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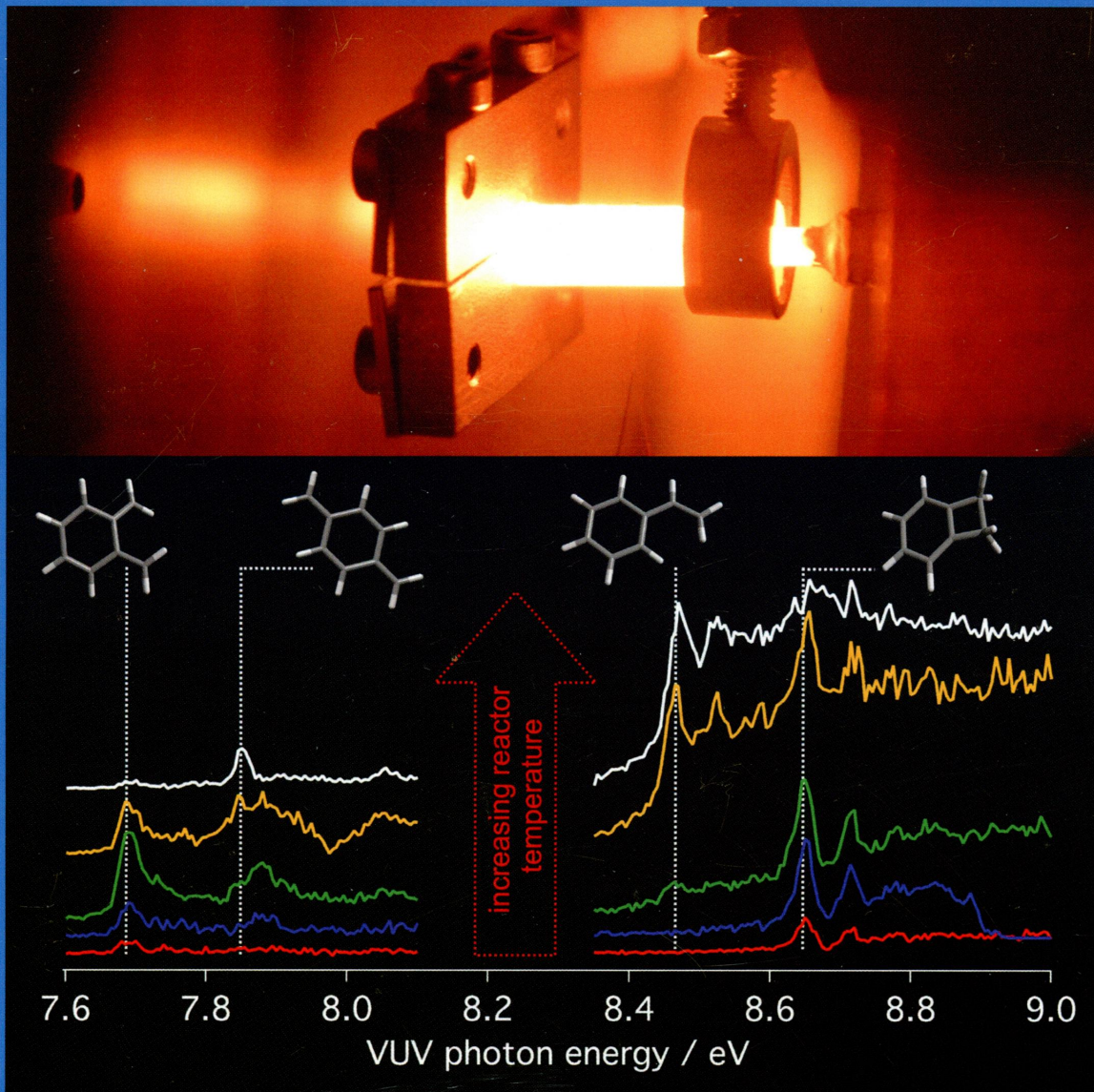
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A



High-Temperature
Xylyl Radical
Decomposition and
Rearrangement
Dynamics Probed
by Tunable VUV
Synchrotron Radiation
(see page 5A)

ISOLATED MOLECULES, CLUSTERS, RADICALS, AND IONS; ENVIRONMENTAL CHEMISTRY,
GEOCHEMISTRY, AND ASTROCHEMISTRY; THEORY



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ON THE COVER: The collage shows the glowing tubular reactor at ~1300 K, which is used to explore the decomposition and rearrangement dynamics of gas-phase *o*-xylyl radicals. *o*-Xylylene, formed by direct hydrogen abstraction of the xylyl radical, further isomerizes in a multistep reaction to yield styrene. The latter species is known to form in particularly large quantities from the oxidation of *o*-xylene compared to the meta and para isomers. This study, benefiting from isomer specific product detection, can explain these finding by utilizing imaging photoelectron photoion coincidence (iPEPICO) spectroscopy (lower panel) and VUV synchrotron radiation at the Swiss Light Source. See page 3593.

Articles

Kinetics and Dynamics

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dx.doi.org/10.1021/jp5009434

Kinetics of the Gas-Phase Reactions of Chlorine Atoms with Naphthalene, Acenaphthene, and Acenaphthylene

Matthieu Riva, Robert M. Healy, Pierre-Marie Flaud, Emilie Perraudin, John C. Wenger,* and Eric Villenave*

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dx.doi.org/10.1021/jp500993k

Atmospheric Reaction of Cl + Methacrolein: A Theoretical Study on the Mechanism, and Pressure- and Temperature-Dependent Rate Constants

Cuihong Sun, Baoen Xu, and Shaowen Zhang*

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dx.doi.org/10.1021/jp501205d

Rate Constants and Kinetic Isotope Effects for Methoxy Radical Reacting with NO₂ and O₂

Jiajue Chai, Hongyi Hu, Theodore S. Dibble,* Geoffrey S. Tyndall,* and John J. Orlando

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dx.doi.org/10.1021/jp501331c

Dynamics of Ferroelectric Bis(imidazolium) Pentachloroantimonate(III) by Means of Nuclear Magnetic Resonance ¹H Relaxometry and Dielectric Spectroscopy

A. Piecha-Bisiorek, R. Jakubas, W. Medycki, M. Florek-Wojciechowska, M. Wojciechowski, and D. Kruk*

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dx.doi.org/10.1021/jp502414e

Quasi-Classical Trajectory Study of the Vibrational and Translational Effects on the O(³P) + CD₄ Reaction

Joaquín Espinosa-García*


Spectroscopy, Photochemistry, and Excited States

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[dx.doi.org/10.1021/jp407342q](https://doi.org/10.1021/jp407342q)

Intramolecular Charge Transfer of Push–Pull Pyridinium Salts in the Singlet Manifold

Benedetta Carlotti, Giuseppe Consiglio, Fausto Elisei, Cosimo G. Fortuna, Ugo Mazzucato, and Anna Spalletti*

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[dx.doi.org/10.1021/jp501117n](https://doi.org/10.1021/jp501117n)

Isomer-Specific Product Detection of Gas-Phase Xylyl Radical Rearrangement and Decomposition Using VUV Synchrotron Photoionization


Patrick Hemberger,* Adam J. Trevitt, Thomas Gerber, Edward Ross, and Gabriel da Silva

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[dx.doi.org/10.1021/jp501398g](https://doi.org/10.1021/jp501398g)

Hyperporphyrin Effects in the Spectroscopy of Protonated Porphyrins with 4-Aminophenyl and 4-Pyridyl Meso Substituents

Chenyi Wang and Carl C. Wamser*

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[dx.doi.org/10.1021/jp5033383](https://doi.org/10.1021/jp5033383)

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Theoretical Study of the Oxidation Mechanisms of Naphthalene Initiated by Hydroxyl Radicals: The H Abstraction Pathway

Abolfazl Shiroudi and Michael S. Deleuze*

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Adenine Formation without HCN

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Molecular Structure, Quantum Chemistry, and General Theory

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Structures of Cycloserine and 2-Oxazolidinone Probed by X-ray Photoelectron Spectroscopy: Theory and Experiment





Marawan Ahmed, Feng Wang, Robert G. Acres, and Kevin C. Prince*

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[dx.doi.org/10.1021/jp500794s](https://doi.org/10.1021/jp500794s)


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Shigeki Yamamoto,* Tatsuya Furukawa, Petr Bouř,* and Yukihiro Ozaki

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Correction to "How Critical Are the van der Waals Interactions in Polymer Crystals?"
Chun-Sheng Liu, Ghanshyam Pilania, Chenchen Wang, and Ramamurthy Ramprasad*

 Supporting Information available via online article