THE JOURNAL OF PHYSICAL CHEMISTRY A



Larger Cover

April 4, 2013

Volume 117, Issue 13

Pages 2665-2890

REVIEW ARTICLE

Excitons in Conjugated Polymers: A Tale of Two Particles

William Barford

pp 2665-2671

Publication Date (Web): February 21, 2013 (Review Article)

DOI: 10.1021/jp310110r

Section:

Physical Properties of Synthetic High Polymers

KINETICS AND DYNAMICS

Structures and Electronic Properties of the SiAu_n (n = 17-20) Clusters

Huai-Wen Yang, Wen-Cai Lu, Li-Zhen Zhao, Wei Qin, Wen-Hua Yang, and Xu-Yan Xue

pp 2672-2677

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

DOI: 10.1021/jp3004807

Section:

General Physical Chemistry

Ab Initio Thermal Rate Calculations of HO + HO = O(³P) + H₂O Reaction and Isotopologues

Thanh Lam Nguyen and John F. Stanton

pp 2678-2686

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

DOI: 10.1021/jp312246q

Section:

Physical Organic Chemistry

Solvent Effects on Intramolecular Charge Transfer Dynamics in a Fullerene Derivative

Craig T. Chapman, Wenkel Liang, and Xiaosong Li

pp 2687-2691

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

DOI: 10.1021/jp312525j

Section:

General Physical Chemistry

Large Scale Computational Chemistry Modeling of the Oxidation of Highly Oriented Pyrolytic Graphite

Savio Poovathingal, Thomas E. Schwartzentruber, Sriram Goverapet Srinivasan, and Adri C. T. van Duin

pp 2692-2703

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

DOI: 10.1021/jp3125999

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Oxyhalogen-Sulfur Chemistry: Kinetics and Mechanism of Oxidation of Captopril by Acidified Bromate and Aqueous Bromine

G. P. Kapungu and G. Rukweza , Thai Tran, Wilbes Mbiya, Risikat Adigun, Patrick Ndungu, Bice Martincigh, and Reuben H. Simoyi

pp 2704-2717

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

DOI: 10.1021/jp312672w

Section:

Physical Organic Chemistry

Dissociation of Propyl Radicals and Other Reactions on a C₃H₇ Potential

James A. Miller and Stephen J. Klippenstein

pp 2718-2727

Publication Date (Web): March 6, 2013 (Article)

DOI: 10.1021/jp312712p

Section:

Physical Organic Chemistry

Thermal Intramolecular Transformation of Key Intermediates in the Photooxidation of *para*-Allyl-Substituted Phenyl Azide

Ekaterina M. Chainikova, Evgeniy Yu. Pankratyev, Aigul N. Teregulova, Rail R. Gataullin, and Rustam L. Safiullin

pp 2728-2737

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

DOI: 10.1021/jp401038g

Section:

Physical Organic Chemistry

SPECTROSCOPY, PHOTOCHEMISTRY, AND EXCITED STATES

White Light Generation by Carbonyl Based Indole Derivatives Due to Proton Transfer: An Efficient Fluorescence Sensor

Nidhi Singla, Venkata Srinu Bhadram, Chandrabhas Narayana, and Papia Chowdhury

pp 2738-2752

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

DOI: 10.1021/jp310331n

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Comparing Femtosecond Multiphoton Dissociative Ionization of Tetrathiafulvene with Imaging Photoelectron Photoion Coincidence Spectroscopy

Paul M. Mayer, David Staedter, Valerie Blanchet, Patrick Hemberger, and Andras Bodi

pp 2753-2759

Publication Date (Web): March 6, 2013 (Article)

DOI: 10.1021/jp311066y

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Solvent Effects in Calculated Vibrational Raman Optical Activity Spectra of α -Helices

Sandra Luber

pp 2760-2770

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

DOI: 10.1021/jp400105u

Section:

General Biochemistry

What Factors Affect the ⁵D₀ Energy of Eu³+? An Investigation of Nephelauxetic Effects

Peter A. Tanner, Yau Yuen Yeung, and Lixin Ning

pp 2771-2781

Publication Date (Web): March 7, 2013 (Article)

DOI: 10.1021/jp400247r

Section:

General Physical Chemistry

Synthesis and Optical Properties of Pyrrolo[3,2-b]pyrrole-2,5(1H,4H)-dione (iDPP)-Based Molecules

Mindaugas Kirkus, Stefan Knippenberg, David Beljonne, Jérôme Cornil, René A. J. Janssen, and Stefan C. J. Meskers

pp 2782-2789

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

DOI: 10.1021/jp400256s

Section:

Physical Organic Chemistry

Nonadiabatic Photodynamics of a Retinal Model in Polar and Nonpolar Environment

Matthias Ruckenbauer, Mario Barbatti, Thomas Müller, and Hans Lischka

pp 2790-2799

Publication Date (Web): March 7, 2013 (Article)

DOI: 10.1021/jp400401f





Physical Organic Chemistry

Ground State Conformational Preferences and CH Stretch–Bend Coupling in a Model Alkoxy Chain: 1,2-Diphenoxyethane

Evan G. Buchanan, Edwin L. Sibert, III, and Timothy S. Zwier

pp 2800-2811

Publication Date (Web): March 12, 2013 (Article)

DOI: 10.1021/jp400691a

Section:

Physical Organic Chemistry

MOLECULAR STRUCTURE, QUANTUM CHEMISTRY, AND GENERAL THEORY Are the Intramolecular O-H···F and O-H···Cl Hydrogen Bonds Maintained in Solution? A Theoretical Study

Peter I. Nagy

pp 2812-2826

Publication Date (Web): March 12, 2013 (Article)

DOI: 10.1021/jp310596c

Section:

General Physical Chemistry

Recognition of a Novel Type X=N-Hal···Hal (X = C, S, P; Hal = F, Cl, Br, I) Halogen Bonding

Pavel V. Gushchin, Maxim L. Kuznetsov, Matti Haukka, and Vadim Yu. Kukushkin

pp 2827-2834

Publication Date (Web): March 7, 2013 (Article)

DOI: 10.1021/jp3112149

Section:

Inorganic Chemicals and Reactions

New Acceptor–Bridge–Donor Strategy for Enhancing NLO Response with Long-Range Excess Electron Transfer from the NH₂...M/M₃O Donor (M = Li, Na, K) to Inside the Electron Hole Cage $C_{20}F_{19}$ Acceptor through the Unusual σ Chain Bridge (CH₂)₄

Yang Bai, Zhong-Jun Zhou, Jia-Jun Wang, Ying Li, Di Wu, Wei Chen, Zhi-Ru Li, and Chia-Chung Sun

pp 2835-2843

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

DOI: 10.1021/jp3120594

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

New Parameterization Scheme of DFT-D for Graphitic Materials

Karol Strutyński, Manuel Melle-Franco, and José A. N. F. Gomes

pp 2844-2853

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

DOI: 10.1021/jp312239n

Section:

General Physical Chemistry

Vibrational and Electronic Structure Analysis of a Carbon Dioxide Interaction with Functionalized Single-Walled Carbon Nanotubes

Edson Nunes Costa Paura, Wiliam F. da Cunha, Pedro H. de Oliveira Neto, Geraldo M. e Silva, Joao B. L. Martins, and Ricardo Gargano

pp 2854-2861

Publication Date (Web): February 20, 2013 (Article)

DOI: 10.1021/jp312622s

Section:

General Physical Chemistry

Density Functional Study of Organocatalytic Cross-Aldol Reactions between Two Aliphatic Aldehydes: Insight into Their Functional Differentiation and Origins of Chemo- and Stereoselectivities

Aiping Fu, Chengyan Zhao, Hongliang Li, Fenghui Tian, Shuping Yuan, Yunbo Duan, and Zonghua, Wang

pp 2862-2872

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

DOI: 10.1021/jp3126363

Section:

Physical Organic Chemistry

Energetics of Nonbonded Ortho Interactions in Alkylbenzenes

Filipe Agapito, Rui C. Santos, and José A. Martinho Simões

pp 2873-2878

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

DOI: 10.1021/jp400475q

Section:

Physical Organic Chemistry

Systematic Study of the Basis Set Superposition Error in Core–Electron Correlation Effects

Tobias Schwabe

pp 2879-2883

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

DOI: 10.1021/jp401495u

Section:

General Physical Chemistry

Validation of Double-Hybrid Density Functionals for Electric Response Properties of Transition-Metal Systems: A New Paradigm Based on Physical Considerations

Mojtaba Alipour

pp 2884-2890

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

DOI: 10.1021/jp4016596

Section:

General Physical Chemistry