

MAY 16, 2013

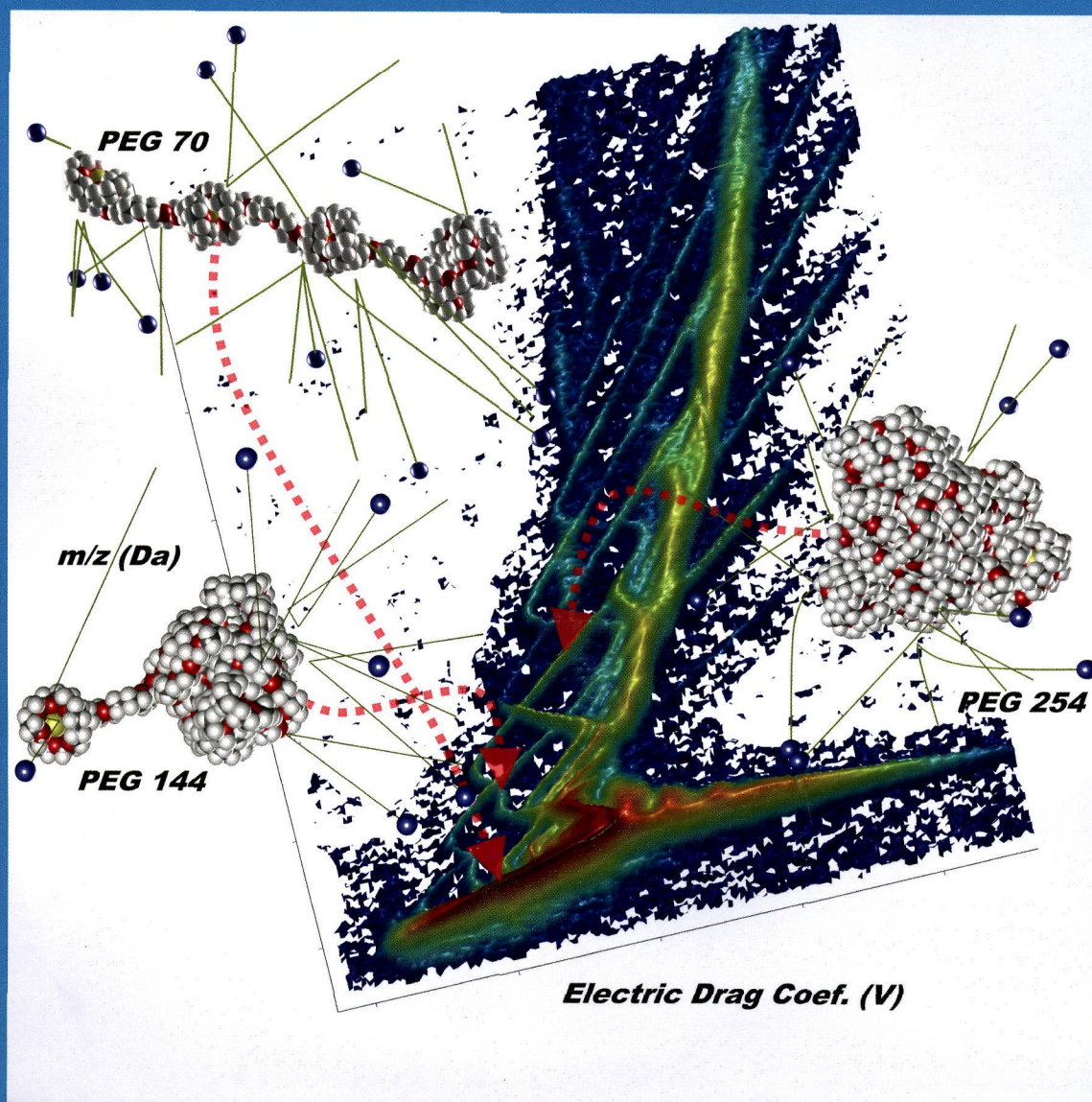
VOLUME 117

NUMBER 19

pubs.acs.org/JPCA

# THE JOURNAL OF PHYSICAL CHEMISTRY

# A



Ion Mobility in Gases  
from Nonspecular  
Scattering Models  
(see page 5A)

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



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

www.acs.org

# THE JOURNAL OF PHYSICAL CHEMISTRY A

May 16, 2013

Volume 117, Issue 19

Pages 3877-4072

## ***Kinetics and Dynamics***

### ***Coulomb Fission in Dielectric Dication Clusters: Experiment and Theory on Steps That May Underpin the Electrospray Mechanism***

Xiaojing Chen, Elena Bichoutskaia, and Anthony J. Stace

pp 3877–3886

**Publication Date (Web):** April 23, 2013 (Article)

**DOI:** 10.1021/jp311950p

 Section:

Electric Phenomena

### ***Ion Mobilities in Diatomic Gases: Measurement versus Prediction with Non-Specular Scattering Models***

Carlos Larriba and Christopher J. Hogan, Jr.

pp 3887–3901

**Publication Date (Web):** March 14, 2013 (Article)

**DOI:** 10.1021/jp312432z

 Section:

Unit Operations and Processes

### ***Kinetics of Several Oxygenated Carbon-Centered Free Radical Reactions with NO<sub>2</sub>***

Matti P. Rissanen, Suula L. Arppe, and Raimo S. Timonen

pp 3902–3908

**Publication Date (Web):** April 15, 2013 (Article)

**DOI:** 10.1021/jp401999e

 Section:

Physical Organic Chemistry

***Spectroscopy, Photochemistry, and Excited States  
Exciplex Formation in Blended Spin-Cast Films of Fluorene-Linked Dyes  
and Bisphthalimide Quenchers***

David J. Stewart, Matthew J. Dalton, Rachel N. Swiger, Thomas M. Cooper, Joy E. Haley, and Loon-Seng Tan

pp 3909–3917

**Publication Date (Web):** April 12, 2013 (Article)

**DOI:** 10.1021/jp312029e

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

***Autocatalytic Chemiluminescence Sheds New Light on the Classic  
Permanganate–Oxalate Reaction***

Christopher M. Hindson, Zoe M. Smith, Neil W. Barnett, Graeme R. Hanson, Kieran F. Lim, and Paul S. Francis

pp 3918–3924

**Publication Date (Web):** May 3, 2013 (Article)

**DOI:** 10.1021/jp312603m

 Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

***Temperature Dependence of the Excited-State Proton-Transfer Reaction of  
Quinone-cyanine-7***

Ron Simkovitch, Shay Shomer, Rinat Gepshtein, Doron Shabat, and Dan Huppert

pp 3925–3934

**Publication Date (Web):** April 18, 2013 (Article)

**DOI:** 10.1021/jp3128669

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

***Photophysics of Xanthone: A Quantum Chemical Perusal***

Vidisha Rai-Constapel, Mihajlo Etinski, and Christel M. Marian

pp 3935–3944

**Publication Date (Web):** April 16, 2013 (Article)

**DOI:** 10.1021/jp401755j

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

***Fluorescence Quenching of Hydrogen-Bonded Coumarin 102-Phenol Complex: Effect of Excited-State Hydrogen Bonding Strength***

Nabajeet Barman, Debabrata Singha, and Kalyanasis Sahu

pp 3945–3953

**Publication Date (Web):** April 25, 2013 (Article)

**DOI:** 10.1021/jp4019298

Section:

Physical Organic Chemistry

***Accurate Modeling of Infrared Multiple Photon Dissociation Spectra: The Dynamical Role of Anharmonicities***

Pascal Parneix, Marie Basire, and Florent Calvo

pp 3954–3959

**Publication Date (Web):** April 12, 2013 (Article)

**DOI:** 10.1021/jp402459f

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

***Physical and Chemical Response of FeCl<sub>3</sub>/FeCl<sub>4</sub><sup>-</sup> Spin Probes on the Functionalizing of Ionic Liquids***

Reinhard Stößer and Werner Herrmann

pp 3960–3971

**Publication Date (Web):** April 18, 2013 (Article)

**DOI:** 10.1021/jp403260r

Section:

Magnetic Phenomena

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

***Synergistic Effects between SO<sub>2</sub> and HCOOH on  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>***

Ling-Yan Wu, Sheng-Rui Tong, Li Zhou, Wei-Gang Wang, and Mao-Fa Ge

pp 3972–3979

**Publication Date (Web):** April 19, 2013 (Article)

**DOI:** 10.1021/jp400195f

 Section:

Air Pollution and Industrial Hygiene

***Characterization of Combustion-Generated Carbonaceous Nanoparticles by Size-Dependent Ultraviolet Laser Photoionization***

Mario Commodo, Lee Anne Sgro, Patrizia Minutolo, and Andrea D'Anna

pp 3980–3989

**Publication Date (Web):** April 15, 2013 (Article)

**DOI:** 10.1021/jp401061d

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

***The Influence of Molecular Structure and Aerosol Phase on the Heterogeneous Oxidation of Normal and Branched Alkanes by OH***

Christopher R. Ruehl, Theodora Nah, Gabriel Isaacman, David R. Worton, Arthur W. H. Chan, Katheryn R. Kolesar, Christopher D. Cappa, Allen H. Goldstein, and Kevin R. Wilson

pp 3990–4000

**Publication Date (Web):** April 23, 2013 (Article)

**DOI:** 10.1021/jp401888q

 Section:

Physical Organic Chemistry

***Molecular Structure, Quantum Chemistry, and General Theory Prediction of Clathrate Structure Type and Guest Position by Molecular Mechanics***

Everly B. Fleischer and Kenneth C. Janda

pp 4001–4010

**Publication Date (Web):** April 19, 2013 (Article)

**DOI:** 10.1021/jp311351j

 Section:

General Physical Chemistry

## ***The Nature of the Interaction of Dimethylselenide with IIIA Group Element Compounds***

Timur I. Madzhidov and Galina A. Chmutova

pp 4011–4024

**Publication Date (Web):** April 16, 2013 (Article)

**DOI:** 10.1021/jp312383f

 Section:

General Physical Chemistry

## ***Interference Energy in C–H and C–C Bonds of Saturated Hydrocarbons: Dependence on the Type of Chain and Relationship to Bond Dissociation Energy***

Francisco Senna Vieira, Felipe Fantuzzi, Thiago Messias Cardozo, and Marco Antonio Chaer Nascimento

pp 4025–4034

**Publication Date (Web):** April 10, 2013 (Article)

**DOI:** 10.1021/jp4005746

 Section:

Physical Organic Chemistry

## ***High-Resolution Infrared and Electron-Diffraction Studies of Trimethylenecyclopropane ([3]-Radialene)***

Corey Wright, Joshua Holmes, Joseph W. Nibler, Kenneth Hedberg, James D. White, Lise Hedberg, Alfons Weber, and Thomas A. Blake

pp 4035–4043

**Publication Date (Web):** April 17, 2013 (Article)

**DOI:** 10.1021/jp401813t

 Section:

Physical Organic Chemistry

## ***Accurate Study of the Two Lowest Singlet States of HN<sub>3</sub>: Stationary Structures and Energetics at the MRCI Complete Basis Set Limit***

B. R. L. Galvão and A. J. C. Varandas

pp 4044–4050

**Publication Date (Web):** April 15, 2013 (Article)

**DOI:** 10.1021/jp402090s

 Section:

General Physical Chemistry

***Crystal Structures, UV Spectra of Solid Iodide Anionic Water Clusters  $I^-(H_2O)_{1-4}$ , and Electrochemical Reaction of  $I^-(H_2O)_{1-4} \rightarrow I \cdot + e^-(H_2O)_{1-4}$***

Yanxuan Qiu, Meng Yang, Wenbin Chen, Yuzhi Su, Zhenjie Ouyang, Hua Yan, Feixian Gao, and Wen Dong

pp 4051–4056

**Publication Date (Web):** April 24, 2013 (Article)

**DOI:** 10.1021/jp402279k

 Section:

Crystallography and Liquid Crystals

***A Density Functional Theory Investigation into the Binding of the Antioxidants Ergothioneine and Ovothiol to Copper.***

Phil De Luna, Eric A. C. Bushnell, and James W. Gauld

pp 4057–4065

**Publication Date (Web):** April 16, 2013 (Article)

**DOI:** 10.1021/jp402514w

 Section:

Toxicology

***Comments***

***Comment on “Assessment and Validation of Density Functional Approximations for Iron Carbide and Iron Carbide Cation”***

Ilie Fishtik

pp 4066–4071

**Publication Date (Web):** April 1, 2013 (Comment)

**DOI:** 10.1021/jp402263s

 Section:

Thermodynamics, Thermochemistry, and Thermal Properties