+(b^4\Sigma g, v^+)$," Chem. Phys., **231**, 121, (1998) LBNL-43648

19. S. Stimson, Y.-J. Chen, M. Evans, C.-L. Liao, C.Y. Ng, C.-W. Hsu, and P. Heimann "Rotational-resolved pulsed field ionization photoelectron bands for $H2^+(X^2\Sigma g^+, v^+=0, 2, 9$ and $11)$," Chem. Phys. Lett., **289**, 507, (1998) LBNL-43650

# Chemical Dynamics Beamline Publications

18. S. Stimson, M. Evans, C.Y. Ng, C.-W. Hsu, P. Heimann, C. Destandau, G. Chambaud, and P. Rosmus "High resolution vacuum ultraviolet pulsed field ionization photoelectron band for $OCS^+$ ($X^2\Pi$): an experimental and theoretical study," J. Chem. Phys., **108**, 6205, DOI: 10.1063/1.476027, (1998) LBNL-45898

17. R.C. Shiell, M. Evans, S. Stimson, C.-W. Hsu, C.Y. Ng, and J.W. Hepburn, "High resolution study of low-lying correlation satellites in xenon," Phys. Rev. Lett., **80**, 472, DOI: 10.1103/PhysRevLett.80.472, (1998) LBNL-45899

**1997**

16. X. Yang, D.A. Blank, J. Lin. P.A. Heimann, A.M. Wodke, Y.T. Lee, and A.G. Suits, "Chemical reaction dynamics using the Advanced Light Source," in **Synchrotron radiation techniques in industrial, chemical, and materials science**, D'Amico, ed., Plenum Press, New York (1997) LBL-37732

15. P.A. Heimann, M. Koike, C.-W. Hsu, D. Blank, X.M. Yang, A.G. Suits, Y.T. Lee, M. Evans, C.Y. Ng, C. Flaim, and H.A. Padmore, "Performance of the vacuum ultraviolet high-resolution and high-flux beamline for chemical dynamics studies at the Advanced Light Source," Rev. Sci. Instrum., **68**, 1945, DOI: 10.1063/1.1148082, (1997) LBL-46409

14. M. Ahmed, D. Blunt, D. Chen, and A.G. Suits, "UV photodissociation of oxalyl chloride yields four fragments from one photon absorption," J. Chem. Phys., **106**, 7617, DOI: 10.1063/1.473764, (1997) LBNL-39682

13. N. Hemmi and A.G. Suits, "Photodissociation of oxalyl chloride at 193 nm probed via synchrotron radiation," J. Phys. Chem. A, **101**, 6633, DOI: 10.1021/jp970786w, (1997) LBNL-40055

12. X. Yang, D.A. Blank, J. Lin, A.G. Suits, Y.T. Lee, and A.M. Wodtke, "Universal crossed molecular beams apparatus with synchrotron photoionization mass spectromometric product detection," Rev. Sci. Instrum., **68**, 3317, DOI: 10.1063/1.1148291, (1997) LBNL-40194

11. M. Bevsek, M. Ahmed, D.S. Peterka, F.C. Sailes, and A.G. Suits, "Direct detection and spectroscopy of O4*," Faraday Discussion, **108**, 131, DOI: 10.1039/A705535H, (1997) LBNL-40633

10. C.-W. Hsu, P. Heimann, M. Evans, S. Stimson, P.T. Fenn, and C.Y. Ng, "A high resolution pulsed field ionization photoelectron study of O2 using third generation undulator synchrotron radiation," J. Chem. Phys., **106**, 8931, DOI: 10.1063/1.473956, (1997) LBNL-45900

9. C.-W. Hsu, M. Evans, C.Y. Ng, and P. Heimann, "High resolution threshold and pulsed field ionization photoelectron spectroscopy using multi-bunch synchrotron radiation," Rev. Sci. Instrum., **68**, 1694, DOI: 10.1063/1.1147977, (1997) LBNL-45901

8. J.W. Keister, T. Baer, M.D. Evans, C.Y. Ng, and C.-W. Hsu, "Methyl loss kinetics of energy-selected 1,3-butadiene radical cations," J. Phys. Chem., **101**, 1866, DOI: 10.1021/jp9629001, (1997) LBNL-45902

7. P.M. Mayer, J.W. Keister, T. Baer, C.-W. Hsu, M.D. Evans, and C.Y. Ng "The fragmentation of dimethylamine dimer ions: accurate neutral and ionic dimer binding energies by a combined PEPICO, variation RRKM, and ab initio approach," J. Phys. Chem., **101**, 1270, DOI: 10.1021/jp9627077 (1997) LBNL-45903

6. D.A. Blank, "Molecular beam studies of unimolecular and bimolecular chemical reaction dynamics using VUV synchrotron radiation as a product probe," Ph.D. thesis, UC Berkeley, (1997) LBNL-41061

# Chemical Dynamics Beamline Publications

5. M. Evans, C.Y. Ng, C.-W. Hsu, and P. Heimann, "A high resolution energy-selected kinetic energy release study of the process SF6 + hv → $SF5^+$ + F + $e^-$: heat of formation of $SF5^+$," J. Chem. Phys., **106**, 978, DOI: 10.1063/1.473963, (1997) LBNL-45904

4. J.-C. Huang, Y.-S. Cheung, M.D. Evans, C.-X. Liao, C.Y. Ng, C.-W. Hsu, P.A. Heimann, H. Lefebvre-Brion, and C. Cossart-Magos, "A high resolution VUV photoionization, photoelectron and pulsed field ionization study of CS2 near the $CS2^+$ thresholds," J. Chem. Phys., **106**, 864, DOI: 10.1063/1.473967, (1997) LBNL-45905

**1996**

3. P.A. Heimann, M. Koike, C.-W. Hsu, M. Evans, C.Y. Ng, D. Blank, X.M. Yang, C. Flaim, A.G. Suits, and Y.T. Lee, "Performance of the VUV high resolution and high flux beamline for chemical dynamics studies at the Advanced Light Source," in **Optics for high-brightness synchrotron radiation beamlines II**, Proc. SPIE., 2856, **90**, DOI: 10.1117/12.259853, (1996) LBNL-39138

2. C.-W. Hsu, K.T. Lu, M.D. Evans, Y.J. Chen, C.Y. Ng, and P. Heimann, "A high resolution photoionization study of Ne and Ar: observation of mass analyzed threshold ions using synchrotron radiation and direct current electric fields," J. Chem. Phys., **105**, 3950, DOI: 10.1063/1.472268, (1996) LBNL-45907

**1995**

1. A.G. Suits, P.A. Heimann, X. Yang, M.D. Evans, C. Hsu, K. Lu, and Y.T. Lee, "A differentially pumped harmonic filter on the chemical dynamics beamline at the Advanced Light Source," Rev. Sci. Instrum., **66**, 4841, DOI: 10.1063/1.1146161, (1995) LBNL-37427