

June 20, 2013

Volume 117, Issue 24

Pages 7145-7488

Biophysical Chemistry and Biomolecules

UV Resonance Raman and DFT Studies of Arginine Side Chains in Peptides: Insights into Arginine Hydration

Zhenmin Hong, Jonathan Wert, and Sanford A. Asher

pp 7145–7156

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

DOI: 10.1021/jp404030u

 Section:

Physical Organic Chemistry

The FMO Complex in a Glycerol–Water Mixture

Mortaza Aghtar, Johan Strümpfer, Carsten Olbrich, Klaus Schulten, and Ulrich Kleinekathöfer

pp 7157–7163

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

DOI: 10.1021/jp311380k

 Section:

Plant Biochemistry

Sonolysis of High Macroviscosity Systems: Hen Albumen Hydrogel

Keith M. Krise, Ellen R. Forsyth, Kay M. DiMarco, and Bratoljub H. Milosavljevic

pp 7164–7168

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

DOI: 10.1021/jp312818f

 Section:

General Biochemistry

Dominant Stable Radicals in Irradiated Sucrose: g Tensors and Contribution to the Powder Electron Paramagnetic Resonance Spectrum

Hendrik De Cooman, Joke Keysabyl, Jevgenij Kusakovskij, Andy Van Yperen-De Deyne, Michel Waroquier, Freddy Callens, and Henk Vrielinck

pp 7169–7178

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

DOI: 10.1021/jp400053h

 Section:

Magnetic Phenomena

The Protein Environment of the Bacteriopheophytin Anion Modulates Charge Separation and Charge Recombination in Bacterial Reaction Centers

Jie Pan, Rafael G. Saer, Su Lin, Zhi Guo, J. Thomas Beatty, and Neal W. Woodbury

pp 7179–7189

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

DOI: 10.1021/jp400132k

 Section:

General Biochemistry

“Strange Kinetics” in the Temperature Dependence of Methionine Ligand Rebinding Dynamics in Cytochrome c

Ping Zhang, Steven Wooseok Ahn, and John E. Straub

pp 7190–7202

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

DOI: 10.1021/jp400481m

 Section:

General Biochemistry

Time-Resolved Fluorescence Studies of Fullerene Derivatives

Alessandra Andreoni, Luca Nardo, Maria Bondani, Baozhong Zhao, and Joan E. Roberts

pp 7203–7209

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

DOI: 10.1021/jp400877h

 Section:

Pharmaceuticals

The Structure and Function of Quinones in Biological Solar Energy Transduction: A Cyclic Voltammetry, EPR, and Hyperfine Sub-Level Correlation (HYSCORE) Spectroscopy Study of Model Naphthoquinones

Christopher S. Coates, Jessica Ziegler, Katherine Manz, Jacob Good, Bernard Kang, Sergey Milikisiyants, Ruchira Chatterjee, Sijie Hao, John H. Golbeck, and K. V. Lakshmi

pp 7210–7220

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

DOI: 10.1021/jp401024p

 Section:

General Biochemistry

Quantifying Coulombic and Solvent Polarization-Mediated Forces Between DNA Helices

Zhaojian He and Shi-Jie Chen

pp 7221–7227

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

DOI: 10.1021/jp4010955

 Section:

General Biochemistry

Unusual Emitting States of the Kindling Fluorescent Protein: Appearance of the Cationic Chromophore in the GFP Family

Bella L. Grigorenko, Igor V. Polyakov, Alexander P. Savitsky, and Alexander V. Nemukhin

pp 7228–7234

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

DOI: 10.1021/jp402149q

 Section:

General Biochemistry

Photocycle of Exiguobacterium sibiricum Rhodopsin Characterized by Low-Temperature Trapping in the IR and Time-Resolved Studies in the Visible

Andrei K. Dioumaev, Lada E. Petrovskaya, Jennifer M. Wang, Sergei P. Balashov, Dmitriy A. Dolgikh, Mikhail P. Kirpichnikov, and Janos K. Lanyi

pp 7235–7253

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

DOI: 10.1021/jp402430w

 Section:

General Biochemistry

Free Energy of Solvated Salt Bridges: A Simulation and Experimental Study

Andrew D. White, Andrew J. Keefe, Jean-Rene Ella-Menye, Ann K. Nowinski, Qing Shao, Jim Pfaendtner, and Shaoyi Jiang

pp 7254–7259

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

DOI: 10.1021/jp4024469

 Section:

General Biochemistry

On the pH Dependent Behavior of the Firefly Bioluminescence: Protein Dynamics and Water Content in the Active Pocket

Hyun Woo Kim and Young Min Rhee

pp 7260–7269

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

DOI: 10.1021/jp4024553

 Section:

Enzymes

Quantum Confinement of the Covalent Bond beyond the Born–Oppenheimer Approximation

A. Sarsa, J. M. Alcaraz-Pelegrina, C. Le Sech, and S. A. Cruz

pp 7270–7276

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

DOI: 10.1021/jp402727b

 Section:

General Physical Chemistry

On the Initial Binding of Alginate by Calcium Ions. The Tilted Egg-Box Hypothesis

Massimiliano Borgogna, Gudmund Skjåk-Bræk, Sergio Paoletti, and Ivan Donati

pp 7277–7282

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

DOI: 10.1021/jp4030766

 Section:

General Biochemistry

Thermostabilization of the β_1 -Adrenergic Receptor Correlates with Increased Entropy of the Inactive State

Michiel J. M. Niesen, Supriyo Bhattacharya, Reinhard Grisshammer, Christopher G. Tate, and Nagarajan Vaidehi

pp 7283–7291

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

DOI: 10.1021/jp403207c

 Section:

General Biochemistry

DNA Interaction with Hoechst 33258: Stretching Experiments Decouple the Different Binding Modes

E. F. Silva, E. B. Ramos, and M. S. Rocha

pp 7292–7296

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

DOI: 10.1021/jp403945e

 Section:

General Biochemistry

Resolution of Organic Polymorphic Crystals by Raman Spectroscopy

Martin Dračinský, Eliška Procházková, Jiří Kessler, Jaroslav Šebestík, Pavel Matějka, and Petr Bouř

pp 7297–7307

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

DOI: 10.1021/jp404382f

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Ultrafast Fluorescence Quenching Dynamics of Atto655 in the Presence of N-Acetyltyrosine and N-Acetyltryptophan in Aqueous Solution: Proton-Coupled Electron Transfer versus Electron Transfer

Ying Zhang, Shuwei Yuan, Rong Lu, and Anchi Yu

pp 7308–7316

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

DOI: 10.1021/jp404466f

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

On the Shape of the Phonon Spectral Density in Photosynthetic Complexes

Adam Kell, Ximao Feng, Mike Reppert, and Ryszard Jankowiak

pp 7317–7323

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

DOI: 10.1021/jp405094p

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Biomaterials, Surfactants, and Membranes
Aggregation Thermodynamics of Sodium Octanoate Micelles Studied by Means of Molecular Dynamics Simulations

Kalil Bernardino and André F. de Moura

pp 7324–7334

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

DOI: 10.1021/jp312840y

 Section:

Surface Chemistry and Colloids

Deuterium NMR Investigation of the Lyotropic Phases of Alkyl β -Glycoside/D₂O Systems

Omar Misran, Bakir A. Timimi, Thorsten Heidelberg, Akihiko Sugimura, and Rauzah Hashim

pp 7335–7344

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

DOI: 10.1021/jp401787b

 Section:

Surface Chemistry and Colloids

Probing the Structure and Dynamics of Confined Water in AOT Reverse Micelles

Anna Victoria Martinez, Laura Dominguez, Edyta Małolepsza, Adam Moser, Zack Ziegler, and John E. Straub

pp 7345–7351

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

DOI: 10.1021/jp402270e

 Section:

Surface Chemistry and Colloids

Liquids; Chemical and Dynamical Processes in Solution
Dynamics of the Higher Lying Excited States of Cyanine Dyes. An Ultrafast Fluorescence Study

Cesar A. Guarin, Juan. P. Villabona-Monsalve, Rafael López-Arteaga, and Jorge Peon

pp 7352–7362

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

DOI: 10.1021/jp400278t

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Long-Range Diffusion in Xylitol–Water Mixtures

Khalid Elamin, Stefano Cazzato, Johan Sjöström, Stephen M. King, and Jan Swenson

pp 7363–7369

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

DOI: 10.1021/jp401633g



Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

Chain Length Dependent Excited-State Decay Processes of Diluted PF2/6 Solutions

João Pina, J. Sérgio Seixas de Melo, Niels Koenen, and Ulli Scherf

pp 7370–7380

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

DOI: 10.1021/jp4017163



Section:

Physical Properties of Synthetic High Polymers

Energy Dispersive XAFS: Characterization of Electronically Excited States of Copper(I) Complexes

Moniek Tromp, Andrew J. Dent, Jon Headspith, Timothy L. Easun, Xue-Zhong Sun, Michael W. George, Olivier Mathon, Grigory Smolentsev, Michelle L. Hamilton, and John Evans

pp 7381–7387

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

DOI: 10.1021/jp4020355



Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Interactions of Ionic Liquids and Acetone: Thermodynamic Properties, Quantum-Chemical Calculations, and NMR Analysis

Elia Ruiz, Victor R. Ferro, Jose Palomar, Juan Ortega, and Juan Jose Rodriguez

pp 7388–7398

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

DOI: 10.1021/jp402331y



Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

Liquid–Liquid Extraction of Uranyl by an Amide Ligand: Interfacial Features Studied by MD and PMF Simulations

G. Benay and G. Wipff

pp 7399–7415

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

DOI: 10.1021/jp4028386

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

Effect of Unsaturation on the Absorption of Ethane and Ethylene in Imidazolium-Based Ionic Liquids

Leila Moura, Manas Mishra, Varinia Bernales, Patricio Fuentealba, Agilio A.H. Padua, Catherine C. Santini, and Margarida F. Costa Gomes

pp 7416–7425

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

DOI: 10.1021/jp403074z

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

U-Shaped Temperature Dependence of Rate Constant of Intramolecular Photoinduced Charge Separation in Zinc–Porphyrin–Bridge–Quinone Compounds

Anna O. Kichigina, Vladimir N. Ionkin, and Anatoly I. Ivanov

pp 7426–7435

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

DOI: 10.1021/jp404222a

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Glasses, Colloids, Polymers, and Soft Matter Structural and Electrochemical Properties of Succinonitrile-Based Gel Polymer Electrolytes: Role of Ionic Liquid Addition

Mohd. Suleman, Yogesh Kumar, and S. A. Hashmi

pp 7436–7443

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

DOI: 10.1021/jp312358x

 Section:

Effect of Carbon Nanotube Dispersion on Glass Transition in Cross-Linked Epoxy–Carbon Nanotube Nanocomposites: Role of Interfacial Interactions

Ketan S. Khare and Rajesh Khare

pp 7444–7454

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

DOI: 10.1021/jp401614p



Section:

Plastics Manufacture and Processing

Shear Thinning Three-Dimensional Colloidal Assemblies of Chitosan and Poly(lactic acid) Nanoparticles

Rémi Roux, Catherine Ladavière, Alexandra Montembault, Laurent David, and Thierry Delair

pp 7455–7464

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

DOI: 10.1021/jp4017486



Section:

Pharmaceuticals

Plasticizing Effect of K⁺ Ions and Succinonitrile on Electrical Conductivity of [Poly(ethylene oxide)–Succinonitrile]/KI–I₂ Redox-Couple Solid Polymer Electrolyte

Ravindra Kumar Gupta and Hee-Woo Rhee

pp 7465–7471

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

DOI: 10.1021/jp4025798



Section:

Plastics Manufacture and Processing

A Step toward the Development of High-Temperature Stable Ionic Liquid-in-Oil Microemulsions Containing Double-Chain Anionic Surface Active Ionic Liquid

Vishal Govind Rao, Chiranjib Banerjee, Surajit Ghosh, Sarthak Mandal, Jagannath Kuchlyan, and Nilmoni Sarkar

pp 7472–7480

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

DOI: 10.1021/jp403265p

 Section:

Surface Active Agents and Detergents

A Comparative Study of Urea-Induced Aggregation of Collapsed Poly(N-isopropylacrylamide) and Poly(N,N-diethylacrylamide) Chains in Aqueous Solutions

Yijie Lu, Xiaodong Ye, Kejin Zhou, and Wenjing Shi

pp 7481–7488

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

DOI: 10.1021/jp403555b

 Section:

Physical Properties of Synthetic High Polymers