

# THE JOURNAL OF PHYSICAL CHEMISTRY A



Larger Cover

April 11, 2013

Volume 117, Issue 14

Pages 2891-3142

## **KINETICS AND DYNAMICS**

### **Collision-Induced Dissociation Studies on $\text{Fe}(\text{O}_2)_n^+$ ( $n = 1-6$ ) Clusters: Application of a New Technique Based on Crossed Molecular Beams**

Michalis Velegarakis, Claudia Mihesan, and Maria Jadraque

pp 2891-2898

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

DOI: 10.1021/jp310617e

 Section:

General Physical Chemistry

### **Probing the Photoisomerization of $\text{CHBr}_3$ and $\text{CHI}_3$ in Solution with Transient Vibrational and Electronic Spectroscopy**

Thomas J. Preston, Michael A. Shaloski, and F. Fleming Crim

pp 2899-2907

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

DOI: 10.1021/jp310737d

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

### **Heterogeneous Ozonolysis of Folpet and Dimethomorph: A Kinetic and Mechanistic Study**

Mariam J. Al Rashidi, Abdelkhaleq Chakir, and Estelle Roth

pp 2908-2915

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

DOI: 10.1021/jp3114896

 Section:

Agrochemical Bioregulators

### **Kinetics of the Gas Phase Reaction $\text{CH}_3 + \text{HO}_2$**

Manuvesh Sangwan and Lev N. Krasnoperov

pp 2916-2923

Publication Date (Web): March 4, 2013 (Article)

DOI: 10.1021/jp4000889

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

### **Kinetics and Mechanism of the Alkaline Decomposition of Hexathionate Ion**

Changwei Pan, Yang Liu, Attila K. Horváth, Zhen Wang, Ying Hu, Chen Ji, Yuemin Zhao, and Qingyu Gao

pp 2924-2931

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

DOI: 10.1021/jp400339u

 Section:

Physical Organic Chemistry

### **Reactivity of First-Row Transition Metal Monocations ( $\text{Sc}^+$ , $\text{Ti}^+$ , $\text{V}^+$ , $\text{Zn}^+$ ) with Methyl Fluoride: A Computational Study**

Pilar Redondo, Adrián Varela-Álvarez, Víctor Manuel Rayón, Antonio Largo, José Ángel Sordo, and Carmen Barrientos

pp 2932-2943

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

DOI: 10.1021/jp400366k

 Section:

Physical Organic Chemistry

**SPECTROSCOPY, PHOTOCHEMISTRY, AND EXCITED STATES**

## **Bis(porphyrin)–Anthraquinone Triads: Synthesis, Spectroscopy, and Photochemistry**

L. Giribabu, P. Silviya Reeta, Ravi Kumar Kanaparthi, Malladi Srikanth, and Y. Soujanya

pp 2944-2951

Publication Date (Web): March 19, 2013 (Article)

DOI: 10.1021/jp312134a

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

## **Structural Rearrangement in the Formation of Jet-Cooled Complexes of Chiral (S)-1,2,3,4-Tetrahydro-3-isoquinolinemethanol with Methyl Lactate: Chirality Effect in Conformer Selection**

Ahmed Mahjoub, Katia Le Barbu-Debus, and Anne Zehnacker

pp 2952-2960

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

DOI: 10.1021/jp400998e

Section:

Physical Organic Chemistry

## **Collision-Induced Dissociation and Infrared Photodissociation Studies of Methane Adsorption on $V_5O_{12}^+$ and $V_5O_{13}^+$ Clusters**

Bo Xu, Yan-Xia Zhao, Xun-Lei Ding, Qing-Yu Liu, and Sheng-Gui He

pp 2961-2970

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

DOI: 10.1021/jp401169p

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

## **Initial Processes of Proton Transfer in Salicylideneaniline Studied by Time-Resolved Photoelectron Spectroscopy**

Taro Sekikawa, Oliver Schalk, Guorong Wu, Andrey E. Boguslavskiy, and Albert Stolow

pp 2971-2979

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

DOI: 10.1021/jp4016036

Section:

Physical Organic Chemistry

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

**Enhancement of Gaseous Iodine Emission by Aqueous Ferrous Ions during the Heterogeneous Reaction of Gaseous Ozone with Aqueous Iodide**

Yosuke Sakamoto, Shinichi Enami, and Kenichi Tonokura

pp 2980-2986

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

DOI: 10.1021/jp308407j

 Section:

Mineralogical and Geological Chemistry

**Photochemical Aging of Light-Absorbing Secondary Organic Aerosol Material**

Neha Sareen, Samar G. Moussa, and V. Faye McNeill

pp 2987-2996

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

DOI: 10.1021/jp309413j

 Section:

Air Pollution and Industrial Hygiene

**Glycolaldehyde Monomer and Oligomer Equilibria in Aqueous Solution:  
Comparing Computational Chemistry and NMR Data**

Jeremy Kua, Melissa M. Galloway, Katherine D. Millage, Joseph E. Avila, and David O. De Haan

pp 2997-3008

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

DOI: 10.1021/jp312202j

 Section:

Physical Organic Chemistry

**Sputtering Effects and Water Formation on an Amorphous Silicate Surface**

Dapeng Jing, Jiao He, Massimo Bonini, John R. Brucato, and Gianfranco Vidali

pp 3009-3016

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

DOI: 10.1021/jp312816k

 Section:

Surface Chemistry and Colloids

**MOLECULAR STRUCTURE, QUANTUM CHEMISTRY, AND GENERAL THEORY**  
**Computational Study of the Coordination of Methane to First Row Transition Metal Dication Complexes**

Gavin W. Roffe and Hazel Cox

pp 3017-3024

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

DOI: 10.1021/jp309739s

 Section:

Organometallic and Organometalloidal Compounds

**Two-Dimensional Penning Ionization Electron Spectroscopy of Open-Shell Metallocenes: Outer Valence Ionic States of Vanadocene and Nickelocene**

Naoki Kishimoto, Miku Kimura, and Koichi Ohno

pp 3025-3033

Publication Date (Web): March 27, 2013 (Article)

DOI: 10.1021/jp310308k

 Section:

Organometallic and Organometalloidal Compounds

**Hydrogen Bonding in the Gas-Phase: The Molecular Structures of 2-Hydroxybenzamide ( $C_7H_7NO_2$ ) and 2-Methoxybenzamide ( $C_8H_9NO_2$ ), Obtained by Gas-Phase Electron Diffraction and Theoretical Calculations**

Kirsten Aarset, Elizabeth M. Page, and David A. Rice

pp 3034-3040

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

DOI: 10.1021/jp311003d

 Section:

Physical Organic Chemistry

**Anharmonic Vibrational Analysis of the Gas-Phase Infrared Spectrum of 1,1-Difluoroethylene Using the Operator Van Vleck Canonical Perturbation Theory**

Sergey V. Krasnoshchekov, Norman C. Craig, and Nikolay F. Stepanov

pp 3041-3056

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

DOI: 10.1021/jp311398z

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

**DFT Studies of Trans and Cis Influences in the Homolysis of the Co–C Bond in Models of the Alkylcobalamins**

Penny P. Govender, Isabelle Navizet, Christopher B. Perry, and Helder M. Marques

pp 3057-3068

Publication Date (Web): March 19, 2013 (Article)

DOI: 10.1021/jp311788t

 Section:

General Biochemistry

**Excited States of Large Open-Shell Molecules: An Efficient, General, and Spin-Adapted Approach Based on a Restricted Open-Shell Ground State Wave function**

Michael Roemelt and Frank Neese

pp 3069-3083

Publication Date (Web): March 19, 2013 (Article)

DOI: 10.1021/jp3126126

 Section:

General Physical Chemistry

**Probing Stereoelectronic Interactions in an O–N–O Unit by the Atomic Energies: Experimental and Theoretical Electron Density Study**

Yulia V. Nelyubina and Konstantin A. Lyssenko

pp 3084-3092

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

DOI: 10.1021/jp312835y

 Section:

Physical Organic Chemistry

**Probing the Electronic Properties of  $W_3O_x^{-/0}$  ( $x = 0-2$ ) and  $W_3^{2-}$  Clusters: The Aromaticity of  $W_3$  and  $W_3^{2-}$**

Shu-Juan Lin, Xian-Hui Zhang, Lei Xu, Bin Wang, Yong-Fan Zhang, and Xin Huang

pp 3093-3099

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

DOI: 10.1021/jp400673s

 Section:

General Physical Chemistry

### **Bond Order Analysis Based on the Laplacian of Electron Density in Fuzzy Overlap Space**

Tian Lu and Feiwu Chen

pp 3100-3108

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

DOI: 10.1021/jp4010345

 Section:

General Physical Chemistry

### **First Principles Studies toward the Design of Silylene Superbases: A Density Functional Theory Study**

Abul Kalam Biswas, Rabindranath Lo, and Bishwajit Ganguly

pp 3109-3117

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

DOI: 10.1021/jp401076j

 Section:

General Physical Chemistry

### **What Can We Learn about Dispersion from the Conformer Surface of *n*-Pentane?**

Jan M. L. Martin

pp 3118-3132

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

DOI: 10.1021/jp401429u

 Section:

Physical Organic Chemistry

### **Phosphorus As a Simultaneous Electron-Pair Acceptor in Intermolecular P $\cdots$ N Pnictogen Bonds and Electron-Pair Donor to Lewis Acids**

Janet E. Del Bene, Ibon Alkorta, Goar Sánchez-Sanz, and José Elguero

pp 3133-3141

**Publication Date (Web):** March 27, 2013 (Article)

**DOI:** 10.1021/jp401480y

