

THE JOURNAL OF PHYSICAL CHEMISTRY A



Larger Cover

April 18, 2013

Volume 117, Issue 15

Pages 3143-3252

KINETICS AND DYNAMICS

Reactions and Reaction Rate of Atmospheric SO_2 and $\text{O}_3^- (\text{H}_2\text{O})_n$ Collisions via Molecular Dynamics Simulations

Nicolai Bork, Ville Loukonen, and Hanna Vehkamäki

pp 3143-3148

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

DOI: 10.1021/jp311103z

 Section:

General Physical Chemistry

SPECTROSCOPY, PHOTOCHEMISTRY, AND EXCITED STATES

Benchmark Studies on the Building Blocks of DNA. 3. Watson–Crick and Stacked Base Pairs

Péter G. Szalay, Thomas Watson, Ajith Perera, Victor Lotrich, and Rodney J. Bartlett

pp 3149-3157

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

DOI: 10.1021/jp3100975

 Section:

General Biochemistry

Multisite Constrained Model of *trans*-4-(*N,N*-Dimethylamino)-4'-nitrostilbene for Structural Elucidation of Radiative and Nonradiative Excited States

Cheng-Kai Lin, Yu-Fu Wang, Yuan-Chung Cheng, and Jye-Shane Yang

pp 3158-3164

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

DOI: 10.1021/jp310770s

 Section:

Physical Organic Chemistry

Conformational Effects on the Lowest Excited States of Benzoyl-Pyrrolopyridazine: Insights from PCM Time-Dependent DFT

Dan Maftei, Gheorghita Zbancioc, Ionel Humelnicu, and Ionel Mangalagiu

pp 3165-3175

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

DOI: 10.1021/jp311396m

 Section:

Physical Organic Chemistry

Two- and Three-Body Dissociation Dynamics of Temporary Negative Ion NF_3^-

Hong-Kai Li, Lei Xia, Xian-Jin Zeng, and Shan Xi Tian

pp 3176-3182

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

DOI: 10.1021/jp400026c

 Section:

General Physical Chemistry

Comparable Strength of OH–O versus OH– π Hydrogen Bonds in Hydrogen-Bonded 2,3-Benzofuran Clusters with Water and Methanol

Hiroko Sasaki, Shigeyuki Daicho, Yuji Yamada, and Yoshinori Nibu

pp 3183-3189

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

DOI: 10.1021/jp400676x

 Section:

Physical Organic Chemistry

Amino→Imino Tautomerization upon in Vacuo Sublimation of 2-Methyltetrazole-Saccharinate as Probed by Matrix Isolation Infrared Spectroscopy

A. Ismael, A. Gómez-Zavaglia, A. Borba, M. L. S. Cristiano, and R. Fausto

pp 3190-3197

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

DOI: 10.1021/jp401360c

 Section:

Physical Organic Chemistry

**ENVIRONMENTAL AND ATMOSPHERIC CHEMISTRY, AEROSOL PROCESSES,
GEOCHEMISTRY, AND ASTROCHEMISTRY**

**An Isotherm-Based Thermodynamic Model of Multicomponent Aqueous
Solutions, Applicable Over the Entire Concentration Range**

Cari S. Dutcher, Xinlei Ge, Anthony S. Wexler, and Simon L. Clegg

pp 3198-3213

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

DOI: 10.1021/jp310860p

 Section:

Thermodynamics, Thermochemistry, and Thermal Properties

**MOLECULAR STRUCTURE, QUANTUM CHEMISTRY, AND GENERAL THEORY
Isomer-Selective Vibrational Spectroscopy of Jet-Cooled Phenol–Acetylene
Aggregates**

Markus Böning, Benjamin Stuhlmann, Gernot Engler, and Karl Kleinermanns

pp 3214-3220

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

DOI: 10.1021/jp3125796

 Section:

Physical Organic Chemistry

Estimating Chloride Polarizability in a Water Solution

Marco Masia

pp 3221-3226

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

DOI: 10.1021/jp400304g

 Section:

General Physical Chemistry

Molecular Structures for FeS_4^{-0} As Determined from an ab Initio Study of the Anion Photoelectron Spectra

Van Tan Tran and Marc F. A. Hendrickx

pp 3227-3234

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

DOI: 10.1021/jp401343j

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Computational Investigation of the Pyrolysis Product Selectivity for α -Hydroxy Phenethyl Phenyl Ether and Phenethyl Phenyl Ether: Analysis of Substituent Effects and Reactant Conformer Selection

Ariana Beste and A. C. Buchanan III

pp 3235-3242

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

DOI: 10.1021/jp4015004

 Section:

Physical Organic Chemistry

Complexes between Dihydrogen and Amine, Phosphine, and Arsine Derivatives. Hydrogen Bond versus Pnictogen Interaction

Stawomir J. Grabowski, Ibon Alkorta, and José Elguero

pp 3243-3251

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

DOI: 10.1021/jp4016933

 Section:

General Physical Chemistry