

August 1, 2013

Volume 117, Issue 30

Pages 6389-6716

Kinetics and Dynamics

Dissociation of Proton Bound Ketone Dimers in Asymmetric Electric Fields with Differential Mobility Spectrometry and in Uniform Electric Fields with Linear Ion Mobility Spectrometry

Xinxia An, Gary A. Eiceman, Riikka-Marjaana Räsänen, Jaime E. Rodriguez, and John A. Stone

pp 6389–6401

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

DOI: 10.1021/jp401640t



Section:

Physical Organic Chemistry

A Microreactor and Imaging Platform for Studying Chemical Oscillators

Dameng Guo, Yuefang Li, and Bo Zheng

pp 6402–6408

Publication Date (Web): July 2, 2013 (Article)

DOI: 10.1021/jp4030014



Section:

Biochemical Methods

Quasiclassical Trajectory Studies of the $O(^3P) + CX_4(v_k = 0, 1) \rightarrow OX(v) + CX_3(n_1n_2n_3n_4)$ [$X = H$ and D] Reactions on an Ab Initio Potential Energy Surface

Gábor Czakó, Rui Liu, Minghui Yang, Joel M. Bowman, and Hua Guo

pp 6409–6420

Publication Date (Web): June 28, 2013 (Article)

DOI: 10.1021/jp4038107



Section:

Physical Organic Chemistry

Structure, Kinetics, and Thermodynamics of the Aqueous Uranyl(VI) Cation

Sebastien Kerisit and Chongxuan Liu

pp 6421–6432

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

DOI: 10.1021/jp404594p



Section:

General Physical Chemistry

Evolution of Structure–Reactivity Correlations for the Hydrogen Abstraction Reaction by Hydroxyl Radical and Comparison with That by Chlorine Atom

Marvin L. Poutsma

pp 6433–6449

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

DOI: 10.1021/jp404749z



Section:

Physical Organic Chemistry

Product Branching Fractions of the CH + Propene Reaction from Synchrotron Photoionization Mass Spectrometry

Adam J. Trevitt, Matthew B. Prendergast, Fabien Goulay, John D. Savee, David L. Osborn, Craig A. Taatjes, and Stephen R. Leone

pp 6450–6457

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

DOI: 10.1021/jp404965k



Section:

Physical Organic Chemistry

Rate Rules, Branching Ratios, and Pressure Dependence of the HO₂ + Olefin Addition Channels

Stephanie M. Villano, Hans-Heinrich Carstensen, and Anthony M. Dean

pp 6458–6473

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

DOI: 10.1021/jp405262r



Section:

Physical Organic Chemistry

Spectroscopy, Photochemistry, and Excited States

Vibrational Spectroscopy of Picolinamide and Water: From Dimers to Condensed Phase

Vladimir Jovanović, Yasunori Miyazaki, Takayuki Ebata, and Milena Petković

pp 6474–6482

Publication Date (Web): July 2, 2013 (Article)

DOI: 10.1021/jp402033c



Section:

Physical Organic Chemistry

Light-Induced Magnetostructural Anomalies in a Polymer Chain Complex of Cu(hfac)₂ with tert-Butylpyrazolynitroxides

Irina Yu. Drozdov, Svyatoslav E. Tolstikov, Evgeny V. Tretyakov, Sergey L. Veber, Victor I. Ovcharenko, Renad Z. Sagdeev, Elena G. Bagryanskaya, and Matvey V. Fedin

pp 6483–6488

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

DOI: 10.1021/jp403977n



Section:

Magnetic Phenomena

Experimental and Computational Exploration of Ground and Excited State Properties of Highly Strained Ruthenium Terpyridine Complexes

Paul J. Vallett and Niels H. Damrauer

pp 6489–6507

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

DOI: 10.1021/jp404248z



Section:

Inorganic Chemicals and Reactions

Microwave and Infrared Spectra, Adjusted r_0 Structural Parameters, Conformational Stabilities, Vibrational Assignments, and Theoretical Calculations of Cyclobutylcarboxylic Acid Chloride

Joshua J. Klaassen, Ikhlas D. Darkhalil, Bhushan S. Deodhar, Todor K. Gounev, Ranil M. Gurusinghe, Michael J. Tubergen, Peter Groner, and James R. Durig

pp 6508–6524

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

DOI: 10.1021/jp404510n



Section:

Physical Organic Chemistry

Matrix Infrared Spectra and Density Functional Calculations for New iso-Halomethanes: $\text{CHCl}_2\text{-Cl}$, CHFCl-Cl , $\text{CFCl}_2\text{-Cl}$, $\text{CHBr}_2\text{-Br}$, and $\text{CBr}_3\text{-Br}$ in Solid Argon

Han-Gook Cho and Lester Andrews

pp 6525–6535

Publication Date (Web): June 26, 2013 (Article)

DOI: 10.1021/jp4046534



Section:

Physical Organic Chemistry

Spin State Diagrams of $3d^n$ Cations in Tetragonally Distorted Octahedral Sites

Michael Pollet and Alla Artemenko

pp 6536–6547

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

DOI: 10.1021/jp4047787



Section:

General Physical Chemistry

Deciphering the Photophysical Role of Conjugated Diyne in Butadiynyl Fluorophores: Synthesis, Photophysical and Theoretical Study

Avik Kumar Pati, Monalisa Mohapatra, Pokhraj Ghosh, Santosh J. Gharpure, and Ashok K. Mishra

pp 6548–6560

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

DOI: 10.1021/jp404809g



Section:

Physical Organic Chemistry

Insight into Magnesium Coordination Environments in Benzoate and Salicylate Complexes through ^{25}Mg Solid-State NMR Spectroscopy

Kevin M. N. Burgess, Yang Xu, Matthew C. Leclerc, and David L. Bryce

pp 6561–6570

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

DOI: 10.1021/jp405145b



Section:

Magnetic Phenomena

Hydrated Alkali Metal Ions: Spectroscopic Evidence for Clathrates

Richard J. Cooper, Terrence M. Chang, and Evan R. Williams

pp 6571–6579

Publication Date (Web): June 28, 2013 (Article)

DOI: 10.1021/jp405147h



Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Excited-State Dynamics in Nitro-Naphthalene Derivatives: Intersystem Crossing to the Triplet Manifold in Hundreds of Femtoseconds

R. Aaron Vogt, Christian Reichardt, and Carlos E. Crespo-Hernández

pp 6580–6588

Publication Date (Web): June 26, 2013 (Article)

DOI: 10.1021/jp405656n



Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

***Environmental and Atmospheric Chemistry, Aerosol Processes, Geochemistry, and Astrochemistry
Size-Resolved Sea Spray Aerosol Particles Studied by Vibrational Sum Frequency Generation***

Carlena J. Ebben, Andrew P. Ault, Matthew J. Ruppel, Olivia S. Ryder, Timothy H. Bertram, Vicki H. Grassian, Kimberly A. Prather, and Franz M. Geiger

pp 6589–6601

Publication Date (Web): July 2, 2013 (Article)

DOI: 10.1021/jp401957k



Section:

Air Pollution and Industrial Hygiene

Modeling the Interaction of Nanoparticles with Mineral Surfaces: Adsorbed C₆₀ on Pyrophyllite

Runliang Zhu, Marco Molinari, Thomas V. Shapley, and Stephen C. Parker

pp 6602–6611

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

DOI: 10.1021/jp402835v

 Section:

Surface Chemistry and Colloids

Using Singlet Molecular Oxygen to Probe the Solute and Temperature Dependence of Liquid-Like Regions in/on Ice

Jonathan P. Bower and Cort Anastasio

pp 6612–6621

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

DOI: 10.1021/jp404071y

 Section:

Mineralogical and Geological Chemistry

***Molecular Structure, Quantum Chemistry, and General Theory
Alternative Approach to Calculate Two-Center Overlap Matrix through
Deformed Exponential Function***

Fernando C. Rangel, Arthur A. Mamiya, Heibbe C. B. de Oliveira, Fernando M. C. Vieira, and Kleber C. Mundim

pp 6622–6628

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

DOI: 10.1021/jp401631a

 Section:

General Physical Chemistry

Theoretical Study on the Gas Phase Reaction of Allyl Alcohol with Hydroxyl Radical

Yunju Zhang, Kai Chao, Jingyu Sun, Zhongmin Su, Xiumei Pan, Jingping Zhang, and Rongshun Wang

pp 6629–6640

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

DOI: 10.1021/jp402142b

 Section:

Physical Organic Chemistry

Cooperative Roles of Charge Transfer and Dispersion Terms in Hydrogen-Bonded Networks of (H₂O)_n, n = 6, 11, and 16

Suehiro Iwata, Pradipta Bandyopadhyay, and Sotiris S. Xantheas

pp 6641–6651

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

DOI: 10.1021/jp403837z

 Section:

General Physical Chemistry

Sulfur-Containing Flavors: Gas Phase Structures of Dihydro-2-methyl-3-thiophenone

Halima Mouhib, Vinh Van, and Wolfgang Stahl

pp 6652–6656

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

DOI: 10.1021/jp4041748

 Section:

Physical Organic Chemistry

Theoretical Studies of Potential Energy Surface and Bound States of the Strongly Bound He($1S$)–BeO ($1\Sigma^+$) Complex

Michał Hapka, Jacek Kłos, Tatiana Korona, and Grzegorz Chałasiński

pp 6657–6663

Publication Date (Web): June 24, 2013 (Article)

DOI: 10.1021/jp404467b

 Section:

General Physical Chemistry

Is There a Simple Way to Reliable Simulations of Infrared Spectra of Organic Compounds?

Sergey A. Katsyuba, Elena E. Zvereva, and Timur I. Burganov

pp 6664–6670

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

DOI: 10.1021/jp404574m

 Section:

Physical Organic Chemistry

Decoding Nitric Oxide Release Rates of Amine-Based Diazeniumdiolates

Yan-Ni Wang, Jack Collins, Ryan J. Holland, Larry K. Keefer, and Joseph Ivanic

pp 6671–6677

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

DOI: 10.1021/jp404589p

 Section:

Pharmaceuticals

Effects of the Cage Unit Size and Number of Cage Units As Well As Bridge Unit on the Second Order Nonlinear Optical Response in Multicage Electride Molecules

Zhen-Bo Liu, Yan-Chun Li, Jia-Jun Wang, Yang Bai, Di Wu, and Zhi-Ru Li

pp 6678–6686

Publication Date (Web): July 2, 2013 (Article)

DOI: 10.1021/jp404671w

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Influence of the Substituents on the CH... π Interaction: Benzene–Methane Complex

S. Karthikeyan, V. Ramanathan, and Brijesh Kumar Mishra

pp 6687–6694

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

DOI: 10.1021/jp404972f

 Section:

Physical Organic Chemistry

Influence of Nucleation Precursors on the Reaction Kinetics of Methanol with the OH Radical

Jonas Elm, Merete Bilde, and Kurt V. Mikkelsen

pp 6695–6701

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

DOI: 10.1021/jp4051269

 Section:

Physical Organic Chemistry

Combined Spectroelectrochemical and Theoretical Study of Electron-Rich Dendritic 2,5-Diaminothiophene Derivatives: N,N,N',N'-Tetrakis-(4-diphenylamino-phenyl)-thiophene-2,5-diamine

Vladimír Lukeš, Peter Rapta, Kinga Haubner, Marco Rosenkranz, Horst Hartmann, and Lothar Dunsch

pp 6702–6711

Publication Date (Web): July 2, 2013 (Article)

DOI: 10.1021/jp405212e



Section:

Physical Organic Chemistry

Cage versus Prism: Electronic Energies of the Water Hexamer

Jonathan J. Foley, IV and David A. Mazziotti

pp 6712–6716

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

DOI: 10.1021/jp405739d



Section:

General Physical Chemistry