

FM
J80/pa

OCTOBER 9, 2014

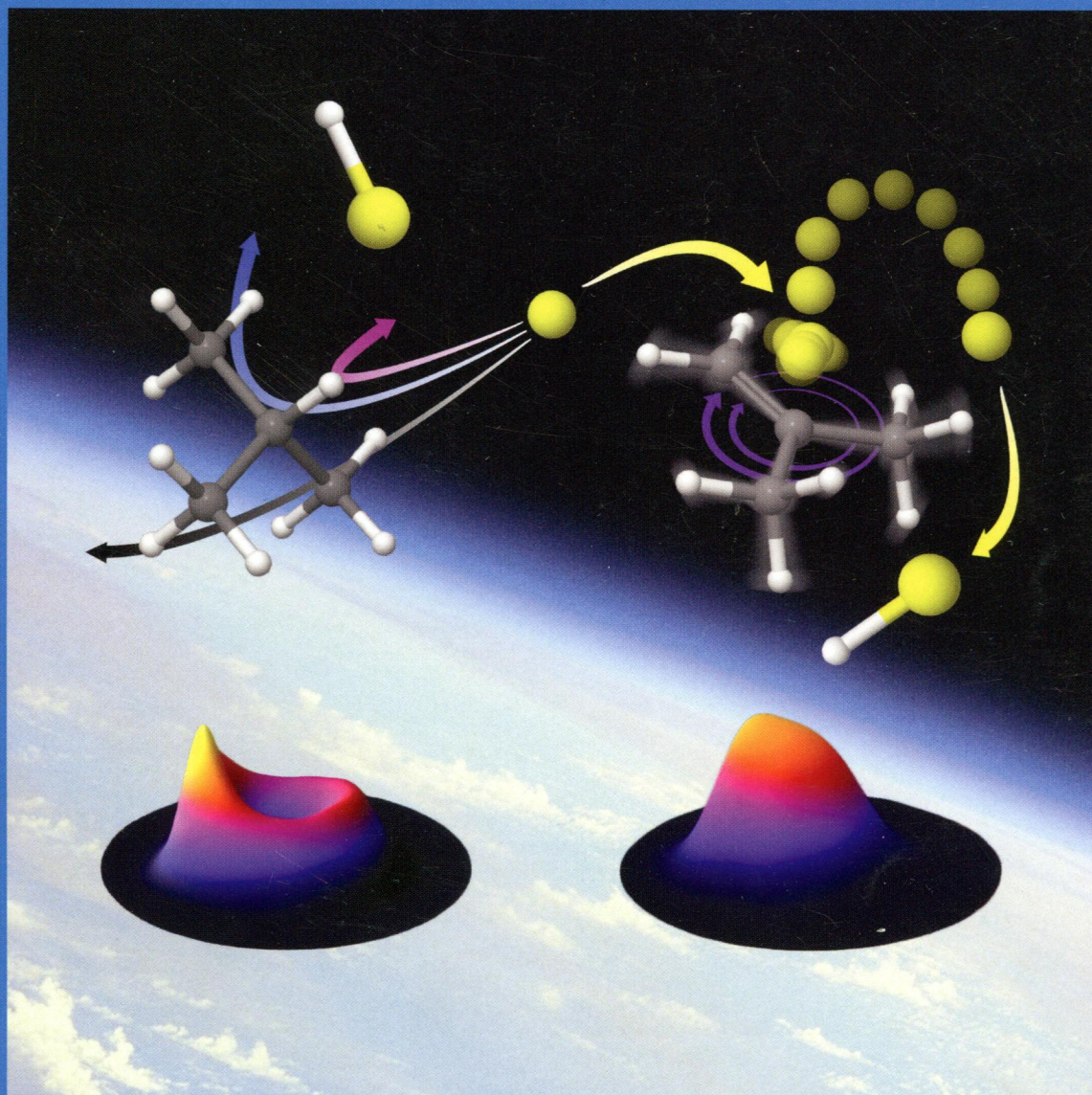
VOLUME 118

NUMBER 40

pubs.acs.org/JPCA

THE JOURNAL OF PHYSICAL CHEMISTRY

A



Roaming Dynamics
in Chlorine Atom
Addition/Elimination
Reactions with
Isobutene
(see page 9281)

ISOLATED MOLECULES, CLUSTERS, RADICALS, AND IONS; ENVIRONMENTAL CHEMISTRY,
GEOCHEMISTRY, AND ASTROCHEMISTRY; THEORY



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

ON THE COVER: Roaming dynamics in chlorine atom addition/elimination reactions with isobutene. Background photo courtesy of NASA (see page 9281).

Feature Article

- 9281 [dx.doi.org/10.1021/jp504804n](https://doi.org/10.1021/jp504804n)
Dynamics of Chlorine Atom Reactions with Hydrocarbons: Insights from Imaging the Radical Product in Crossed Beams
 Baptiste Joalland, Yuanyuan Shi, Armando D. Estillore, Alexander Kamasah, Alexander M. Mebel, and Arthur G. Suits*

Articles

Kinetics and Dynamics

- 9296 [dx.doi.org/10.1021/jp503570e](https://doi.org/10.1021/jp503570e)
Kinetic Modeling of α -Hydrogen Abstractions from Unsaturated and Saturated Oxygenate Compounds by Hydrogen Atoms
 Paschalis D. Paraskevas, Maarten K. Sabbe, Marie-Françoise Reyniers,* Nikos G. Papayannakos, and Guy B. Marin

- 9310 [dx.doi.org/10.1021/jp503794j](https://doi.org/10.1021/jp503794j)
Modeling Spin-Forbidden Monomer Self-Initiation Reactions in Spontaneous Free-Radical Polymerization of Acrylates and Methacrylates
 Shi Liu, Sriraj Srinivasan, Jianmin Tao, Michael C. Grady, Masoud Soroush, and Andrew M. Rappe*

- 9319 [dx.doi.org/10.1021/jp504132q](https://doi.org/10.1021/jp504132q)
Radiation-Induced Pink Nickel Oligomeric Clusters in Water. Pulse Radiolysis Study
 Mohamed Larbi Hioul, Mingzhang Lin, Jacqueline Belloni, Nassira Kéghouche, and Jean-Louis Marignier*

- 9330 [dx.doi.org/10.1021/jp504912j](https://doi.org/10.1021/jp504912j)
Kinetics and Dynamics on the Formation of $S_2(X^3\Sigma_g^-, a^1\Delta_g)$ in the $S(^1D) + OCS$ Reaction
 Jun Yamashita, Keigo Fujihara, Osamu Takahashi, Hiroshi Kohguchi, and Katsuyoshi Yamasaki*

- 9338 [dx.doi.org/10.1021/jp505742u](https://doi.org/10.1021/jp505742u)
Mechanism of Thermal Decomposition of Tetrabromobisphenol A (TBBA)
 Mohammednoor Altarawneh* and Bogdan Z. Dlugogorski

Unimolecular Reactions of 1,1,1-Trichloroethane, 1,1,1-Trichloropropane, and 3,3,3-Trifluoro-1,1,1-trichloropropane: Determination of Threshold Energies by Chemical Activation

Martha A. Turpin, Kylie C. Smith, George L. Heard, D. W. Setser, and Bert E. Holmes*

Experimental Binding Energies for the Metal Complexes $[\text{Mg}(\text{CH}_3\text{OH})_n]^{2+}$, $[\text{Ca}(\text{CH}_3\text{OH})_n]^{2+}$, and $[\text{Sr}(\text{CH}_3\text{OH})_n]^{2+}$ for n in the Range 4–20

E. Bruzzi and A. J. Stace*

Spectroscopy, Photochemistry, and Excited States**Thermochemistry of C_7H_{16} to $\text{C}_{10}\text{H}_{22}$ Alkane Isomers: Primary, Secondary, and Tertiary C–H Bond Dissociation Energies and Effects of Branching**

Jason M. Hudzik, Joseph W. Bozzelli,* and John M. Simmie

Octacoordinate Metal Carbonyls of Lanthanum and Cerium: Experimental Observation and Theoretical Calculation

Hua Xie, Jie Wang, Zhengbo Qin, Lei Shi, Zichao Tang,* and Xiaopeng Xing*

ZEKE Photoelectron Spectroscopy of p -Fluorophenol $\cdots\text{H}_2\text{S}/\text{H}_2\text{O}$ Complexes and Dissociation Energy Measurement Using the Birge–Spencer Extrapolation Method

Surjendu Bhattacharyya and Sanjay Wategaonkar*

Demonstration of Multiple Logic Operations in a Heteroditopic Pyrene–Phenylimidazole–Terpyridine Conjugate Based on Optical Responses by Selective Anions and Cations: An Experimental and Theoretical Investigation

Srikanta Karmakar, Dinesh Maity, Sourav Mardanya, and Sujoy Baitalik*

X-ray Spectroscopic Study of Solvent Effects on the Ferrous and Ferric Hexacyanide Anions

T. J. Penfold, M. Reinhard, M. H. Rittmann-Frank, I. Tavernelli, U. Tavernisberger, C. J. Milne, P. Glatzel, and M. Chergui*

Synthesis, Microwave Spectrum, Quantum Chemical Calculations, and Conformational Composition of a Novel Primary Phosphine, Cyclopropylethynylphosphine, $(\text{C}_3\text{H}_5\text{C}\equiv\text{CPH}_2)$

Harald Møllendal,* Svein Samdal, Jürgen Gauss, and Jean-Claude Guillemin*

9429



dx.doi.org/10.1021/jp506740r

Quantum Chemical Investigations on the Nonradiative Deactivation Pathways of Cytosine Derivatives
Akira Nakayama,* Shohei Yamazaki, and Tetsuya Taketsugu

9438



dx.doi.org/10.1021/jp507201a

Tunneling Dynamics of the NH_3 (\bar{A}) State Observed by Time-Resolved Photoelectron and H Atom Kinetic Energy Spectroscopies
Hui Yu, Nicholas L. Evans, Adam S. Chatterley, Gareth M. Roberts, Vasilios G. Stavros, and Susanne Ullrich*

9445

dx.doi.org/10.1021/jp507401y

Room Temperature Hole-Burning of X-ray Induced Sm^{2+} in Nanocrystalline $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{FCl}_{0.5}\text{Br}_{0.5}:\text{Sm}^{3+}$ Prepared by Mechanochemistry
Xianglei Wang, Hans Riesen,* Marion A. Stevens-Kalceff, and Rajitha Papakutty Rajan

9451



dx.doi.org/10.1021/jp5080626

Role of Bad Dihedral Angles: Methylfluorenes Act as Energy Barriers for Excitons and Polarons of Oligofluorenes
Tomoyasu Mani* and John R. Miller*

Environmental and Atmospheric Chemistry, Aerosol Processes, Geochemistry, and Astrochemistry

9460



dx.doi.org/10.1021/jp501380j

Kinetic and Dynamic Investigations of OH Reaction with Styrene
Joeson Cho, Masoud Roueintan, and Zhuangjie Li*

9471

dx.doi.org/10.1021/jp503572c

Reactive and Nonreactive Ozone Uptake during Aging of Oleic Acid Particles
Maxence Mendez, Nicolas Visez,* Sylvie Gosselin, Vincent Crenn, Veronique Riffault, and Denis Petitprez

9482



dx.doi.org/10.1021/jp507180g

Experimental Study of the Reactions of Limonene with OH and OD Radicals: Kinetics and Products
Tristan Braure, Yuri Bedjanian,* Manolis N. Romanias, Julien Morin, Véronique Riffault, Alexandre Tomas, and Patrice Coddeville

Molecular Structure, Quantum Chemistry, and General Theory

9491



dx.doi.org/10.1021/jp501289s









Negative Muon Chemistry: The Quantum Muon Effect and the Finite Nuclear Mass Effect
Edwin Posada, Félix Moncada, and Andrés Reyes*

9500



dx.doi.org/10.1021/jp5029257

Properties of Complexes Formed by Na^+ , Mg^{2+} , and Fe^{2+} Binding with Benzene Molecules
Sujitha Kolakkandy, Subha Pratihar, Adelia J. A. Aquino, Hai Wang, and William L. Hase*

- 9512  [dx.doi.org/10.1021/jp505183z](https://doi.org/10.1021/jp505183z)
Reactivity of CH_3 with OH Radicals: X-Abstraction Reaction Pathways (X = H, I), Atmospheric Chemistry, and Nuclear Safety
Mária Sudolská, Florent Louis,* and Ivan Černušák*
-
- 9521  [dx.doi.org/10.1021/jp5061107](https://doi.org/10.1021/jp5061107)
Substituted Corannulenes and Sumanenes as Fullerene Receptors. A Dispersion-Corrected Density Functional Theory Study
Daniela Josa, Jesús Rodríguez-Otero,* Enrique M. Cabaleiro-Lago, Lucas A. Santos, and Teodorico C. Ramalho
-
- 9529  [dx.doi.org/10.1021/jp506256a](https://doi.org/10.1021/jp506256a)
Anionic Halide...Alcohol Clusters in the Solid State
Pavel V. Gushchin, Maxim L. Kuznetsov, Matti Haukka, and Vadim Yu. Kukushkin*
-
- 9540  [dx.doi.org/10.1021/jp506355f](https://doi.org/10.1021/jp506355f)
Conformational, Spectroscopic, and Molecular Dynamics DFT Study of Precursors for New Potential Antibacterial Fluoroquinolone Drugs
Sandra Dorotíková, Kristína Plevová, Lukáš Bučinský,* Michal Malček, Peter Herich, Lenka Kucková, Miroslava Bobeničová, Stanislava Šoralová, Jozef Kožíšek, Marek Fronc, Viktor Milata, and Dana Dvoranová
-
- 9552  [dx.doi.org/10.1021/jp506663x](https://doi.org/10.1021/jp506663x)
Traditional and Ion-Pair Halogen-Bonded Complexes Between Chlorine and Bromine Derivatives and a Nitrogen-Heterocyclic Carbene
Oscar Donoso-Tauda,* Pablo Jaque, José Elguero, and Ibon Alkorta*
-
- 9561  [dx.doi.org/10.1021/jp506860t](https://doi.org/10.1021/jp506860t)
Accuracy of Dispersion Interactions in Semiempirical and Molecular Mechanics Models: The Benzene Dimer Case
Karol Strutyński, José A. N. F. Gomes, and Manuel Melle-Franco*
-
- 9568  [dx.doi.org/10.1021/jp506874q](https://doi.org/10.1021/jp506874q)
Temperature-Induced Reversible First-Order Single Crystal to Single Crystal Phase Transition in Boc- $\gamma^4(R)$ Val-Val-OH: Interplay of Enthalpy and Entropy
Rumpa Pal, M. B. Madhusudana Reddy, Bhimareddy Dinesh, Padmanabhan Balam, and Tayur N. Guru Row*
-
- 9575  [dx.doi.org/10.1021/jp5070598](https://doi.org/10.1021/jp5070598)
Effect of Ionic Charge on the $\text{CH}\cdots\pi$ Hydrogen Bond
Binod Nepal and Steve Scheiner*
-
- 9588  [dx.doi.org/10.1021/jp507129y](https://doi.org/10.1021/jp507129y)
Spin-Rotation and NMR Shielding Constants in XF Molecules (X = B, Al, Ga, In, and Tl)
Michał Jaszuński,* Taye B. Demissie, and Kenneth Ruud

Simple but Useful Scheme toward Understanding of Intramolecular Magnetic Interactions: Benzene-Bridged Oxoverdazyl Diradicals

Kyoung Chul Ko, Young Geun Park, Daeheum Cho, and Jin Yong Lee*

AuToGraFS: Automatic Topological Generator for Framework Structures

Matthew A. Addicoat,* Damien E. Coupry, and Thomas Heine

