

ПН
780/ра

AUGUST 8, 2013

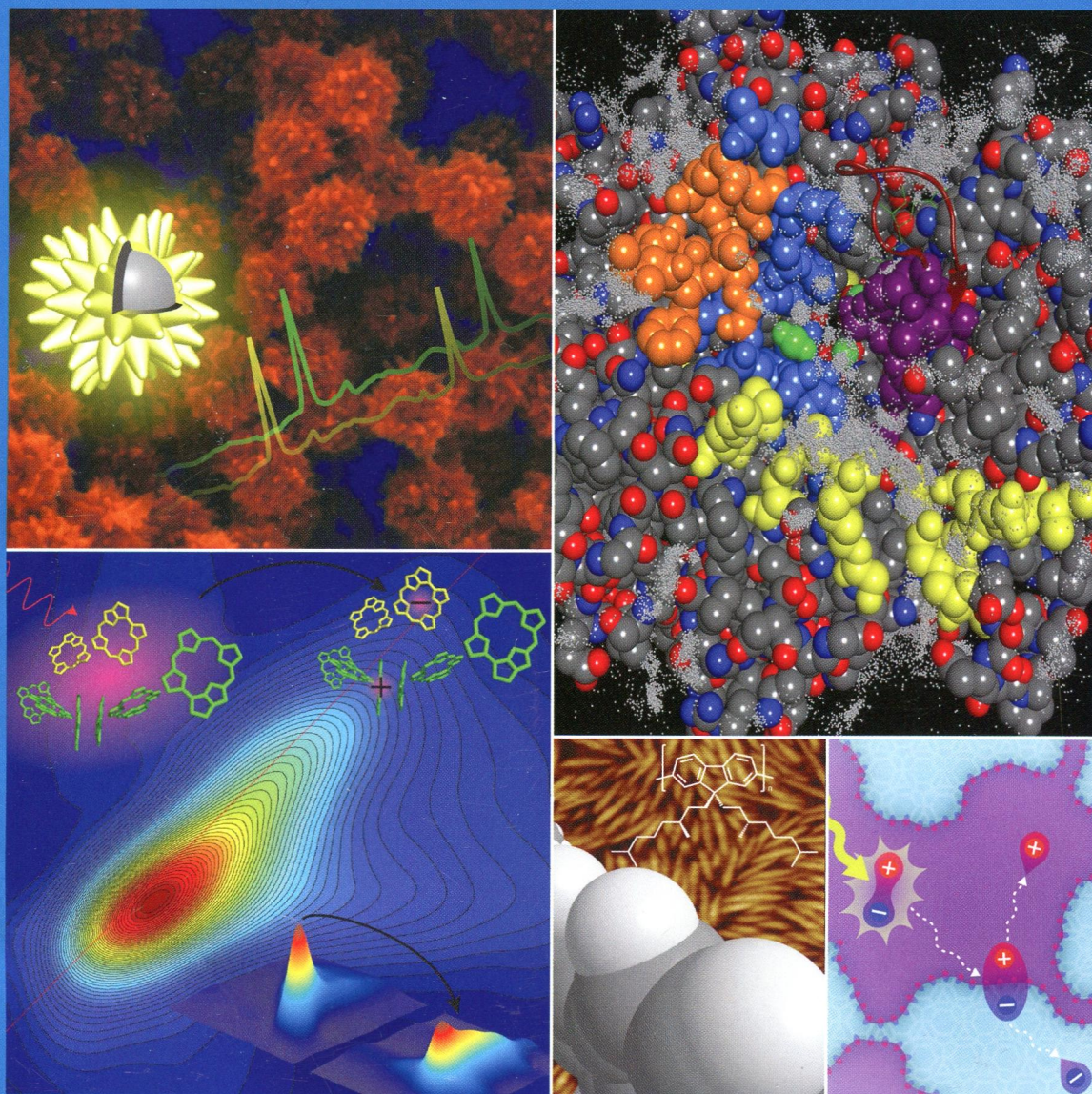
VOLUME 117

NUMBER 31

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

August 8, 2013

Volume 117, Issue 31

Pages 6717-6904

Kinetics and Dynamics

Unimolecular Isomerization of CH₂FCD₂Cl via the Interchange of Cl and F Atoms: Assignment of the Threshold Energy to the 1,2-Dyotropic Rearrangement

Mary K. Tucker, Samuel M. Rossabi, Corey E. McClintock, George L. Heard, D. W. Setser, and Bert E. Holmes

pp 6717–6723

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

DOI: 10.1021/jp4032767

 Section:

Physical Organic Chemistry

Dehydration of Isobutanol and the Elimination of Water from Fuel Alcohols

Claudette M. Rosado-Reyes and Wing Tsang, Ionut M. Alecu, Shamel S. Merchant, and William H. Green

pp 6724–6736

Publication Date (Web): June 27, 2013 (Article)

DOI: 10.1021/jp4045513

 Section:

Physical Organic Chemistry

Small Reorganization Energies of Photoinduced Electron Transfer between Spherical Fullerenes

Yuki Kawashima, Kei Ohkubo, and Shunichi Fukuzumi

pp 6737–6743

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

DOI: 10.1021/jp4047165

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Multichannel RRKM-TST and Direct-Dynamics CVT Study of the Reaction of Hydrogen Sulfide with Ozone

S. Hosein Mousavipour, Maryam Mortazavi, and Omid Hematti

pp 6744–6756

Publication Date (Web): July 9, 2013 (Article)

DOI: 10.1021/jp404738d

 Section:

Mineralogical and Geological Chemistry

Hydrogen Abstraction from n-Butyl Formate by H[•] and HO₂[•]

Wassja A. Kopp, Raymond T. Langer, Malte Döntgen, and Kai Leonhard

pp 6757–6770

Publication Date (Web): July 3, 2013 (Article)

DOI: 10.1021/jp4063675

 Section:

Physical Organic Chemistry

***Spectroscopy, Photochemistry, and Excited States
Hydrogen Bond Donors Accelerate Vibrational Cooling of Hot Purine
Derivatives in Heavy Water***

Yuyuan Zhang, Jinqun Chen, and Bern Kohler

pp 6771–6780

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

DOI: 10.1021/jp4040002

 Section:

Physical Organic Chemistry

Infrared Investigations of 4-Hydroxycyanobenzene Single Crystals

E. Capria, L. Benevoli, A. Perucchi, B. Fraboni, M. Tessarolo, Stefano Lupi, and A. Fraleoni-Morgera

pp 6781–6788

Publication Date (Web): July 5, 2013 (Article)

DOI: 10.1021/jp405058h

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Proton Transfer in Nucleobases is Mediated by Water

Kirill Khistyayev, Amir Golan, Ksenia B. Bravaya, Natalie Orms, Anna I. Krylov, and Musahid Ahmed

pp 6789–6797

Publication Date (Web): June 27, 2013 (Article)

DOI: 10.1021/jp406029p

 Section:

General Biochemistry

Symmetry Breaking and Hole Localization in Multiple Core Electron Ionization

V. Carravetta and H. Ågren

pp 6798–6802

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

DOI: 10.1021/jp406602y

 Section:

General Physical Chemistry

***Molecular Structure, Quantum Chemistry, and General Theory
Structure and Properties of Small Aurocarbons: A Selective Study***

C. N. Ramachandran and Fedor Y. Naumkin

pp 6803–6808

Publication Date (Web): July 29, 2013 (Article)

DOI: 10.1021/jp4035858

 Section:

General Physical Chemistry

***Barrierless Inter and Intramolecular Proton Transfer; A DFT Study of
Tautomerism in Microsolvated and Protonated Systems***

Hossein Tavakol

pp 6809–6816

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

DOI: 10.1021/jp4038232

 Section:

Physical Organic Chemistry

***Formation of H₂O₂ on Au₂₀ and Au₁₉Pd Clusters: Understanding the Structure
Effect on the Atomic Level***

Anna V. Beletskaya, Daria A. Pichugina, Alexander F. Shestakov, and Nikolay E. Kuz'menko

pp 6817–6826

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

DOI: 10.1021/jp4040437

 Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Application of Time-Dependent Density Functional Theory and Optical Spectroscopy toward the Rational Design of Novel 3,4,5-Triaryl-1-R-1,2-diphospholes

Elena E. Zvereva, Stefan Grimme, Sergey A. Katsyuba, Timur I. Burganov, Almaz A. Zagidullin, Vasily A. Milyukov, and Oleg G. Sinyashin

pp 6827–6834

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

DOI: 10.1021/jp4043914

 Section:

Organometallic and Organometalloidal Compounds

Accurate Prediction of Enthalpies of Formation of Organic Azides by Combining G4 Theory Calculations with an Isodesmic Reaction Scheme

Olga V. Dorofeeva, Oxana N. Ryzhova, and Marina A. Suntsova

pp 6835–6845

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

DOI: 10.1021/jp404484q

 Section:

Thermodynamics, Thermochemistry, and Thermal Properties

Quantum Chemical Investigation on Indole: Vibrational Force Field and Theoretical Determination of Its Aqueous pK_a Value

Andrea Pietropolli Charmet, Giuseppe Quartarone, Lucio Ronchin, Claudio Tortato, and Andrea Vavasori

pp 6846–6858

Publication Date (Web): July 30, 2013 (Article)

DOI: 10.1021/jp4049692

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

On the Origins of Large Interaction-Induced First Hyperpolarizabilities in Hydrogen-Bonded π -Electronic Complexes

Robert W. Góra and Bartosz Błasiak

pp 6859–6866

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

DOI: 10.1021/jp405144f

 Section:

Physical Organic Chemistry

Structure, Thermochemical Properties, and Growth Sequence of Aluminum-Doped Silicon Clusters Si_nAl_m ($n = 1-11$, $m = 1-2$) and Their Anions

Nguyen Minh Tam, Truong Ba Tai, Vu Thi Ngan, and Minh Tho Nguyen

pp 6867–6882

Publication Date (Web): July 9, 2013 (Article)

DOI: 10.1021/jp405280c

 Section:

General Physical Chemistry

Theoretical Study on the Water-Assisted Reaction of NCO with HCHO

Benni Du and Weichao Zhang

pp 6883–6892

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

DOI: 10.1021/jp405687c

 Section:

Physical Organic Chemistry

Characterizing Complexes with Pnicogen Bonds Involving sp^2 Hybridized Phosphorus Atoms: $(H_2C=PX)_2$ with $X = F, Cl, OH, CN, NC, CCH, H, CH_3$, and BH_2

Janet E. Del Bene, Ibon Alkorta, and José Elguero

pp 6893–6903

Publication Date (Web): July 30, 2013 (Article)

DOI: 10.1021/jp4063109

 Section:

Organometallic and Organometalloidal Compounds