

SEPTEMBER 5, 2013

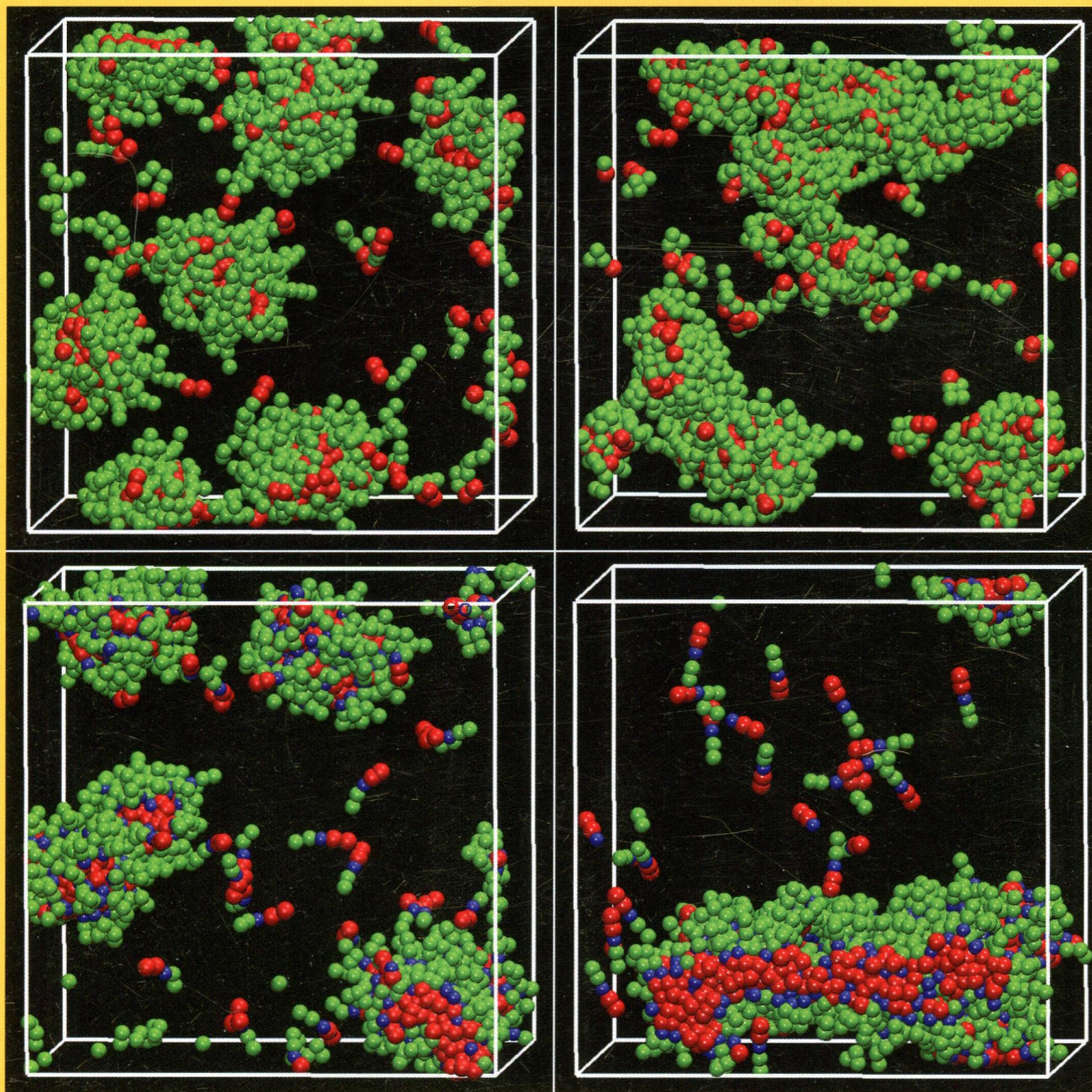
VOLUME 117

NUMBER 35

pubs.acs.org/JPCB

THE JOURNAL OF PHYSICAL CHEMISTRY

B



Self-Assembled
Morphologies in
Micellar Solutions of
Nonionic Surfactants
of Different
Hydrophobicity
and Rigidity
(see page 5A)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

www.acs.org

September 5, 2013

Volume 117, Issue 35

Pages 10053-10342

Biophysical Chemistry and Biomolecules

Toward an Understanding of the Retinal Chromophore in Rhodopsin Mimics

Mark M. Huntress, Samer Gozem, Konstantin R. Malley, Askat E. Jailaubekov, Chrysoula Vasileiou, Mikas Vengris, James H. Geiger, Babak Borhan, Igor Schapiro, Delmar S. Larsen, and Massimo Olivucci

pp 10053–10070

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

DOI: 10.1021/jp305935t

 Section:

General Biochemistry

Combined QM/MM Investigation on the Light-Driven Electron-Induced Repair of the (6–4) Thymine Dimer Catalyzed by DNA Photolyase

Shirin Faraji, Gerrit Groenhof, and Andreas Dreuw

pp 10071–10079

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

DOI: 10.1021/jp401662z

 Section:

Enzymes

“Amide Resonance” in the Catalysis of 1,2- α -L-Fucosidase from *Bifidobacterium bifidum*

Jingli Liu, Min Zheng, Chunchun Zhang, and Dingguo Xu

pp 10080–10092

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

DOI: 10.1021/jp402110j

 Section:

Enzymes

Cation- π Interactions: Accurate Intermolecular Potential from Symmetry-Adapted Perturbation Theory

Kay Ansorg, Maxim Tafipolsky, and Bernd Engels

pp 10093–10102

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

DOI: 10.1021/jp403578r

 Section:

Physical Organic Chemistry

Binding of O₂ and NO to Heme in Heme-Nitric Oxide/Oxygen-Binding (H-NOX) Proteins. A Theoretical Study

Meng-Sheng Liao, Ming-Ju Huang, and John D. Watts

pp 10103–10114

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

DOI: 10.1021/jp403998u

 Section:

General Biochemistry

Design and Evaluation of an i-Motif-Based Allosteric Control Mechanism in DNA-Hairpin Molecular Devices

Irina V. Nesterova, Siddieg O. Elsiddieg, and Evgueni E. Nesterov

pp 10115–10121

Publication Date (Web): August 13, 2013 (Article)

DOI: 10.1021/jp405230g

 Section:

Biochemical Methods

Side-by-Side Comparison of DNA Damage Induced by Low-Energy Electrons and High-Energy Photons with Solid TpTpT Trinucleotide

Yeunsoo Park, Anita R. Peoples, Guru S. Madugundu, Léon Sanche, and J. Richard Wagner

pp 10122–10131

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

DOI: 10.1021/jp405397m

 Section:

Radiation Biochemistry

Hydration of Cations: A Key to Understanding of Specific Cation Effects on Aggregation Behaviors of PEO-PPO-PEO Triblock Copolymers

Jacob C. Lutter, Tsung-yu Wu, and Yanjie Zhang

pp 10132–10141

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

DOI: 10.1021/jp405709x

 Section:

Physical Properties of Synthetic High Polymers

Ionic Liquid-Induced Formation of the α -Helical Structure of β -Lactoglobulin

Takahiro Takekiyo, Yoshihiro Koyama, Kumiko Yamazaki, Hiroshi Abe, and Yukihiro Yoshimura

pp 10142–10148

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

DOI: 10.1021/jp405834n

 Section:

General Biochemistry

β (16–22) Peptides Can Assemble into Ordered β -Barrels and Bilayer β -Sheets, while Substitution of Phenylalanine 19 by Tryptophan Increases the Population of Disordered Aggregates

Luogang Xie, Yin Luo, and Guanghong Wei

pp 10149–10160

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

DOI: 10.1021/jp405869a

 Section:

General Biochemistry

Catalytic Mechanism of Hyaluronate Lyase from *Spectrooccus pneumoniae*: Quantum Mechanical/Molecular Mechanical and Density Functional Theory Studies

Min Zheng and Dingguo Xu

pp 10161–10172

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

DOI: 10.1021/jp406206s

 Section:

Enzymes

Photochemical and Optical Properties of Water-Soluble Xanthophyll Antioxidants: Aggregation vs Complexation

Nikolay E. Polyakov, Adam Magyar, and Lowell D. Kispert

pp 10173–10182

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

DOI: 10.1021/jp4062708

 Section:

General Biochemistry

***Biomaterials, Surfactants, and Membranes
Simulations of Anionic Lipid Membranes: Development of Interaction-Specific Ion Parameters and Validation Using NMR Data***

Richard M. Venable, Yun Luo, Klaus Gawrisch, Benoît Roux, and Richard W. Pastor

pp 10183–10192

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

DOI: 10.1021/jp401512z

 Section:

Biochemical Methods

Reaction Field Analysis and Lipid Bilayer Location for Lipophilic Fluorophores

Edward G. Randles and Peter R. Bergethon

pp 10193–10202

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

DOI: 10.1021/jp402861x

 Section:

Biochemical Methods

Novel Spiropyran Amphiphiles and Their Application as Light-Responsive Liquid Crystalline Components

Kristian J. Tangso, Wye-Khay Fong, Tamim Darwish, Nigel Kirby, Ben J. Boyd, and Tracey L. Hanley

pp 10203–10210

Publication Date (Web): August 3, 2013 (Article)

DOI: 10.1021/jp403840m

 Section:

Biomolecules and Their Synthetic Analogs

***Liquids; Chemical and Dynamical Processes in Solution
NMR and Raman Spectroscopy Monitoring of Proton/Deuteron Exchange in
Aqueous Solutions of Ionic Liquids Forming Hydrogen Bond: A Role of Anions,
Self-Aggregation, and Mesophase Formation***

Vytautas Klimavicius, Zofia Gdaniec, Jonas Kausteklis, Valdemaras Aleksa, Kestutis Aidas, and Vytautas Balevicius

pp 10211–10220

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

DOI: 10.1021/jp4021245

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

***Solvation Effects on Self-Association and Segregation Processes in tert-
Butanol–Aprotic Solvent Binary Mixtures***

A. R. Abdel Hamid, R. Lefort, Y. Lechaux, A. Moréac, A. Ghoufi, C. Alba-Simionesco, and D. Morineau

pp 10221–10230

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

DOI: 10.1021/jp402380f

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

***Osmotic Virial Coefficients of Hydroxyethyl Starch from Aqueous
Hydroxyethyl Starch–Sodium Chloride Vapor Pressure Osmometry***

Jingjiang Cheng, Martin Gier, Lisa U. Ross-Rodriguez, Vinay Prasad, Janet A. W. Elliott, and Andreas Sputtek

pp 10231–10240

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

DOI: 10.1021/jp403377b

 Section:

Industrial Carbohydrates

***Size Effect on Nucleation Rate for Homogeneous Crystallization of Nanoscale
Water Film***

Yongjun Lü, Xiangxiong Zhang, and Min Chen

pp 10241–10249

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

DOI: 10.1021/jp404403k

 Section:

Surface Chemistry and Colloids

Molecular Dynamic Simulations and Vibrational Analysis of an Ionic Liquid Analogue

Sasha L. Perkins, Paul Painter, and Coray M. Colina

pp 10250–10260

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

DOI: 10.1021/jp404619x

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

On the Thermodynamics and Kinetics of Hydrophobic Interactions at Interfaces

Srivathsan Vembanur, Amish J. Patel, Sapna Sarupria, and Shekhar Garde

pp 10261–10270

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

DOI: 10.1021/jp4050513

 Section:

Surface Chemistry and Colloids

Systematic Study of the Thermophysical Properties of Imidazolium-Based Ionic Liquids with Cyano-Functionalized Anions

Catarina M. S. S. Neves, Kiki Adi Kurnia, João A. P. Coutinho, Isabel M. Marrucho, José N. Canongia Lopes, Mara G. Freire, and Luís Paulo N. Rebelo

pp 10271–10283

Publication Date (Web): August 13, 2013 (Article)

DOI: 10.1021/jp405913b

 Section:

Physical Organic Chemistry

Volumetric Study of the Mixtures n-Hexane + Isomeric Chlorobutane: Experimental Characterization and Volume Translated Peng–Robinson Predictions

Hernando Guerrero, Pilar Cea, Ignacio Gascón, Félix M. Royo, and Carlos Lafuente

pp 10284–10292

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

DOI: 10.1021/jp407380a

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

***Glasses, Colloids, Polymers, and Soft Matter
Terminally Grafted Chain Layers in Oligomer–Monomer Solutions:
Predictions from a Density Functional Theory***

M. Borówko, S. Sokołowski, and T. Staszewski

pp 10293–10303

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

DOI: 10.1021/jp4027546

 Section:

Physical Properties of Synthetic High Polymers

***Calculations of Critical Micelle Concentration by Dissipative Particle
Dynamics Simulations: The Role of Chain Rigidity***

Ming-Tsung Lee, Aleksey Vishnyakov, and Alexander V. Neimark

pp 10304–10310

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

DOI: 10.1021/jp4042028

 Section:

Surface Chemistry and Colloids

***Molar Volumes of Ethylcyclohexane and Butyronitrile Glasses Resulting from
Vapor Deposition: Dependence on Deposition Temperature and Comparison
to Alkylbenzenes***

Hideyuki Nakayama, Kio Omori, Katsunobu Ino-u-e, and Kikujiro Ishii

pp 10311–10319

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

DOI: 10.1021/jp404256r

 Section:

General Physical Chemistry

***Small Angle X-ray Scattering Investigation of Norbornene-Terminated
Syndiotactic Polypropylene and Corresponding Comb-Like
Poly(macromonomer)***

Finizia Auriemma, Claudio De Rosa, Rocco Di Girolamo, and Amelia Silvestre, Amelia M. Anderson-Wile and Geoffrey W. Coates

pp 10320–10333

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

DOI: 10.1021/jp404394y

 Section:

Physical Properties of Synthetic High Polymers

Low-Concentration Polymers Inhibit and Accelerate Crystal Growth in Organic Glasses in Correlation with Segmental Mobility

C. Travis Powell, Ting Cai, Mariko Hasebe, Erica M. Gunn, Ping Gao, Geoff Zhang, Yuchuan Gong, and Lian Yu

pp 10334–10341

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

DOI: 10.1021/jp406418n

 Section:

Plastics Manufacture and Processing