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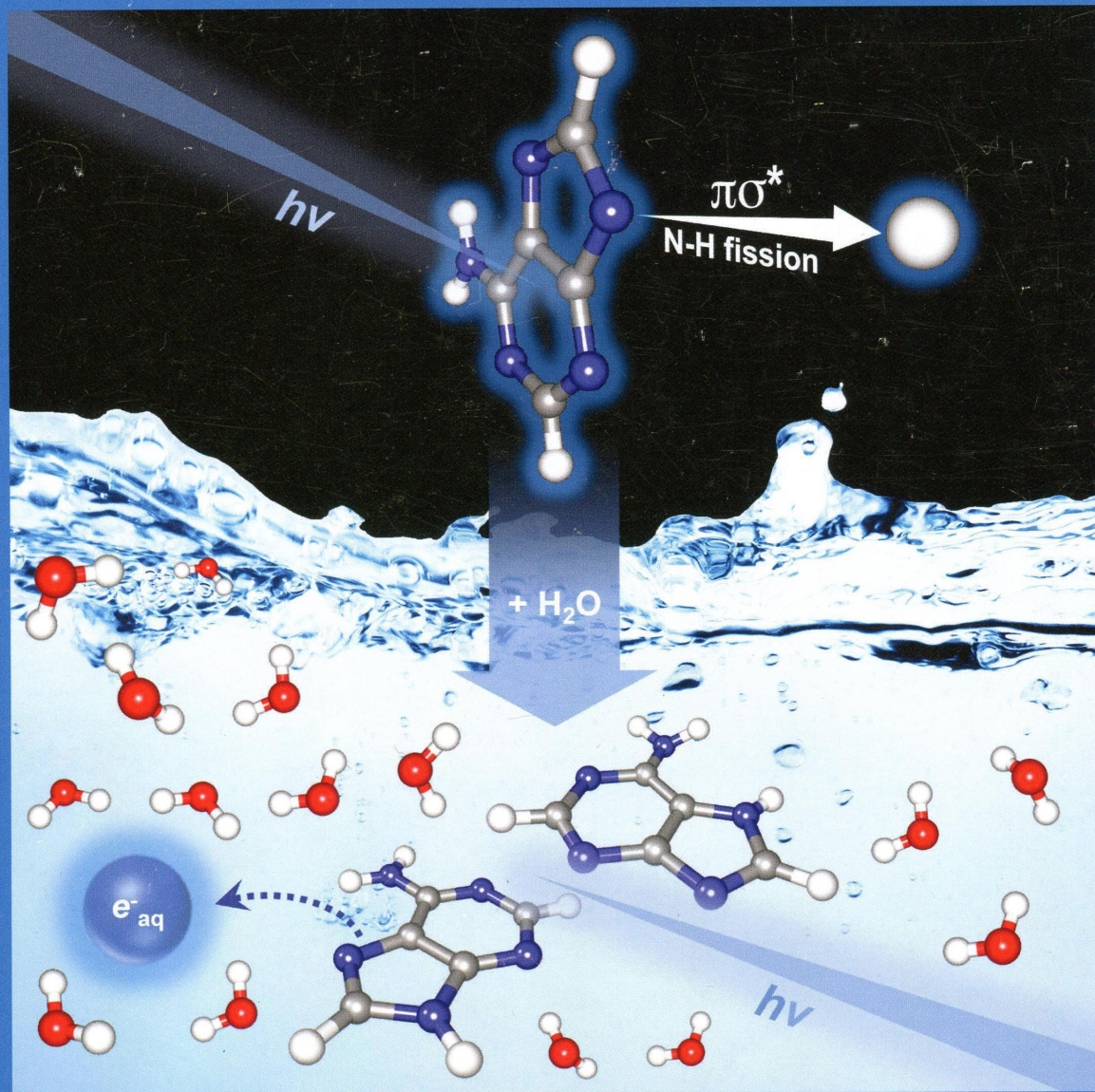
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A



Exploring the Role of
N–H Bond Dissociation
in the Photochemistry
of Aqueous Adenine
(see page 11211)

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




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ON THE COVER: Ultrafast transient absorption spectroscopy measurements on adenine in D_2O reveal that N–H bond cleavage, mediated by a repulsive ${}^1\pi\sigma^*$ state, is not an active excited state deactivation channel for excitation wavelengths longer than 220 nm. This behavior is in contrast to the isolated nucleobase in the gas phase and is traced to the 3s Rydberg character of the ${}^1\pi\sigma^*$ state in the vertical Franck-Condon region. The Rydberg character renders this state susceptible to Pauli repulsion in aqueous media and strongly blue shifts the threshold for accessing the N–H bond scission channel, relative to the gas phase. See page 11211.

Articles

Kinetics and Dynamics

11119 

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Thermal Decomposition Mechanisms of Alkylimidazolium Ionic Liquids with Cyano-Functionalized Anions

Steven D. Chambreau, Adam C. Schenk, Anna J. Sheppard, Gregory R. Yandek, Ghanshyam L. Vaghjiani,* John Maciejewski, Christine J. Koh, Amir Golan, and Stephen R. Leone

11133

DOI: 10.1021/jp5095849

Dynamics Simulations and Statistical Modeling of Thermal Decomposition of 1-Ethyl-3-methylimidazolium Dicyanamide and 1-Ethyl-2,3-dimethylimidazolium Dicyanamide

Jianbo Liu,* Steven D. Chambreau, and Ghanshyam L. Vaghjiani

11145

DOI: 10.1021/jp5038156

Detailed Mechanistic Studies into the Reactivities of Thiourea and Substituted Thiourea Oxoacids: Decompositions and Hydrolyses of Dioxides in Basic Media

Merfat M. Aslabban, Risikat Ajibola Adigun, William DeBenedetti, Wilbes Mbiya, Morgen Mhike, Kayode Morakinyo, Adenike Otoikhian, Tinashe Ruwona, and Reuben H. Simoyi*

11155 

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Kinetics of C–C and C–H Bond Cleavage in Phenyl Alkane Radical Cations Generated by Photoinduced Electron Transfer

Douglas Cyr and Paritosh Das*

11168

DOI: 10.1021/jp5100507

A Full-Dimensional Global Potential Energy Surface of $H_3O^+(\bar{a}^3A)$ for the $OH^+(\bar{X}^3\Sigma^-) + H_2(\bar{X}^1\Sigma_g^+) \rightarrow H(^2S) + H_2O^+(\bar{X}^2B_1)$ Reaction

Anyang Li and Hua Guo*

11177

DOI: 10.1021/jp510130x

Ultrafast Dissociation Dynamics of $[\text{Fe}(\text{CO})_5]_n$ Clusters Induced by Femtosecond IR Radiation

Denis G. Poydashev,* Valery N. Likhman, Victor O. Kompanets, Sergey V. Chekalin, and Evgeny A. Ryabov*

Spectroscopy, Photochemistry, and Excited States11185 

DOI: 10.1021/jp507050y

Vacuum Ultraviolet Photoionization Study of Gas Phase Vitamins A and B1 Using Aerosol Thermodesorption and Synchrotron Radiation

Héloïse Dossmann,* Adrián Schwarzenberg, Denis Lesage, Marie Pérot-Taillandier, Carlos Afonso, Barbara Cunha de Miranda, and Gustavo A. Garcia

11193 

DOI: 10.1021/jp507863b

Matrix Isolation Study of the Conformations and Photochemistry of S-Ethyl Fluorothioformate, $\text{FC}(\text{O})\text{SCH}_2\text{CH}_3$

Lucas S. Rodríguez Pirani, Mauricio F. Erben,* Helge Willner, Rosana M. Romano, and Carlos O. Della Védova*

11204 

DOI: 10.1021/jp507926x

Structural Determination and Gas-Phase Synthesis of Monomeric, Unsolvated IZnCH_3 ($\bar{X}^1\text{A}_1$): A Model Organozinc Halide

Matthew P. Bucchino, Justin P. Young, Phillip M. Sheridan,* and Lucy M. Ziurys

11211 

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On the Participation of Photoinduced N–H Bond Fission in Aqueous Adenine at 266 and 220 nm: A Combined Ultrafast Transient Electronic and Vibrational Absorption Spectroscopy Study

Gareth M. Roberts,* Hugo J. B. Marroux, Michael P. Grubb, Michael N. R. Ashfold, and Andrew J. Orr-Ewing*

11226 

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Dissociative Photoionization and Threshold Photoelectron Spectra of Polycyclic Aromatic Hydrocarbon Fragments: An Imaging Photoelectron Photoion Coincidence (iPEPICO) Study of Four Substituted Benzene Radical Cations

Brandi West, Alicia Sit, Andras Bodi, Patrick Hemberger, and Paul M. Mayer*

11235 

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Decomposition of Diazomeldrum's Acid: A Threshold Photoelectron Spectroscopy Study

Melanie Lang, Fabian Holzmeier, Ingo Fischer,* and Patrick Hemberger*

11244 

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Ab Initio Study of Energy Transfer Pathways in Dinuclear Lanthanide Complex of Europium(III) and Terbium(III) Ions

Ksenia A. Romanova,* Alexandra Ya. Freidzon, Alexander A. Bagaturyants, and Yuri G. Galyametdinov

11253

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Excitonic Splitting, Delocalization, and Vibronic Quenching in the Benzonitrile Dimer

Franziska A. Balmer, Philipp Ottiger, and Samuel Leutwyler*

11262 

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Direct Observation of Hole Shift and Characterization of Spin States in Radical Ion Pairs Generated from Photoinduced Electron Transfer of (Phenothiazine)_n-Anthraquinone ($n = 1, 3$) Dyads
Ayumu Karimata, Shuichi Suzuki, Masatoshi Kozaki, Kenshi Kimoto, Koichi Nozaki,* Hironori Matsushita, Noriaki Ikeda,* Kimio Akiyama,* Daisuke Kosumi, Hideki Hashimoto, and Keiji Okada*

11272 

DOI: 10.1021/jp510142g

Fermi Resonance Effects in the Vibrational Spectroscopy of Methyl and Methoxy Groups
Edwin L. Sibert III, Daniel P. Tabor, Nathanael M. Kidwell, Jacob C. Dean, and Timothy S. Zwier*

Molecular Structure, Quantum Chemistry, and General Theory

11282

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Complex Frequency-Dependent Polarizability through the $\pi \rightarrow \pi^*$ Excitation Energy of Azobenzene Molecules by a Combined Charge-Transfer and Point-Dipole Interaction Model
Shokouh Haghdani, Nazanin Davari, Runar Sandnes, and Per-Olof Åstrand*

11293 

DOI: 10.1021/jp5082164

Charge Delocalization in an Organic Mixed Valent Bithiophene Is Greater Than in a Structurally Analogous Biselenophene
Ann Christin Jahnke, Jonny Proppé, Mariana Spulber, Cornelia G. Palivan, Carmen Herrmann,* and Oliver S. Wenger*

11304 

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The Localization–Delocalization Matrix and the Electron-Density-Weighted Connectivity Matrix of a Finite Graphene Nanoribbon Reconstructed from Kernel Fragments
Matthew J. Timm, Chérif F. Matta,* Lou Massa, and Lulu Huang

11317

DOI: 10.1021/jp5088042

First-Principles Computational Visualization of Localized Surface Plasmon Resonance in Gold Nanoclusters
Kenji Iida, Masashi Noda, Kazuya Ishimura, and Katsuyuki Nobusada*

11323

DOI: 10.1021/jp5091685

From Dissipative Dynamics to Studies of Heat Transfer at the Nanoscale: Analysis of the Spin-Boson Model
Nazim Boudjada and Dvira Segal*