

**NOVEMBER 14, 2013** 

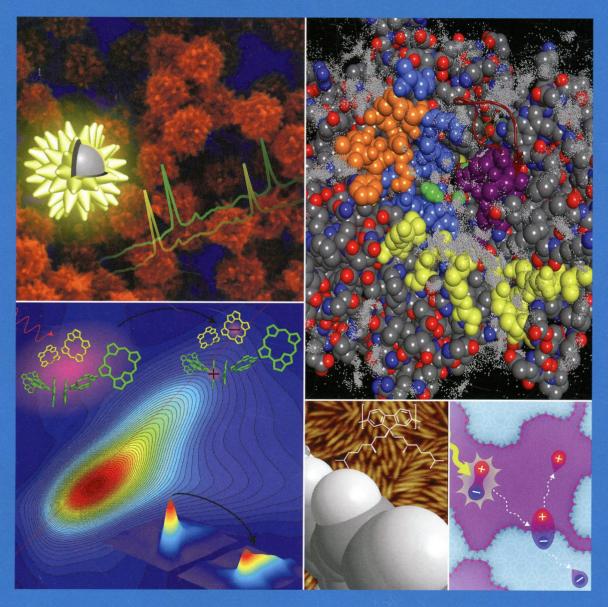
**VOLUME 117** 

**NUMBER 45** 

pubs.acs.org/JPCA

# THE JOURNAL OF PHYSICAL CHEMISTRY

A



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





November 14, 2013 Volume 117, Issue 45 Pages 11383-11604

#### **Kinetics and Dynamics**

Reinvestigation of the Elementary Chemical Kinetics of the Reaction  $C_2H_5$  + HBr (HI)  $\rightarrow C_2H_6$  + Br (I $^{\bullet}$ ) in the Range 293–623 K and Its Implication on the Thermochemical Parameters of  $C_2H_5$  Free Radical

N. Leplat, A. Wokaun, and M. J. Rossi

pp 11383-11402

Publication Date (Web): October 17, 2013 (Article)

**DOI:** 10.1021/jp403761r

Section:

**Physical Organic Chemistry** 

Theoretical Study of Excess Electron Attachment Dynamics to the Guanine– Cytosine Base Pair: Electronic Structure Calculations and Ring–Polymer Molecular Dynamics Simulations

Yuji Sugioka, Takehiro Yoshikawa, and Toshiyuki Takayanagi pp 11403–11410

Publication Date (Web): October 22, 2013 (Article)

DOI: 10.1021/jp4067058

Section:

**Physical Organic Chemistry** 

Time-Dependent Wave Packet Quantum Scattering and Quasi-Classical Trajectory Calculations of the  $H + FCl(v=0,j=0) \rightarrow HF + Cl/HCl + F$  Reaction

Juan Zhao, Xiangyang Miao, and Yi Luo

pp 11411-11419

Publication Date (Web): October 14, 2013 (Article)

**DOI:** 10.1021/jp4070592

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Experimental and Modeling Study of the Reaction  $C_2F_4$  (+ M)  $\Rightarrow$   $CF_2$  +  $CF_2$  (+ M)

C.J. Cobos, A.E. Croce, K. Luther, L. Sölter, E. Tellbach, and J. Troe pp 11420–11429

Publication Date (Web): October 8, 2013 (Article)

**DOI:** 10.1021/jp408363s

Section:

**Physical Organic Chemistry** 

## Modeling of Energy Transfer From Vibrationally Excited CO<sub>2</sub> Molecules: Cross Sections and Probabilities for Kinetic Modeling of Atmospheres, Flows, and Plasmas

Andrea Lombardi, Noelia Faginas-Lago, Leonardo Pacifici, and Alessandro Costantini pp 11430–11440

Publication Date (Web): October 14, 2013 (Article)

**DOI:** 10.1021/jp408522m

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

#### Spectroscopy, Photochemistry, and Excited States

## Vibrational Energy Flow between Modes by Dynamic Mode Coupling in THIATS J-Aggregates

Daisuke Hasegawa, Kazuaki Nakata, Eiji Tokunaga, Kotaro Okamura, Juan Du, and Takayoshi Kobayashi pp 11441–11448

Publication Date (Web): October 10, 2013 (Article)

**DOI:** 10.1021/jp4015228

Section:

Physical Organic Chemistry

#### Excimer Luminescence From Nonresonantly Excited Pyrene and Perylene Molecules in Solution

Kazuya Nakagawa, Yudai Numata, Heisuke Ishino, Daichi Tanaka, Takayoshi Kobayashi, and Eiji Tokunaga pp 11449–11455

Publication Date (Web): October 14, 2013 (Article)

**DOI:** 10.1021/jp402330n

Section:

Physical Organic Chemistry

### Electronic Excitations in Fischer-Type Cr and W Aminocarbene Complexes: A Combined ab Initio and Experimental Study

Hana Kvapilová, Irena Hoskovcová, Megumi Kayanuma, Chantal Daniel, and Stanislav Záliš pp 11456–11463

Publication Date (Web): October 11, 2013 (Article)

**DOI:** 10.1021/jp4074027

Section:

Organometallic and Organometalloidal Compounds

## Raman Spectrum of Pyrope Garnet. A Quantum Mechanical Simulation of Frequencies, Intensities, and Isotope Shifts

Lorenzo Maschio, Bernard Kirtman, Simone Salustro, Claudio M. Zicovich-Wilson, Roberto Orlando, and Roberto Dovesi
pp 11464–11471

Publication Date (Web): October 14, 2013 (Article)

**DOI:** 10.1021/jp4099446

Section:

Mineralogical and Geological Chemistry

#### Low Frequency Resonant Impulsive Raman Modes Reveal Inversion Mechanism for Azobenzene

David P. Hoffman, Scott R. Ellis, and Richard A. Mathies pp 11472–11478

Publication Date (Web): October 18, 2013 (Article)

**DOI:** 10.1021/jp408470a

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

# Efficiency of Intramolecular Charge Separation from the Second Excited State: Suppression of the Hot Charge Recombination by Electron Transfer to the Secondary Acceptor

Serguei V. Feskov and Anatoly I. Ivanov

pp 11479-11489

Publication Date (Web): October 8, 2013 (Article)

**DOI:** 10.1021/jp408516q

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

### IR Spectroscopy of Gas Phase $V(CO_2)_n^+$ Clusters: Solvation-Induced Electron Transfer and Activation of $CO_2$

Allen M. Ricks, Antonio D. Brathwaite, and Michael A. Duncan pp 11490–11498

Publication Date (Web): October 21, 2013 (Article)

**DOI:** 10.1021/jp4089035

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

#### Magnetic Circular Dichroism Spectroscopy of N-Confused Porphyrin and Its Ionized Forms

Christopher J. Ziegler, Nathan R. Erickson, Michael R. Dalby, and Victor N. Nemykin pp 11499–11508

Publication Date (Web): October 16, 2013 (Article)

**DOI:** 10.1021/jp409013d

Section:

Physical Organic Chemistry

### Simple Recipes for Separating Excited-State Absorption and Cascading Signals by Polarization-Sensitive Measurements

Maxim F. Gelin and Wolfgang Domcke

pp 11509-11513

Publication Date (Web): October 21, 2013 (Article)

**DOI:** 10.1021/jp409436z

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

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

## Ion-Induced Reorientation and Distribution of Pentanone in the Air–Water Boundary Layer

Kathryn L. Plath, Nicholas A. Valley, and Geraldine L. Richmond pp 11514–11527

Publication Date (Web): October 31, 2013 (Article)

**DOI:** 10.1021/jp408188x

Section:

Surface Chemistry and Colloids

#### Molecular Structure, Quantum Chemistry, and General Theory

#### Relative Contribution of Combined Kinetic and Exchange Energy Terms vs the Electronic Component of Molecular Electrostatic Potential in Hardness Potential Derivatives

Rituparna Bhattacharjee and Ram Kinkar Roy

pp 11528-11539

Publication Date (Web): October 1, 2013 (Article)

**DOI:** 10.1021/jp406685p

Section:

Physical Organic Chemistry

#### Cyclic $\pi$ Electron Delocalization in Fluoroborazines

Marija Baranac-Stojanović

pp 11540-11547

Publication Date (Web): October 21, 2013 (Article)

**DOI:** 10.1021/jp407454x

Section:

Organometallic and Organometalloidal Compounds

### Experimental Characterization of $C-X\cdots Y-C$ (X=Br, I; Y=F, CI) Halogen-Halogen Bonds

Dieter Hauchecorne and Wouter A. Herrebout pp 11548–11557

Publication Date (Web): October 15, 2013 (Article)

DOI: 10.1021/jp4077323

Section:

**Physical Organic Chemistry** 

## Tuning Amidoximate to Enhance Uranyl Binding: A Density Functional Theory Study

Carter W. Abney, Shubin Liu, and Wenbin Lin pp 11558–11565

Publication Date (Web): October 18, 2013 (Article)

**DOI:** 10.1021/jp408460x

Section:

General Physical Chemistry

#### Topology of the Electron Density of d<sup>0</sup> Transition Metal Compounds at Subatomic Resolution

Kilian Batke and Georg Eickerling pp 11566–11579

Publication Date (Web): October 10, 2013 (Article)

**DOI:** 10.1021/jp408576y

Section:

General Physical Chemistry

### Density-Dependent Onset of the Long-Range Exchange: A Key to Donor-Acceptor Properties

Marcin Modrzejewski, Łukasz Rajchel, Grzegorz Chalasinski, and Małgorzata M. Szczesniak pp 11580–11586

Publication Date (Web): October 16, 2013 (Article)

**DOI:** 10.1021/jp4088404

Section:

General Physical Chemistry

#### Face-Capping $\mu^3$ -BO in $B_6(BO)_7$ : Boron Oxide Analogue of $B_6H_7$ with Rhombic 4c–2e Bonds

Jin-Chang Guo, Hai-Gang Lu, Hua-Jin Zhai, and Si-Dian Lipp 11587–11591

Publication Date (Web): October 22, 2013 (Article)

**DOI:** 10.1021/jp4089723

Section:

**General Physical Chemistry** 

## Properties of Complexes $H_2C=(X)P:PXH_2$ , for X=F, Cl, OH, CN, NC, CCH, H, $CH_3$ , and $BH_2: P\cdots P$ Pnicogen Bonding at $\sigma$ -Holes and $\pi$ -Holes

Janet E. Del Bene, Ibon Alkorta, and José Elguero pp 11592–11604

Publication Date (Web): November 4, 2013 (Article)

**DOI:** 10.1021/jp409016q

Section:

General Physical Chemistry