

F001  
J80/pa

OCTOBER 16, 2014

VOLUME 118

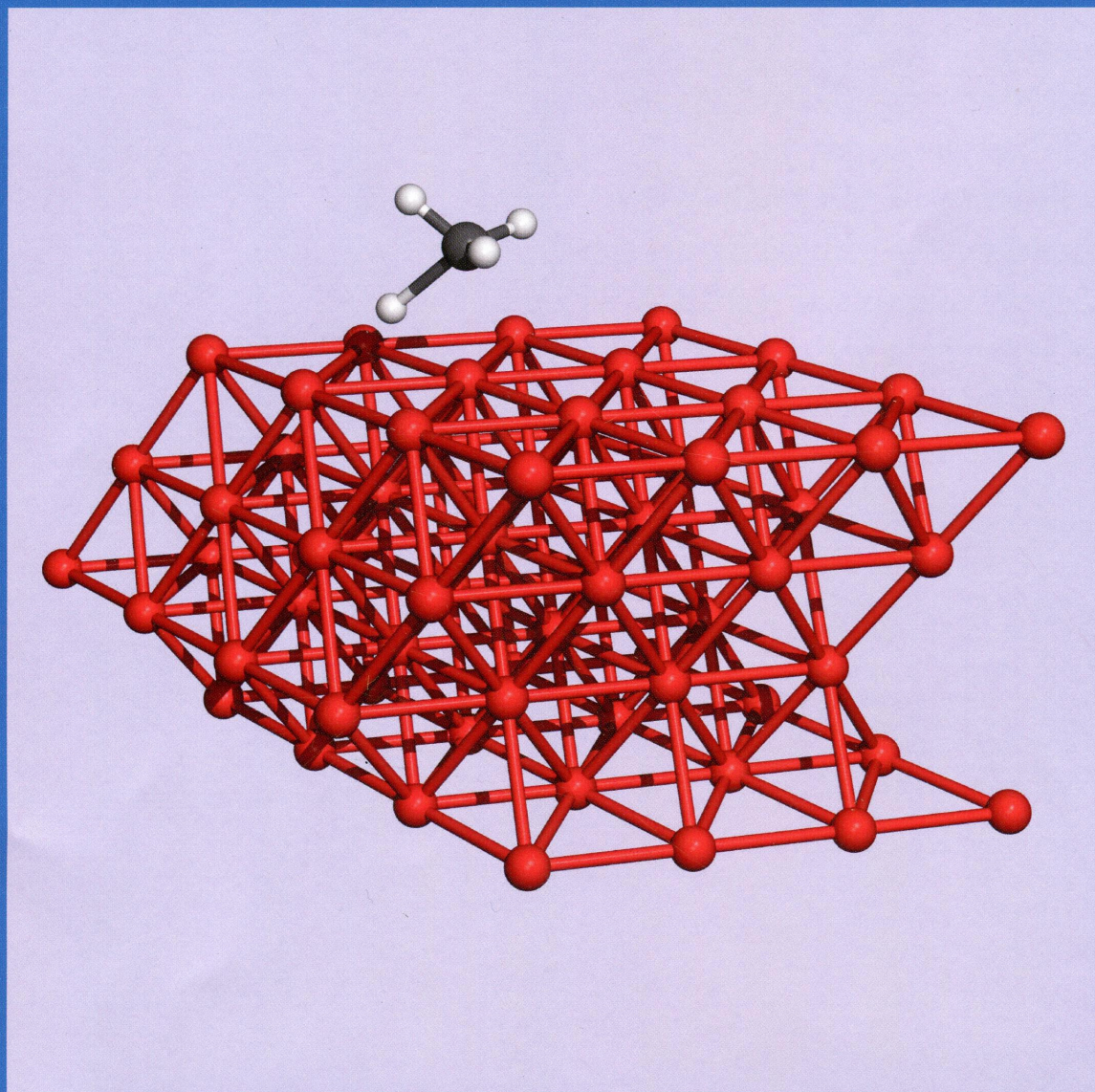
NUMBER 41

pubs.acs.org/JPCA

THE JOURNAL OF  
PHYSICAL  
CHEMISTRY

A

Transition State for  
Methane Dissociation  
on the (111) Surface  
of Ni  
(see page 9615)



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



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**ON THE COVER:** The rate-limiting step in the steam reforming of natural gas is the dissociative chemisorption of methane on a Ni-based catalyst. Shown on the cover is the transition state for this reaction on a Ni(111) surface. See page 9615.

## Feature Article

9615

[dx.doi.org/10.1021/jp5063644](https://doi.org/10.1021/jp5063644)

**Dissociative Chemisorption of Methane on Ni and Pt Surfaces: Mode-Specific Chemistry and the Effects of Lattice Motion**  
Sven Nave, Ashwani K. Tiwari, and Bret Jackson\*

## Articles

### Kinetics and Dynamics

9632

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[dx.doi.org/10.1021/jp507001r](https://doi.org/10.1021/jp507001r)

**Combined Crossed Molecular Beam and ab Initio Investigation of the Multichannel Reaction of Boron Monoxide (BO;  $X^2\Sigma^+$ ) with Propylene ( $CH_3CHCH_2$ ;  $X^1A'$ ): Competing Atomic Hydrogen and Methyl Loss Pathways**  
Surajit Maity, Beni B. Dangi, Dorian S. N. Parker, Ralf I. Kaiser,\* Yi An, Bing-Jian Sun, and A. H. H. Chang\*

9646

[dx.doi.org/10.1021/jp507696y](https://doi.org/10.1021/jp507696y)

**Collision Energy Dependent Cross Section and Rotational Alignment of NO ( $A^2\Sigma^+$ ) in the Energy-Transfer Reaction of  $N_2$  ( $A^3\Sigma_u^+$ ) + NO ( $X^2\Pi$ )  $\rightarrow$   $N_2$  ( $X^1\Sigma_g^+$ ) + NO ( $A^2\Sigma^+$ )**  
H. Ohoyama\*

### Spectroscopy, Photochemistry, and Excited States

9653

[dx.doi.org/10.1021/jp506272b](https://doi.org/10.1021/jp506272b)

**Quasiperiodic Energy Dependence of Exciton Relaxation Kinetics in the Sexithiophene Crystal**  
Piotr Petelenz\* and Emil Zak

9661

[dx.doi.org/10.1021/jp506890r](https://doi.org/10.1021/jp506890r)

**Solvent Dependent Switching of  $^3MLCT$  and  $^1IL$  Luminescent States in  $[ClRe(CO)_3(Bathocuproinedisulfonate)]^{2-}$ : Spectroscopic and Computational Study**  
Hector H. Martinez Saavedra, Fabricio Ragone, Gustavo T. Ruiz, Pedro M. David Gara,\* and Ezequiel Wolcan\*

9675  [dx.doi.org/10.1021/jp506948h](https://doi.org/10.1021/jp506948h)

**State-by-State Investigation of Destructive Interference in Resonance Raman Spectra of Neutral Tyrosine and the Tyrosinate Anion with the Simplified Sum-over-States Approach**

Jerry B. Cabalo,\* Semion K. Saikin, Erik D. Emmons, Dmitrij Rappoport, and Alán Aspuru-Guzik

9687  [dx.doi.org/10.1021/jp508207f](https://doi.org/10.1021/jp508207f)

**Photodissociation Spectroscopy of the Anionic Copper Nitrate Association Complex  $\text{Cu}(\text{NO}_3)_3^-$**

Sydney H. Kaufman and J. Mathias Weber\*

9692  [dx.doi.org/10.1021/jp5092653](https://doi.org/10.1021/jp5092653)

**Liquid Hot NAGMA Cooled to 0.4 K: Benchmark Thermochemistry of a Gas-Phase Peptide**

Christopher M. Leavitt, Kevin B. Moore III, Paul L. Raston, Jay Agarwal, Grant H. Moody, Caitlyne C. Shirley, Henry F. Schaefer III, and Gary E. Douberly\*

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

9701  [dx.doi.org/10.1021/jp505100x](https://doi.org/10.1021/jp505100x)

**Role of Tunable Acid Catalysis in Decomposition of  $\alpha$ -Hydroxyalkyl Hydroperoxides and Mechanistic Implications for Tropospheric Chemistry**

Manoj Kumar, Daryle H. Busch, Bala Subramaniam, and Ward H. Thompson\*

**Molecular Structure, Quantum Chemistry, and General Theory**

9712  [dx.doi.org/10.1021/jp505404w](https://doi.org/10.1021/jp505404w)

**Phase Transition Thermodynamics of Bisphenols**

José C. S. Costa, Juan Z. Dávalos,\* and Luís M. N. B. F. Santos\*

9720  [dx.doi.org/10.1021/jp507057r](https://doi.org/10.1021/jp507057r)

**Predicting Impact Sensitivities of Nitro Compounds on the Basis of a Semi-empirical Rate Constant**

Didier Mathieu\* and Thibaud Alaime

9727  [dx.doi.org/10.1021/jp507133n](https://doi.org/10.1021/jp507133n)

**Dealing with Quasi-Ring Formation by Two Hydrogen Bonds. Cooperativity Analysis with Delocalization Indices**

L. Guillaumes and S. Simon\*

9734  [dx.doi.org/10.1021/jp5073186](https://doi.org/10.1021/jp5073186)

**Joint Experimental and Theoretical Study on Vibrational Excitation Cross Sections for Electron Collisions with Diacetylene**

Roman Čurík,\* Ivana Paidarová, Michael Allan, and Petr Čárský\*

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[dx.doi.org/10.1021/jp507386j](https://doi.org/10.1021/jp507386j)**Electronic Structure of Cesium Butyratouranilate(VI) as Derived from DFT-assisted Powder X-ray Diffraction Data**

Anna V. Vologzhanina,\* Anton V. Savchenkov, Artem O. Dmitrienko, Alexander A. Korlyukov, Ivan S. Bushmarinov, Denis V. Pushkin, and Larisa B. Serezhkina

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[dx.doi.org/10.1021/jp507471z](https://doi.org/10.1021/jp507471z)**In Silico Studies to Explore the Mutagenic Ability of 5-Halo/Oxy/Li-Oxy-Uracil Bases with Guanine of DNA Base Pairs**

Kalyanashis Jana and Bishwajit Ganguly\*

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[dx.doi.org/10.1021/jp507726m](https://doi.org/10.1021/jp507726m)**Efficient Molecular Dynamics Simulations of Multiple Radical Center Systems Based on the Fragment Molecular Orbital Method**

Hiroya Nakata, Michael W. Schmidt, Dmitri G. Fedorov,\* Kazuo Kitaura, Shinichiro Nakamura, and Mark S. Gordon\*

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[dx.doi.org/10.1021/jp5079899](https://doi.org/10.1021/jp5079899)**Substituent-Modulated Affinities of Halobenzene Derivatives to the HIV-1 Integrase Recognition Site. Analyses of the Interaction Energies by Parallel Quantum Chemical and Polarizable Molecular Mechanics**

Krystal El Hage, Jean-Philip Piquemal, Zeina Hobaika, Richard G. Maroun, and Nohad Gresh\*

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[dx.doi.org/10.1021/jp508278d](https://doi.org/10.1021/jp508278d)**Effect of Acid Identity on the Geometry of Intermolecular Complexes: The Microwave Spectrum and Molecular Structure of Vinyl Chloride–HF**

Helen O. Leung\* and Mark D. Marshall\*

## Comments

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[dx.doi.org/10.1021/jp509101s](https://doi.org/10.1021/jp509101s)**Comment on “Analysis of CF<sup>+</sup>–FC Interactions on Cyclohexane and Naphthalene Frameworks”**

Vincent Tognetti,\* Meziane Yahia-Ouahmed, and Laurent Joubert\*

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[dx.doi.org/10.1021/jp509140n](https://doi.org/10.1021/jp509140n)**Comment on “Negative Thermal Expansion in Single-Component Systems with Isotropic Interactions”**

Vitaly A. Kuzkin\*