ON THE COVER: Soluble aggregates in aqueous solutions of polyion-surfactant ion complex salts and a nonionic surfactant. NMR, scattering, and calorimetric methods reveal that soluble mixed aggregates, containing polyions and mixed micelles of ionic and nonionic surfactants, form when a C16TA polyacrylate complex salt is added to a solution of the nonionic surfactant C12E8. Aggregate growth, ultimately resulting in phase separation, occurs when more and more polyions add to mixed micelles of a nearly constant composition. See page 9745.

Articles

Biophysical Chemistry and Biomolecules

9525  dx.doi.org/10.1021/jp5025153
In Silico Spectroscopy of Tryptophan and Tyrosine Radicals Involved in the Long-Range Electron Transfer of Cytochrome c Peroxidase
Caterina Bemini, Elena Arezzini, Riccardo Basosi, and Adalgisa Sinicropi*

9538  dx.doi.org/10.1021/jp502687q
Systematic Molecular Dynamics, MM–PBSA, and Ab Initio Approaches to the Saquinavir Resistance Mechanism in HIV-1 PR Due to 11 Double and Multiple Mutations
Haralambos Tzoupis,* Georgios Leonis,* Aggelos Avramopoulos, Thomas Mavromoustakos, and Manthos G. Papadopoulos*

9553  dx.doi.org/10.1021/jp503032h
Solid-State NMR Shows That Dynamically Different Domains of Membrane Proteins Have Different Hydration Dependence
Zhengfeng Zhang, Yanke Chen, Xinqi Tang, Jianping Li, Liying Wang, and Jun Yang*

9565  dx.doi.org/10.1021/jp503358n
Solubility and Aggregation of Gly₃ in Water
Deepti Karandur, Ka-Yiu Wong, and B. Montgomery Pettitt*

9573  dx.doi.org/10.1021/jp5047535
Reactivity and Aromaticity of Nucleobases are Sensitive Toward External Electric Field
Biswa Jyoti Dutta and Pradip Kr. Bhattacharyya*

9583  dx.doi.org/10.1021/jp505107g
Affinity of Molecular Ions for DNA Structures Is Determined by Solvent-Accessible Surface Area
Miki Nakano, Hisae Tateishi-Karimata, Shigenori Tanaka, and Naoki Sugimoto*
9595

Polymorphism in 2-X-Adamantane Derivatives (X = Cl, Br)
Philippe Negrier, María Barrio, Josep Ll. Tamarit,* and Denise Mondieig

dx.doi.org/10.1021/jp505280d

9604

Interaction of Extracellular Loop II of κ-Opioid Receptor (196–228) with Opioid Peptide Dynorphin in Membrane Environments as Revealed by Solid State Nuclear Magnetic Resonance, Quartz Crystal Microbalance and Molecular Dynamics Simulation
Atsushi Kira, Namsrai Javkhlanjugs, Takenori Miyamori, Yoshiyuki Sasaki, Masayuki Eguchi, Izuru Kawamura, Kazuyoshi Ueda, and Akira Naito*

dx.doi.org/10.1021/jp505412j

9613

Combination of Transient 2D-IR Experiments and Ab Initio Computations Sheds Light on the Formation of the Charge-Transfer State in Photoexcited Carboxyl Carotenoids
Mariangela Di Donato, Mirela Segado Centellas, Andrea Lapini,* Manuela Lima, Francisco Avila, Fabrizio Santoro,* Chiara Cappelli, and Roberto Righini

dx.doi.org/10.1021/jp505473j

9631

Accurate and Computationally Efficient Prediction of Thermochemical Properties of Biomolecules Using the Generalized Connectivity-Based Hierarchy
Arkajyoti Sengupta, Raghu Nath O. Ramabhadran, and Krishnan Raghavachari*

dx.doi.org/10.1021/jp505544y

9644

Binding Mode Investigations on the Interaction of Lead(II) Acetate with Human Chorionic Gonadotropin
Hao Zhang, Yang Liu, Rui Zhang, Rutao Liu,* and Yadong Chen

dx.doi.org/10.1021/jp505565s

9651

Conformations of Disulfide-Intact and -Reduced Lysozyme Ions Probed by Proton-Transfer Reactions at Various Temperatures
Shinji Nonose,* Kazuki Yamashita, Takuya Okamura, Satoshi Fukase, Minami Kawashima, Ayako Sudo, and Hideo Isono

dx.doi.org/10.1021/jp505621f

9662

Fluorescence Correlation Spectroscopy at Micromolar Concentrations without Optical Nanoconfinement
Ted A. Laurence,* Sonny Ly,* Feliza Bourguet, Nicholas O. Fischer, and Matthew A. Coleman

dx.doi.org/10.1021/jp505881z

9668

Counterion-Assisted Cation Transport in a Biological Calcium Channel
Hao Dong, Michael L. Klein,* and Giacomo Fiorin

dx.doi.org/10.1021/jp5059897
Mapping Central α-Helix Linker Mediated Conformational Transition Pathway of Calmodulin via Simple Computational Approach
Jian Wang, Shaoliang Peng, Benjamin P. Cossins, Xiangke Liao, Kaixian Chen, Qiang Shao,* Xiaojian Zhu,* Jiye Shi,* and Weiliang Zhu

Biomaterials, Surfactants, and Membranes

Dual-Transmission Line Modeling of Electrochemical Processes in Polyaniline–Cellulose Ester Composite Porous Membranes
Asif A. Qaiser*

Aqueous Dual-Tailed Surfactants Simulated on the Alumina Surface
Zhen Liu, Jian-Guo Yu, Edgar A. O’Rear, and Alberto Striolo*

Gel-to-Fluid Phase Transformations in Solid-Supported Phospholipid Bilayers Assembled by the Langmuir–Blodgett Technique: Effect of the Langmuir Monolayer Phase State and Molecular Density
Mohini Ramkaran and Antonella Badia*

Computational Study of Bacterial Membrane Disruption by Cationic Biocides: Structural Basis for Water Pore Formation
Eric H. Hill, David G. Whitten, and Deborah G. Evans*

Liquids; Chemical and Dynamical Processes in Solution

Reversible Multistep Synthesis with Equilibrium Properties Based on a Selection-Oriented Process with a Repetitive Sequence of Steps
Sagi Eppel* and Moshe Portnoy

Glasses, Colloids, Polymers, and Soft Matter

Soluble Aggregates in Aqueous Solutions of Polyion–Surfactant Ion Complex Salts and a Nonionic Surfactant
John Janiak, Matija Tomšič, Dan Lundberg, Gerd Olofsson, Lennart Piculell, and Karin Schillén*

Effects of Added Surfactant on Swelling and Molecular Transport in Drug-Loaded Tablets Based on Hydrophobically Modified Poly(acrylic acid)
Patrik Knöös,* Marie Wahlgren, Daniel Topgaard, Stefan Ulvenlund, and Lennart Piculell*
Supramolecular Interaction between a Hydrophilic Coumarin Dye and Macroyclic Hosts: Spectroscopic and Calorimetric Study
Aninda Chatterjee, Banibrata Maity, and Debabrata Seth*

Immobilization of Hydrophilic Low Molecular-Weight Molecules in Nanoparticles of Chitosan/Poly(sodium 4-styrenesulfonate) Assisted by Aromatic–Aromatic Interactions
Juan Pablo Fuenzalida, Mario E. Flores, Inés Móniz, Miguel Feijoo, Francisco Goycoolea, Hiroyuki Nishiide, and Ignacio Moreno-Villoslada*

Chemical Stabilization and Improved Thermal Resilience of Molecular Arrangements: Possible Formation of a Surface Network of Bonds by Multiple Pulse Atomic Layer Deposition
Muriel de Pauli, Matheus J. S. Matos, Pablo F. Siles, Mariana C. Prado, Bernardo R. A. Neves, Sukarno O. Ferreira, Mário S. C. Mazzoni, and Angelo Malachias*

Study of Molecular Dynamics in Poly(n-alkyl methacrylates) by Light Induced Absorption Anisotropy
S. Grebenkin,* B. Bolshakov, and V. M. Syutkin

Biocolloids Based on Amphiphilic Block Copolymers as a Medium for Enzyme Encapsulation
Victoria Sereti, Maria Zoumpanioti, Vassiliki Papadimitriou, Stergios Pispas, and Aristotelis Xenakis*

Additions and Corrections

Correction to "Rheological Study of Mutarotation of Fructose in Anhydrous State"
Yangyang Wang, Patryk Wlodarczyk, Alexei P. Sokolov, and Marian Paluch*