

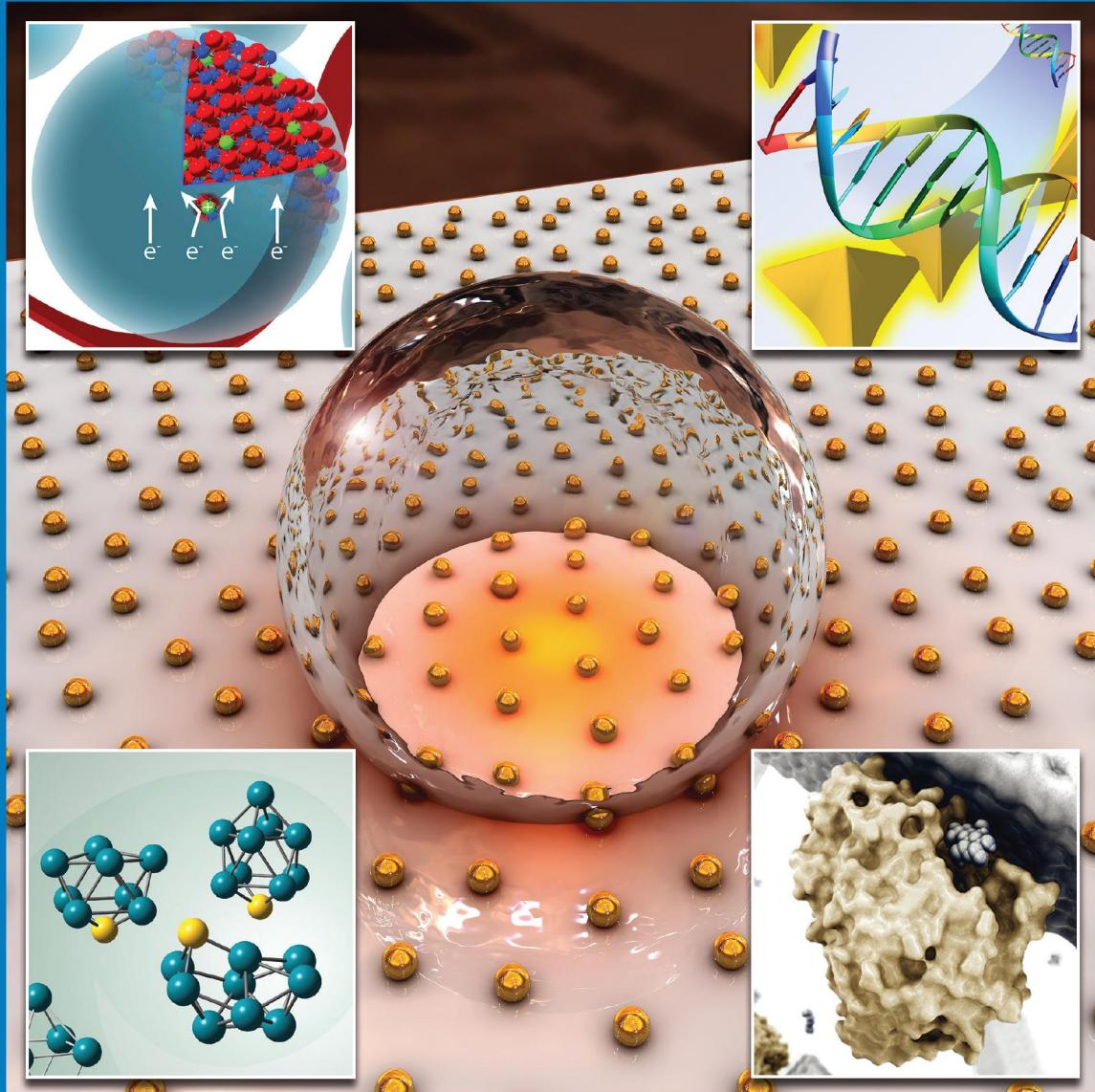
APRIL 2, 2015

VOLUME 119

NUMBER 13

[pubs.acs.org/JPCA](http://pubs.acs.org/JPCA)THE JOURNAL OF  
PHYSICAL  
CHEMISTRY

A



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



ACS Publications  
Most Trusted. Most Cited. Most Read.

[www.acs.org](http://www.acs.org)

# THE JOURNAL OF PHYSICAL CHEMISTRY A

April 2, 2015: Vol. 119, Iss. 13

## Content

### 1. Dependence of the Four-Atom Reaction $\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$ on Temperatures between 20 and 2000 K

J. Ree, Y. H. Kim, and H. K. Shin

*The Journal of Physical Chemistry A* 2015 119 (13), 3147-3160

DOI: 10.1021/jp511505h

### 2. Temperature and Pressure Dependent Rate Coefficients for the Reaction of $\text{C}_2\text{H}_4 + \text{HO}_2$ on the $\text{C}_2\text{H}_4\text{O}_2\text{H}$ Potential Energy Surface

JunJiang Guo, JiaQi Xu, ZeRong Li, NingXin Tan, and XiangYuan Li

*The Journal of Physical Chemistry A* 2015 119 (13), 3161-3170

DOI: 10.1021/jp511991n

### 3. Comparative Kinetics of the 3-Buten-1-ol and 1-Butene Reactions with OH Radicals: A Density Functional Theory/RRKM Investigation

Silvina Peirone, Jorge D. Nieto, Pablo M. Cometto, Thaís da Silva Barbosa, Glauco Favilla

Bauerfeldt, Graciela Arbillal, and Silvia I. Lane

*The Journal of Physical Chemistry A* 2015 119 (13), 3171-3180

DOI: 10.1021/jp512544x

### 4. Transient Absorption Dynamics of Sterically Congested Cu(I) MLCT Excited States

Sofia Garakyanaghi, Evgeny O. Danilov, Catherine E. McCusker, and Felix N. Castellano

*The Journal of Physical Chemistry A* 2015 119 (13), 3181-3193

DOI: 10.1021/acs.jpca.5b00901

### 5. Gas-Phase Kinetics of the $\text{N} + \text{C}_2\text{N}$ Reaction at Low Temperature

James W. Stubbing, Gianmarco Vanuzzo, Audrey Moudens, Jean-Christophe Loison, and Kevin M. Hickson

*The Journal of Physical Chemistry A* 2015 119 (13), 3194-3199

DOI: 10.1021/acs.jpca.5b01259

### 6. Electron Spin Relaxation of $\text{C}_60$ Monoanion in Liquid Solution: Applicability of Kivelson–Orbach Mechanism

Krishnendu Kundu, Daniel R. Kattnig, Boryana Mladenova, Günter Grampp, and Ranjan Das

*The Journal of Physical Chemistry A* 2015 119 (13), 3200-3208

DOI: 10.1021/jp5126409

### 7. Identification of Alcohol Conformers by Raman Spectra in the C–H Stretching Region

Lin Chen, Weiduo Zhu, Ke Lin, Naiyin Hu, Yuanqin Yu, Xiaoguo Zhou, Lan-Feng Yuan, Shui-Ming Hu, and Yi Luo

*The Journal of Physical Chemistry A* 2015 119 (13), 3209-3217

DOI: 10.1021/jp513027r

### 8. Halide Abstraction from Halogenated Acetate Ligands by Actinyls: A Competition between Bond Breaking and Bond Making

Phuong D. Dau and John K. Gibson

*The Journal of Physical Chemistry A* 2015 119 (13), 3218-3224

DOI: 10.1021/acs.jpca.5b00952

### 9. H and D Attachment to Naphthalene: Spectra and Thermochemistry of Cold Gas-Phase 1-C<sub>10</sub>H<sub>9</sub> and 1-C<sub>10</sub>H<sub>8</sub>D Radicals and Cations

Olha Krechkivska, Callan M. Wilcox, Bun Chan, Rebecca Jacob, Yu Liu, Klaas Nauta, Scott H. Kable, Leo Radom, and Timothy W. Schmidt

*The Journal of Physical Chemistry A* 2015 119 (13), 3225-3232

DOI: 10.1021/acs.jpca.5b01652

**10. Controlling Factors in the Rates of Oxidation of Anilines and Phenols by Triplet Methylene Blue in Aqueous Solution**

Paul R. Erickson, Nicolas Walpen, Jennifer J. Guerard, Soren N. Eustis, J. Samuel Arey, and Kristopher McNeill

*The Journal of Physical Chemistry A* 2015 119 (13), 3233-3243

DOI: 10.1021/jp511408f

**11. Isotherm-Based Thermodynamic Model for Electrolyte and Nonelectrolyte Solutions Incorporating Long- and Short-Range Electrostatic Interactions**

Peter B. Ohm, Caitlin Asato, Anthony S. Wexler, and Cari S. Dutcher

*The Journal of Physical Chemistry A* 2015 119 (13), 3244-3252

DOI: 10.1021/jp512646k

**12. Theoretical Study on Structures and Bond Properties of  $\text{NpO}_2\text{m}^+$  Ions and  $\text{NpO}_2(\text{H}_2\text{O})\text{nm}^+$  ( $m = 1-2$ ,  $n = 1-6$ ) Complexes in the Gas Phase and Aqueous Solution**

Yao-Peng Yin, Chen-Zhong Dong, and Xiao-Bin Ding

*The Journal of Physical Chemistry A* 2015 119 (13), 3253-3260

DOI: 10.1021/jp511265j

**13. Investigating the Role of  $\text{CH}_2$  Radicals in the HACA Mechanism**

Peng Liu, He Lin, Yang Yang, Can Shao, Bin Guan, and Zhen Huang

*The Journal of Physical Chemistry A* 2015 119 (13), 3261-3268

DOI: 10.1021/jp5124162

**14. Terahertz Spectroscopy and Computational Investigation of the Flufenamic Acid/Nicotinamide Cocrystal**

Sean P. Delaney and Timothy M. Korter

*The Journal of Physical Chemistry A* 2015 119 (13), 3269-3276

DOI: 10.1021/jp5125519

**15. Electronic Structural Basis for the Atomic Partial Charges of Planar Molecular Systems Derived from Out-of-Plane Dipole Derivatives**

Hajime Torii

*The Journal of Physical Chemistry A* 2015 119 (13), 3277-3284

DOI: 10.1021/jp512884g

**16. Distributed Atomic Polarizabilities of Amino Acids and their Hydrogen-Bonded Aggregates**

Leonardo H. R. Dos Santos, Anna Krawczuk, and Piero Macchi

*The Journal of Physical Chemistry A* 2015 119 (13), 3285-3298

DOI: 10.1021/acs.jpca.5b00069

**17. Theoretical Study of Acene-Bridged Dyes for Dye-Sensitized Solar Cells**

Minjie Li, Li Kou, Ling Diao, Qing Zhang, Zhonggao Li, Qiang Wu, Wencong Lu, and Dengyu Pan

*The Journal of Physical Chemistry A* 2015 119 (13), 3299-3309

DOI: 10.1021/acs.jpca.5b00798

**18. Correction to “Reoxidation of Photoreduced Polyoxotungstate [PW<sub>12</sub>O<sub>40</sub>]<sup>4-</sup> by Different Oxidants in the Presence of a Model Pollutant. Kinetics and Reaction Mechanism”**

Bing Yang, Joseph J. Pignatello, Dong Qu, and Baoshan Xing

*The Journal of Physical Chemistry A* 2015 119 (13), 3310-3310

DOI: 10.1021/acs.jpca.5b02221