THE JOURNAL OF PHYSICAL CHEMISTRY A



Larger Cover

February 21, 2013

Volume 117, Issue 7

Pages 1371-1684

Kinetics and Dynamics

Shock Tube and Chemical Kinetic Modeling Study of the Oxidation of 2,5-Dimethylfuran

Baptiste Sirjean, René Fournet, Pierre-Alexandre Glaude, Frédérique Battin-Leclerc, Weijing Wang, and Matthew A. Oehlschlaeger

pp 1371-1392

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

DOI: 10.1021/jp308901q

Section:

Physical Organic Chemistry

Coulomb Explosion of Dichloroethene Geometric Isomers at 1 PW cm⁻²

Tomoyuki Yatsuhashi, Nobuaki Nakashima, and Juri Azuma

pp 1393-1399

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

DOI: 10.1021/jp310361x

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Active Role of Proton in Excited State Intramolecular Proton Transfer Reaction

Junghwa Lee, Chul Hoon Kim, and Taiha Joo

pp 1400-1405

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

DOI: 10.1021/jp311884b

Section:

Physical Organic Chemistry

Accurate Study on the Quantum Dynamics of the He + HeH⁺ ($X^1\Sigma^+$) Reaction on A New ab Initio Potential Energy Surface for the Lowest $1^1A'$ Electronic Singlet State

Wenwu Xu and Peiyu Zhang

pp 1406-1412

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

DOI: 10.1021/jp312084r

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Spectroscopy, Photochemistry, and Excited States

Optical and Time-Resolved Electron Paramagnetic Resonance Studies of the Excited States of a UV-B Absorber (4-Methylbenzylidene)camphor

Azusa Kikuchi, Kenji Shibata, Ryo Kumasaka, and Mikio Yagi

pp 1413-1419

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

DOI: 10.1021/jp3071772

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Analysis of Low-Lying Gerade Rydberg States of Acetylene Using Two-Photon Resonance Fluorescence Excitation Spectroscopy

Kazuhide Tsuji, Kentaro Misawa, Junichi Awamura, Akio Kawai, and Kazuhiko Shibuya

pp 1420-1427

Publication Date (Web): January 25, 2013 (Article)

DOI: 10.1021/jp308406r

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Excimer of 9-Aminoacridine Hydrochloride Hydrate in Confined Medium: An Integrated Experimental and Theoretical Study

Piyali Mitra, Brotati Chakraborty, Dhananjay Bhattacharyya, and Samita Basu

pp 1428-1438

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

DOI: 10.1021/jp3103639

Section:

Physical Organic Chemistry

Monotrimethylene-Bridged Bis-p-phenylenediamine Radical Cations and Dications: Spin States, Conformations, and Dynamics

Michal Zalibera, Almaz S. Jalilov, Stefan Stoll, Ilia A. Guzei, Georg Gescheidt, and Stephen F. Nelsen

pp 1439-1448

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

DOI: 10.1021/jp3104358

Section:

Physical Organic Chemistry

Energetics and Dynamics of the Low-Lying Electronic States of Constrained Polyenes: Implications for Infinite Polyenes

Ronald L. Christensen, Miriam M. Enriquez, Nicole L. Wagner, Alexandra Y. Peacock-Villada, Corina Scriban, Richard R. Schrock, Tomáš Polívka, Harry A. Frank, and Robert R. Birge

pp 1449-1465

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

DOI: 10.1021/jp310592s

Section:

Physical Organic Chemistry

Determination of Very Rapid Molecular Rotation by Using the Central Electron Paramagnetic Resonance Line

Mark R. Kurban

pp 1466-1473

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

DOI: 10.1021/jp310890h



Physical Organic Chemistry

Mechanism for Different Fluorescence Response of a Coumarin-Amide-Dipicolylamine Linkage to Zn(II) and Cd(II) in Water

Shigehiro Sumiya, Yasuhiro Shiraishi, and Takayuki Hirai

pp 1474-1482

Publication Date (Web): January 23, 2013 (Article)

DOI: 10.1021/jp3111315



Optical, Electron, and Mass Spectroscopy and Other Related Properties

Influence of Intense THz Radiation on Spin State of Photoswitchable Compound Cu(hfac)₂L^{pr}

Sergey L. Veber, Matvey V. Fedin, Ksenia Yu. Maryunina, Kirill N. Boldyrev, Mikhail A. Sheglov, Vitaly V. Kubarev, Oleg A. Shevchenko, Nikolay A. Vinokurov, Gennady N. Kulipanov, Renad Z. Sagdeev, Victor I. Ovcharenko, and Elena G. Bagryanskaya

pp 1483-1491

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

DOI: 10.1021/jp311404t

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Visible Light-Driven Chemistry of Oxalic Acid in Solid Argon, Probed by Raman Spectroscopy

Adriana Olbert-Majkut, Jussi Ahokas, Mika Pettersson, and Jan Lundell

pp 1492-1502

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

DOI: 10.1021/jp311749z

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Electronegativity, Charge Transfer, Crystal Field Strength, and the Point Charge Model Revisited

Peter A. Tanner and Lixin Ning

pp 1503-1507

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

DOI: 10.1021/jp3117566

Section:

General Physical Chemistry

Infrared Spectra of NgBeS (Ng = Ne, Ar, Kr, Xe) and BeS_2 in Noble-Gas Matrices

Qiang Wang and Xuefeng Wang

pp 1508-1513

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

DOI: 10.1021/jp311901a

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Carbonyl Bonding on Oxophilic Metal Centers: Infrared Photodissociation Spectroscopy of Mononuclear and Dinuclear Titanium Carbonyl Cation Complexes

Xiaojie Zhou, Jieming Cui, Zhen Hua Li, Guanjun Wang, Zhipan Liu, and Mingfei Zhou

pp 1514-1521

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

DOI: 10.1021/jp3120429

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Ground State Proton Transfer in Phenol-(NH₃)_n ($n \le 11$) Clusters Studied by Mid-IR Spectroscopy in 3–10 µm Range

Mitsuhiko Miyazaki, Ayako Kawanishi, Iben Nielsen, Ivan Alata, Shun-ichi Ishiuchi, Claude Dedonder, Christophe Jouvet, and Masaaki Fujii

pp 1522-1530

Publication Date (Web): January 25, 2013 (Article)

DOI: 10.1021/jp312074m



Physical Organic Chemistry

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

Theoretical Investigation on Monomer and Solvent Selection for Molecular Imprinting of Nitrocompounds

Julia Saloni, Kiara Walker, and Glake Hill, Jr

pp 1531-1534

Publication Date (Web): January 23, 2013 (Article)

DOI: 10.1021/jp2124839

Section:

Physical Organic Chemistry

Molecular Structure, Quantum Chemistry, and General Theory

Transferability of Atomic Multipoles in Amino Acids and Peptides for Various Density Partitions

Magdalena Woińska and Paulina M. Dominiak

pp 1535-1547

Publication Date (Web): September 26, 2011 (Article)

DOI: 10.1021/jp204010v

Section:

Physical Organic Chemistry

Quantum-Chemical Studies on the Favored and Rare Tautomers of Neutral and Redox Adenine

Ewa D. Raczyńska, Mariusz Makowski, Katarzyna Zientara-Rytter, Katarzyna Kolczyńska, Tomasz M. Stępniewski, and Małgorzata Hallmann

pp 1548-1559

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

DOI: 10.1021/jp3081029

Section:

Physical Organic Chemistry

Impact of Geometry Optimization on Base-Base Stacking Interaction Energies in the Canonical A- and B-Forms of DNA

Ashley Ringer McDonald, Elizabeth J. Denning, and Alexander D. MacKerell, Jr.

pp 1560-1568

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

DOI: 10.1021/jp308364d

Section:

Biochemical Methods

Ab Initio Calculations of Thermochemical Properties of Methanol Clusters

Muhammad Umer and Kai Leonhard

pp 1569-1582

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

DOI: 10.1021/jp308908j

Section:

Thermodynamics, Thermochemistry, and Thermal Properties

Structures, Stabilization Energies, and Binding Energies of Quinoxaline···(H_2O)_n, Quinoxaline Dimer, and Quinoxaline····Cu Complexes: A Theoretical Study

Mwadham M. Kabanda and Eno E. Ebenso

pp 1583-1595

Publication Date (Web): January 23, 2013 (Article)

DOI: 10.1021/jp309356b

Section:

Physical Organic Chemistry

Reactivity Patterns of Imidazole, Oxazole, and Thiazole As Reflected by the Polarization Justified Fukui Functions

Wiktor Beker, Paweł Szarek, Ludwik Komorowski, and Józef Lipiński

pp 1596-1600

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

DOI: 10.1021/jp309390j

Section:

Physical Organic Chemistry

Interaction Between Group IIb Divalent Transition-Metal Cations and 3-Mercaptopropionic Acid: A Computational and Topological Perspective

Sabyasachi Bagchi, Debasish Mandal, Deepanwita Ghosh, and Abhijit K. Das

pp 1601-1613

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

DOI: 10.1021/jp309792v

Section:

General Physical Chemistry

Planar to 3D Transition in the B₆H_v Anions

J. K. Olson and A. I. Boldyrev

pp 1614-1620

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

DOI: 10.1021/jp310162v

Section:

General Physical Chemistry

Pseudo Jahn-Teller Effect and Natural Bond Orbital Analysis of Structural Properties of Tetrahydridodimetallenes M_2H_4 , (M = Si, Ge, and Sn)

Davood Nori-Shargh, Seiedeh Negar Mousavi, and James E. Boggs

pp 1621-1631

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

DOI: 10.1021/jp310389q

Section:

General Physical Chemistry

Bonded Radii and the Contraction of the Electron Density of the Oxygen Atom by Bonded Interactions

Gerald V. Gibbs, Nancy L. Ross, David F. Cox, Kevin M. Rosso, Bo B. Iversen, and Mark A. Spackman

pp 1632-1640

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

DOI: 10.1021/jp310462g



General Physical Chemistry

Anomeric Effect in Halogenated Methanols: A Quantum Theory of Atoms in Molecules Study

David Ferro-Costas, Antonio Vila, and Ricardo A. Mosquera

pp 1641-1650

Publication Date (Web): January 25, 2013 (Article)

DOI: 10.1021/jp310534x

Section:

Physical Organic Chemistry

Tautomerism and Possible Polymorphism in Solid Hydroxypyridines and Pyridones Studied by ¹⁴N NQR

Janez Seliger and Veselko Žagar

pp 1651-1658

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

DOI: 10.1021/jp3117038

Section:

Physical Organic Chemistry

Conformational Analysis and Intramolecular Interactions in Aminofluorobenzoic Acids

Josué M. Silla, Rodrigo A. Cormanich, Roberto Rittner, and Matheus P. Freitas

pp 1659-1664

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

DOI: 10.1021/jp311791g

Section:

Physical Organic Chemistry

Luminescence of BODIPY and Dipyrrin: An MCSCF Comparison of Excited States

Muhammed Buyuktemiz, Selin Duman, and Yavuz Dede

pp 1665-1669

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

DOI: 10.1021/jp311939s



Optical, Electron, and Mass Spectroscopy and Other Related Properties

A New Generation of B_nN_n Rings as a Supplement to Boron Nitride Tubes and Cages

Majid Monajjemi and James E. Boggs

pp 1670-1684

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

DOI: 10.1021/jp312073q

