

TU  
J80/par

APRIL 17, 2014

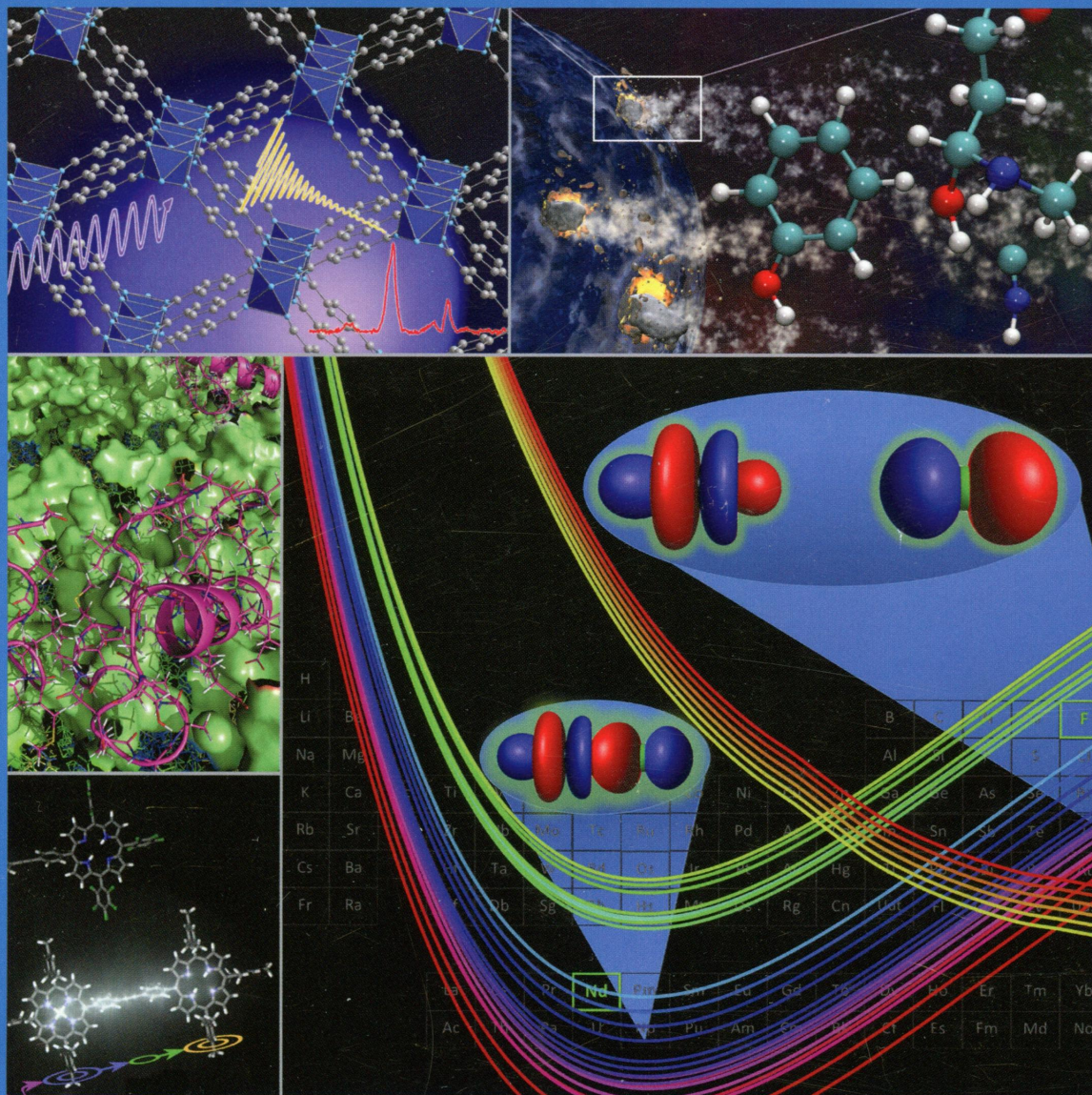
VOLUME 118

NUMBER 15

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



**ON THE COVER:** Collage of cover art from recent issues of *J. Phys. Chem.* Top Left:  $^{17}\text{O}$  Solid-State NMR Spectra Provide Signatures of Various Oxygen Species in Metal-Organic Frameworks (*J. Phys. Chem. C* **2013**, *117* (33), 16953–16960). Center Left: Behavior of Amyloid  $\beta$ -Peptides on a Ganglioside-Containing Membrane Surface (*J. Phys. Chem. B* **2013**, *117* (27), 8085–8094). Bottom Left: Bridge-Mediated EET in Porphyrin Dimers: Electronic Coupling Reduced by Fluorination (*J. Phys. Chem. C* **2013**, *117* (24), 12423–12431). Top Right: Synthesis of Prebiotic Hydrocarbons in Impacts of Simple Icy Mixtures on Early Earth (*J. Phys. Chem. A* **2013**, *117* (24), 5124–5131). Bottom Right: Computed Potential Energy Curves for Quartet, Doublet, and Sextet States of  $\text{NdF}^{2+}$  (*J. Phys. Chem. A* **2013**, *117* (42), 10881–10888).

## Articles

### Kinetics and Dynamics

2683



dx.doi.org/10.1021/jp412444b

**Decomposition Kinetics of Nitroglycerine-Cl<sup>-</sup>(g) in Air at Ambient Pressure with a Tandem Ion Mobility Spectrometer**

Maneeshin Y. Rajapakse, John A. Stone, and Gary A. Eiceman\*

2693

dx.doi.org/10.1021/jp5002995

**Low Temperature Kinetics of the CH<sub>3</sub>OH + OH Reaction**

J. C. Gómez Martín,\* R. L. Caravan, M. A. Blitz, D. E. Heard, and J. M. C. Plane

2702

dx.doi.org/10.1021/jp500627z

**pH Oscillations and Mechanistic Analysis in the Hydrogen Peroxide–Sulfite–Thiourea Reaction System**

Ling Yuan, Tao Yang, Yang Liu, Ying Hu, Yuemin Zhao, Juhua Zheng, and Qingyu Gao\*

2709



dx.doi.org/10.1021/jp501210d

**An Experimental and Theoretical Study on the Formation of 2-Methylnaphthalene (C<sub>11</sub>H<sub>10</sub>/C<sub>11</sub>H<sub>9</sub>D<sub>1</sub>) in the Reactions of the Para-Tolyl (C<sub>7</sub>H<sub>7</sub>) and Para-Tolyl-d<sub>7</sub> (C<sub>7</sub>D<sub>7</sub>) with Vinylacetylene (C<sub>4</sub>H<sub>4</sub>)**

Dorian S. N. Parker, Beni B. Dangi, Ralf I. Kaiser,\* Adeel Jamal, Mikhail N. Ryazantsev, Keiji Morokuma,\* André Korte, and Wolfram Sander

### Spectroscopy, Photochemistry, and Excited States

2719



dx.doi.org/10.1021/jp411237p

**Infrared Photodissociation Spectroscopy of Mass-Selected Homoleptic Cobalt Carbonyl Cluster Cations in the Gas Phase**

Jieming Cui, Xiaojie Zhou, Guanjun Wang, Chaoxian Chi, Zhen Hua Li,\* and Mingfei Zhou\*

2728 

[dx.doi.org/10.1021/jp412073c](https://doi.org/10.1021/jp412073c)

**In Situ Observation on the Dynamic Process of Evaporation and Crystallization of Sodium Nitrate Droplets on a ZnSe Substrate by FTIR-ATR**

Qing-Nuan Zhang, Yun Zhang, Chen Cai, Yu-Cong Guo, Jonathan P. Reid, and Yun-Hong Zhang\*

2738

[dx.doi.org/10.1021/jp4121996](https://doi.org/10.1021/jp4121996)

**Dynamics of Excited Sodium Atoms Attached to Helium Nanodroplets**

Evgeniy Loginov and Marcel Drabbels\*

2749 

[dx.doi.org/10.1021/jp501454v](https://doi.org/10.1021/jp501454v)

**Tetrapositive Plutonium, Neptunium, Uranium, and Thorium Coordination Complexes: Chemistry Revealed by Electron Transfer and Collision Induced Dissociation**

Yu Gong, Guoxin Tian, Linfeng Rao, and John K. Gibson\*

2756 

[dx.doi.org/10.1021/jp501517t](https://doi.org/10.1021/jp501517t)

**Quantum Yields for Photochemical Production of NO<sub>2</sub> from Organic Nitrates at Tropospherically Relevant Wavelengths**

Christina M. Higgins, Louise A. Evans, Guy C. Lloyd-Jones, Dudley E. Shallcross, David P. Tew, and Andrew J. Orr-Ewing\*

2765

[dx.doi.org/10.1021/jp5016142](https://doi.org/10.1021/jp5016142)

**VUV Photodynamics and Chiral Asymmetry in the Photoionization of Gas Phase Alanine Enantiomers**

Maurice Tia, Barbara Cunha de Miranda, Steven Daly, François Gaie-Levrel, Gustavo A. Garcia, Laurent Nahon,\* and Ivan Powis

## Environmental and Atmospheric Chemistry, Aerosol Processes, Geochemistry, and Astrochemistry

2780

[dx.doi.org/10.1021/jp4121029](https://doi.org/10.1021/jp4121029)

**Reactive Molecular Dynamics Simulation on the Disintegration of Kapton, POSS Polyimide, Amorphous Silica, and Teflon during Atomic Oxygen Impact Using the Reaxff Reactive Force-Field Method**

A. Rahnamoun and A. C. T. van Duin\*

## Molecular Structure, Quantum Chemistry, and General Theory

2788 

[dx.doi.org/10.1021/jp412400q](https://doi.org/10.1021/jp412400q)

**Acidities of *cis*-1-COOH-1,7-C<sub>2</sub>B<sub>10</sub>H<sub>11</sub> and Amino Acids Based on Icosahedral Carboranes**

Juan Z. Dávalos,\* Javier González, Rocío Ramos, Drahomír Hnyk,\* Josef Holub, J. Arturo Santaballa, Moisés Canle-L., and Josep M. Oliva\*

2794 

[dx.doi.org/10.1021/jp500211y](https://doi.org/10.1021/jp500211y)

**Experimental and Theoretical Studies of Intramolecular Hydrogen Bonding in 3-Hydroxytetrahydropyran: Beyond AIM Analysis**

Daniela C. Solha, Thaís M. Barbosa, Renan V. Viesser, Roberto Rittner, and Cláudio F. Tormena\*

2801 

[dx.doi.org/10.1021/jp501107b](https://doi.org/10.1021/jp501107b)

**Combined ab Initio Molecular Dynamics and Experimental Studies of Carbon Atom Addition to Benzene**

Michael L. McKee,\* Hans Peter Reisenauer, and Peter R. Schreiner\*

2810 

[dx.doi.org/10.1021/jp501256f](https://doi.org/10.1021/jp501256f)

**Effect of Protonation State and Interposed Connector Groups on Bond Dissociation Enthalpies of Alcohols and Related Systems**

Michael Morris, Bun Chan,\* and Leo Radom\*

2820

[dx.doi.org/10.1021/jp501553j](https://doi.org/10.1021/jp501553j)

**Cooperative Effects and Optimal Halogen Bonding Motifs for Self-Assembling Systems**

Xin Cindy Yan, Patric Schyman, and William L. Jorgensen\*

2827 

[dx.doi.org/10.1021/jp502301n](https://doi.org/10.1021/jp502301n)

**A Combined Theoretical and Cambridge Structural Database Study of  $\pi$ -Hole Pnictogen Bonding Complexes between Electron Rich Molecules and Both Nitro Compounds and Inorganic Bromides (YO<sub>2</sub>Br, Y = N, P, and As)**

Antonio Bauzá, Rafael Ramis, and Antonio Frontera\*


## Additions and Corrections

2835

[dx.doi.org/10.1021/jp5026653](https://doi.org/10.1021/jp5026653)

**Correction to "Analytic Density-Functional Theory Calculations of Pure Vibrational Hyperpolarizabilities: The First Dipole Hyperpolarizability of Retinal and Related Molecules"**

Bin Gao, Magnus Ringholm, Radovan Bast, Kenneth Ruud,\* Andreas J. Thorvaldsen, and Michał Jaszuński

 Supporting Information available via online article