

NOVEMBER 14, 2013

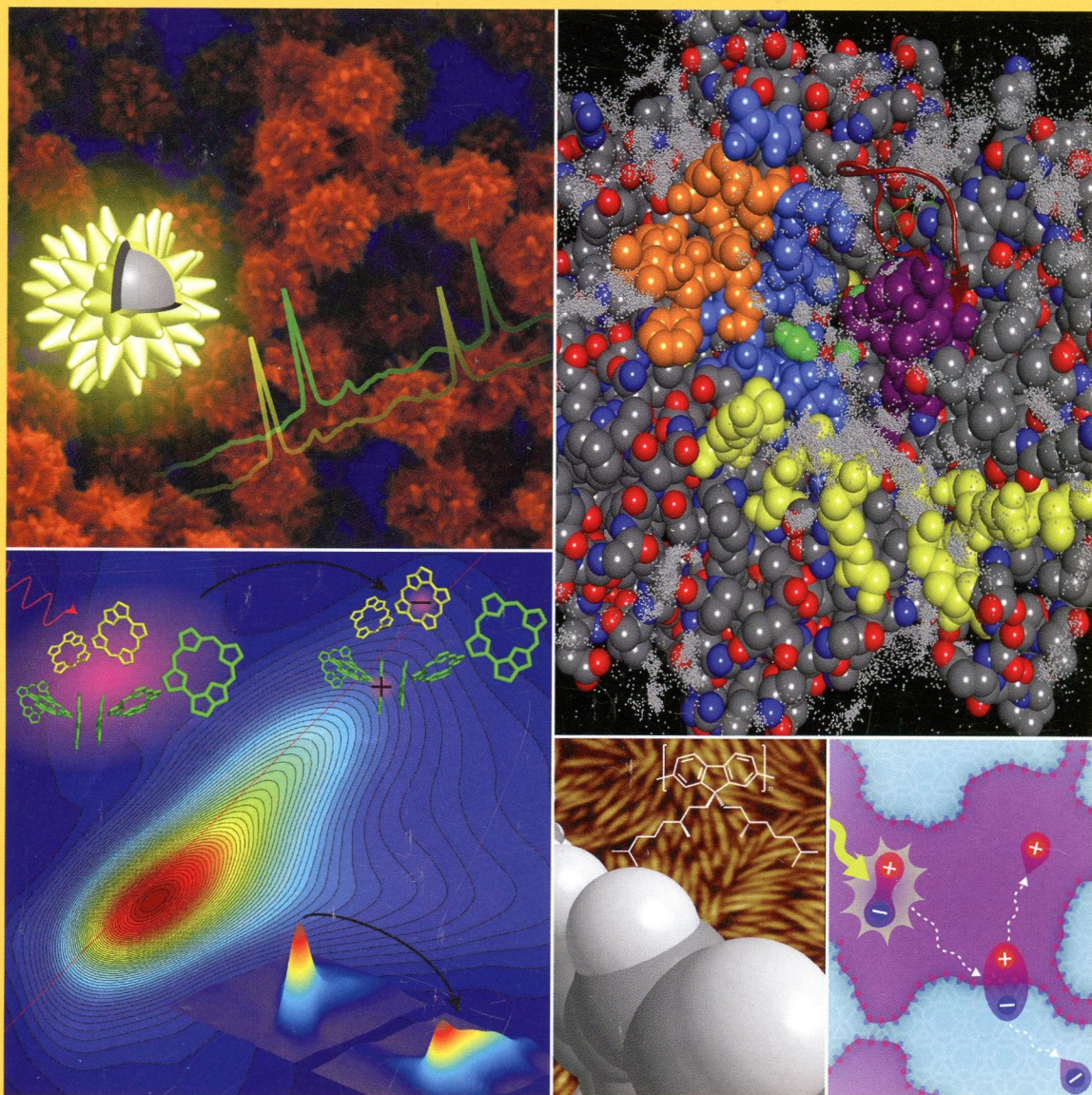
VOLUME 117

NUMBER 45

pubs.acs.org/JPCB

THE JOURNAL OF PHYSICAL CHEMISTRY

B

**BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER**

ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

www.acs.org

November 14, 2013
Volume 117, Issue 45
Pages 13947-14172

Biophysical Chemistry and Biomolecules

Deciphering the Catalysis-Associated Conformational Changes of Human Adenylate Kinase 1 with Single-Molecule Spectroscopy

Chien Y. Lin, Jung Y. Huang, and Leu-Wei Lo

pp 13947–13955

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

DOI: 10.1021/jp4019537

 Section:

Enzymes

Counterion and Polythymidine Loop-Length-Dependent Folding and Thermodynamic Stability of DNA Hairpins Reveal the Unusual Counterion-Dependent Stability of Tetraloop Hairpins

Rajesh K. Nayak and Alan Van Orden

pp 13956–13966

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

DOI: 10.1021/jp404832d

 Section:

General Biochemistry

Calculating Hyperfine Couplings in Large Ionic Crystals Containing Hundreds of QM Atoms: Subsystem DFT Is the Key

Ruslan Kevorkyants, Xiqiao Wang, David M. Close, and Michele Pavanello

pp 13967–13974

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

DOI: 10.1021/jp405154d

 Section:

General Physical Chemistry

Poly(4-styrenesulfonate) as an Inhibitor of A β 40 Amyloid Fibril Formation

Bimlesh Ojha, Haiyang Liu, Samrat Dutta, Praveen P. N. Rao, Ewa P. Wojcikiewicz, and Deguo Du

pp 13975–13984

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

DOI: 10.1021/jp4065467

 Section:

General Biochemistry

Photochemistry of Singlet Oxygen Sensor Green

Sooyeon Kim, Mamoru Fujitsuka, and Tetsuro Majima

pp 13985–13992

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

DOI: 10.1021/jp406638g

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Distribution of Protein Ramachandran Psi (ψ) Angle Using Non-Resonance Visible Raman Scattering Measurements

Susmita Bhattacharya, Sudeshna Ghosh, Nitin Kumar Pandey, Susmitnarayan Chaudhury, Swagata Dasgupta, and Anushree Roy

pp 13993–14000

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

DOI: 10.1021/jp408009y

 Section:

Biochemical Methods

Examination of Tyrosine/Adenine Stacking Interactions in Protein Complexes

Kari L. Copeland, Samuel J. Pellock, James R. Cox, Mauricio L. Cafiero, and Gregory S. Tschumper

pp 14001–14008

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

DOI: 10.1021/jp408027j

 Section:

General Biochemistry

Ultrafast Two-Dimensional Infrared Spectroscopy of Guanine–Cytosine Base Pairs in DNA Oligomers

Christian Greve and Thomas Elsaesser

pp 14009–14017

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

DOI: 10.1021/jp408229k

 Section:

General Biochemistry

Binding Interactions of β -Conglycinin and Glycinin with Vitamin B₁₂

Jing Zhang, Zhigang Tian, Li Liang, Muriel Subirade, and Lingyun Chen

pp 14018–14028

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

DOI: 10.1021/jp408578m

 Section:

General Biochemistry

Small-Angle Neutron Scattering Study of a Monoclonal Antibody Using Free-Energy Constraints

Nicholas J. Clark, Hailiang Zhang, Susan Krueger, Hyo Jin Lee, Randal R. Ketchem, Bruce Kerwin, Sekhar R. Kanapuram, Michael J. Treuheit, Arnold McAuley, and Joseph E. Curtis

pp 14029–14038

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

DOI: 10.1021/jp408710r

 Section:

From Formamide to Adenine: A Self-Catalytic Mechanism for an Abiotic Approach

Jing Wang, Jiande Gu, Minh Tho Nguyen, Greg Springsteen, and Jerzy Leszczynski
pp 14039–14045

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

DOI: 10.1021/jp409296k

 Section:

General Biochemistry

Biomaterials, Surfactants, and Membranes

Amaranth 7S Globulin Langmuir Films and Its Interaction with L- α -Dipalmitoilphosphatidilcholine at the Air-Fluid Interface

Alcione Garcia-Gonzalez, A. L. Flores-Vazquez, A. P. Barba de la Rosa, E. A. Vazquez-Martinez, and J. Ruiz-Garcia

pp 14046–14058

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

DOI: 10.1021/jp405944u

 Section:

Surface Chemistry and Colloids

Free-Energy Landscape for Peptide Amphiphile Self-Assembly: Stepwise versus Continuous Assembly Mechanisms

Tao Yu and George C. Schatz

pp 14059–14064

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

DOI: 10.1021/jp409305e

 Section:

General Biochemistry

Liquids; Chemical and Dynamical Processes in Solution

Dissociation of a Strong Acid in Neat Solvents: Diffusion Is Observed after Reversible Proton Ejection Inside the Solvent Shell

Manoel Veiga-Gutiérrez, Alfonso Brenlla, Carlos Carreira Blanco, Berta Fernández, Sergey A. Kovalenko, Flor Rodríguez-Prieto, Manuel Mosquera, and J. Luis Pérez Lustres

pp 14065–14078

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

DOI: 10.1021/jp4042765

 Section:

Physical Organic Chemistry

Temperature Effect on Dual Fluorescence of 2-(2'-Hydroxyphenyl)benzimidazole and Its Nitrogen Substituted Analogues

Francis A. S. Chipem and Govindarajan Krishnamoorthy

pp 14079–14088

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

DOI: 10.1021/jp405804c

 Section:

Physical Organic Chemistry

Electronic and Nuclear Structural Snapshots in Ligand Dissociation and Recombination Processes of Iron Porphyrin in Solution: A Combined Optical/X-ray Approach

Michael W. Mara, Megan Shelby, Andrew Stickrath, Mike Harpham, Jier Huang, Xiaoyi Zhang, Brian M. Hoffman, and Lin X. Chen

pp 14089–14098

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

DOI: 10.1021/jp407094u

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Prototropical and Photophysical Properties of Ellipticine inside the Nanocavities of Molecular Containers

Krishna Gavvala, Abhigyan Sengupta, Raj Kumar Koninti, and Partha Hazra

pp 14099–14107

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

DOI: 10.1021/jp408280p

 Section:

Pharmaceuticals

Excited-State Proton Transfer of Fluorescein Anion as an Ionic Liquid Component

Catarina A. B. Rodrigues, Cátia Graça, Ermelinda Maçôas, Alexander Fedorov, Carlos A. M. Afonso, and José M. G. Martinho

pp 14108–14114

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

DOI: 10.1021/jp408616r

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Theoretical Study of Salt Effects on the Diels–Alder Reaction of Cyclopentadiene with Methyl Vinyl Ketone Using RISM-SCF Theory

Norio Yoshida, Hidetsugu Tanaka, and Fumio Hirata

pp 14115–14121

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

DOI: 10.1021/jp4091552

 Section:

Physical Organic Chemistry

Glasses, Colloids, Polymers, and Soft Matter

Epoxy-Based Hydrogels Investigated by High-Frequency Dielectric Relaxation Spectroscopy

Ivan Krakovský, Toshiyuki Shikata, and Ryuta Hasegawa

pp 14122–14128

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

DOI: 10.1021/jp4058059

 Section:

Physical Properties of Synthetic High Polymers

Investigations on the Interactions of Proteins with Polyampholyte-Coated Magnetite Nanoparticles

Tao Zhao, Kaimin Chen, and Hongchen Gu

pp 14129–14135

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

DOI: 10.1021/jp407157n

 Section:

Pharmaceuticals

Spin Radical Enhanced Magnetocapacitance Effect in Intermolecular Excited States

Huidong Zang, Jianguo Wang, Mingxing Li, Lei He, Zitong Liu, Deqing Zhang, and Bin Hu

pp 14136–14140

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

DOI: 10.1021/jp407789g

 Section:

Electric Phenomena

Linear and Nonlinear Optical Susceptibilities and the Hyperpolarizability of Borate $\text{LiBaB}_9\text{O}_{15}$ Single-Crystal: Theory and Experiment

A. H. Reshak, Xuean Chen, S. Auluck, H. Kamarudin, Jan Chyský, A. Wojciechowski, and I. V. Kityk

pp 14141–14150

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

DOI: 10.1021/jp4077905

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Modulated Fluorescence of Colloidal Quantum Dots Embedded in a Porous Alumina Membrane

Hao Xu, Li Li, Otto Manneberg, Aman Russom, Kristinn B. Gylfason, Hjalmar Brismar, and Ying Fu

pp 14151–14156

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

DOI: 10.1021/jp409132e

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Effect of p-tert-Butyl Group Substitution on the Quantum Tunneling Rate in Quadruple Proton Rearrangement of Calix[4]arene

Kouhei Ueda and Masaharu Oguni

pp 14157–14162

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

DOI: 10.1021/jp409280s

 Section:

Physical Organic Chemistry

Copper(II) Complexes with 4-Carbomethoxypyrrolidone Functionalized PAMAM-Dendrimers: An EPR Study

Maria Francesca Ottaviani, Michela Cangiotti, Alberto Fattori, Concetta Coppola, Susanna Lucchi, Mario Ficker, Johannes F. Petersen, and Jørn B. Christensen

pp 14163–14172

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

DOI: 10.1021/jp410307z

 Section:

Chemistry of Synthetic High Polymers