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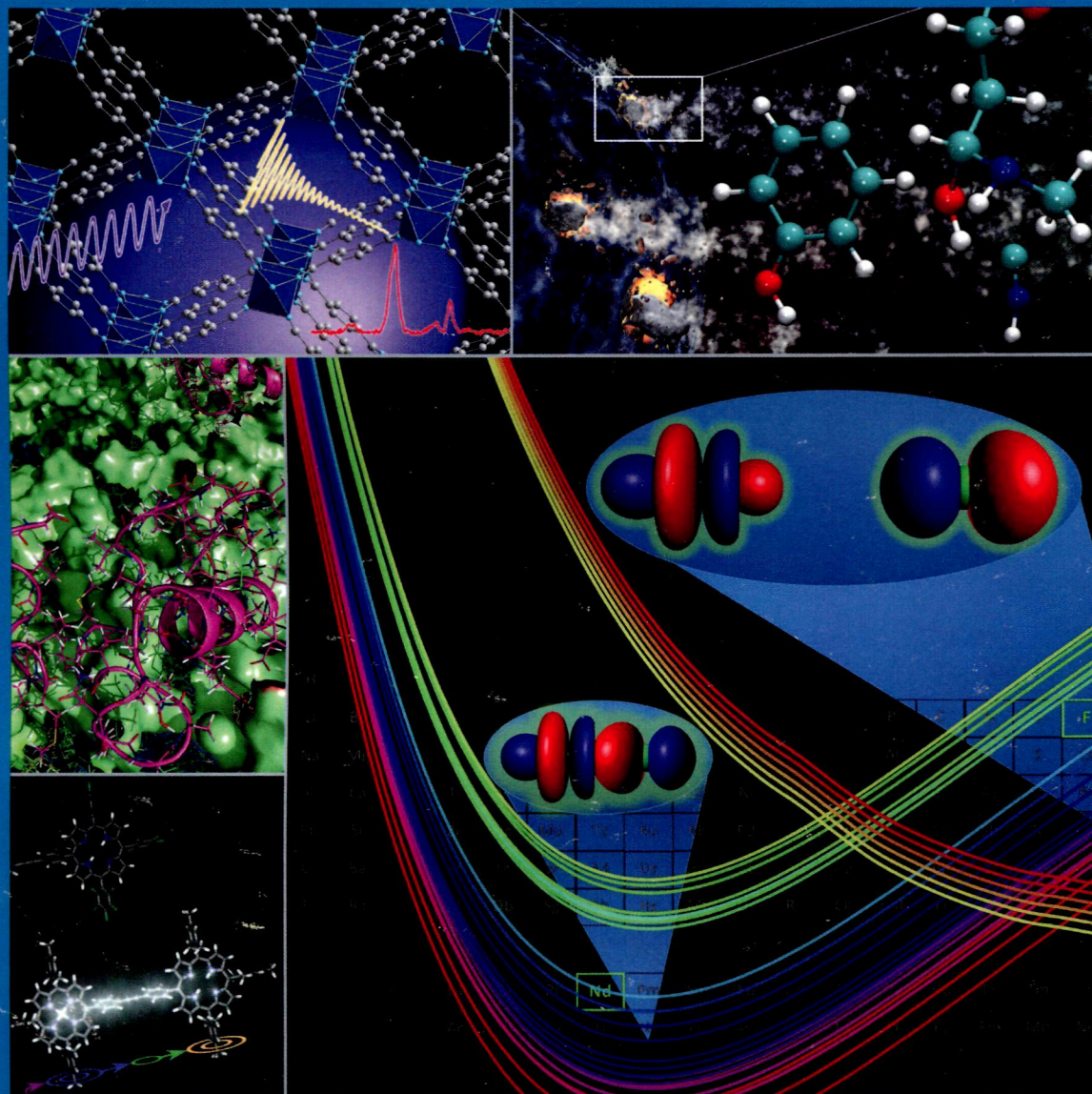
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**ON THE COVER:** Collage of cover art from recent issues of *J. Phys. Chem.* Top Left:  $^{17}\text{O}$  Solid-State NMR Spectra Provide Signatures of Various Oxygen Species in Metal-Organic Frameworks (*J. Phys. Chem. C* **2013**, *117* (33), 16953–16960). Center Left: Behavior of Amyloid  $\beta$ -Peptides on a Ganglioside-Containing Membrane Surface (*J. Phys. Chem. B* **2013**, *117* (27), 8085–8094). Bottom Left: Bridge-Mediated EET in Porphyrin Dimers: Electronic Coupling Reduced by Fluorination (*J. Phys. Chem. C* **2013**, *117* (24), 12423–12431). Top Right: Synthesis of Prebiotic Hydrocarbons in Impacts of Simple Icy Mixtures on Early Earth (*J. Phys. Chem. A* **2013**, *117* (24), 5124–5131). Bottom Right: Computed Potential Energy Curves for Quartet, Doublet, and Sextet States of  $\text{NdF}^{2+}$  (*J. Phys. Chem. A* **2013**, *117* (42), 10881–10888).

## Articles

### Kinetics and Dynamics

4363  [dx.doi.org/10.1021/jp4110147](https://doi.org/10.1021/jp4110147)


**Concentration-Dependent Dynamics of Hydrogen Bonding between Acetonitrile and Methanol As Determined by 1D Vibrational Spectroscopy**

Brian G. Alberding and Benjamin J. Lear\*

4372 [dx.doi.org/10.1021/jp411642w](https://doi.org/10.1021/jp411642w)

**Crossed Beam Reactions of the Phenyl ( $\text{C}_6\text{H}_5$ ;  $X^2A_1$ ) and Phenyl- $d_5$  Radical ( $\text{C}_6\text{D}_5$ ;  $X^2A_1$ ) with 1,2-Butadiene ( $\text{H}_2\text{CCCHCH}_3$ ;  $X^1A'$ )**

Tao Yang, Dorian S. N. Parker, Beni B. Dangi, Ralf I. Kaiser,\* Vadim V. Kislov, and Alexander M. Mebel

4382  [dx.doi.org/10.1021/jp501947y](https://doi.org/10.1021/jp501947y)

**Kinetic Studies of the Reduction of  $[\text{Co}(\text{dmgH})_2(\text{py})(\text{Cl})]$  Revisited: Mechanisms, Products, and Implications**

Axel Kahnt,\* Katrin Peuntinger, Claudia Dammann, Thomas Drewello, Ralf Hermann, Sergej Naumov, Bernd Abel, and Dirk M. Guldi\*

4392  [dx.doi.org/10.1021/jp503702t](https://doi.org/10.1021/jp503702t)

**Investigation of Thermochemistry Associated with the Carbon–Carbon Coupling Reactions of Furan and Furfural Using ab Initio Methods**

Cong Liu, Rajeev S. Assary, and Larry A. Curtiss\*

4405  [dx.doi.org/10.1021/jp503872m](https://doi.org/10.1021/jp503872m)

**Hydrogen Transfer Reaction in Polycyclic Aromatic Hydrocarbon Radicals**

Huiting Liu, Liuming Yan,\* Baohua Yue, and Aijun Li

4415  [dx.doi.org/10.1021/jp5001557](https://doi.org/10.1021/jp5001557)

**Unraveling the Electronic Structure of Azolehemiporphyrazines: Direct Spectroscopic Observation of Magnetic Dipole Allowed Nature of the Lowest  $\pi$ - $\pi^*$  Transition of  $20\pi$ -Electron Porphyrinoids**  
Atsuya Muranaka,\* Shino Ohira, Naoyuki Toriumi, Machiko Hirayama, Fumiko Kyotani, Yukie Mori, Daisuke Hashizume, and Masanobu Uchiyama\*

4425  [dx.doi.org/10.1021/jp5002435](https://doi.org/10.1021/jp5002435)

**Comprehensive Study of Ultrafast Excited-State Proton Transfer in Water and  $D_2O$  Providing the Missing  $RO^{\cdot-} \cdots H^+$  Ion-Pair Fingerprint**  
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4444  [dx.doi.org/10.1021/jp500495b](https://doi.org/10.1021/jp500495b)

**Photodissociation Dynamics of Allyl Chloride at 200 and 266 nm Studied by Time-Resolved Mass Spectrometry and Photoelectron Imaging**  
Huan Shen,\* Jianjun Chen, Linqiang Hua, and Bing Zhang\*

4451  [dx.doi.org/10.1021/jp501084b](https://doi.org/10.1021/jp501084b)

**Visible-Light Activation of the Bimetallic Chromophore–Catalyst Dyad: Analysis of Transient Intermediates and Reactivity toward Organic Sulfides**  
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4464  [dx.doi.org/10.1021/jp501773n](https://doi.org/10.1021/jp501773n)

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Miquel Huix-Rotllant\* and Nicolas Ferré\*

4471  [dx.doi.org/10.1021/jp501888c](https://doi.org/10.1021/jp501888c)

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Malgorzata Kauch and Magdalena Pecul\*

4480 [dx.doi.org/10.1021/jp502324p](https://doi.org/10.1021/jp502324p)

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4484 [dx.doi.org/10.1021/jp503198r](https://doi.org/10.1021/jp503198r)

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Chun C. Mak and Gilles H. Peslherbe\*

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dx.doi.org/10.1021/jp503263f

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N. V. Bashmakova, Ye. O. Shaydyuk, S. M. Levchenko, A. E. Masunov,\* O. V. Przhonska, J. L. Bricks, O. D. Kachkovsky, Yu. L. Slominsky, Yu. P. Piryatinski, K. D. Belfield, and M. V. Bondar\*

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dx.doi.org/10.1021/jp503761g

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Dmitry Khuseynov, Andrew R. Dixon, Daniel J. Dokuchitz, and Andrei Sanov\*

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dx.doi.org/10.1021/jp504107k

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Caixia Wang, Jiwen Jian, Guanjun Wang, Zhen Hua Li,\* and Mingfei Zhou\*

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dx.doi.org/10.1021/jp504689q

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Mamoru Fujitsuka,\* Chao Lu, Takahiro Iwamoto, Eiichi Kayahara, Shigeru Yamago, and Tetsuro Majima\*

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

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dx.doi.org/10.1021/jp500077f

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Runrun Wu, Shanshan Pan, Yun Li, and Liming Wang\*

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dx.doi.org/10.1021/jp500224j

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Karen J. Castle,\* Labe A. Black, and Tara J. Pedersen

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dx.doi.org/10.1021/jp502434t

**Radical-Induced *Cis*–*Trans* Isomerization of Fatty Acids: A Theoretical Study**

Yu-Zan Tzeng and Ching-Han Hu\*

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dx.doi.org/10.1021/jp502541y

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Victoria E. J. Berryman, Matthew G. Baker, and Russell J. Boyd\*

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[dx.doi.org/10.1021/jp502857d](https://doi.org/10.1021/jp502857d)

**A Simple Method for the Prediction of the Detonation Performances of Metal-Containing Explosives**

Yuan Wang, Jichuan Zhang, Hui Su, Shenghua Li,\* Shaowen Zhang, and Siping Pang\*

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[dx.doi.org/10.1021/jp503929g](https://doi.org/10.1021/jp503929g)

**DFT Modeling of CO<sub>2</sub> Interaction with Various Aqueous Amine Structures**

Tugba Davran-Candan\*

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## Additions and Corrections

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**Correction to "Phase-Matching and Dilution Effects in Two-Dimensional Femtosecond Stimulated Raman Spectroscopy"**

Barbara Dunlap, Kristina C. Wilson, and David W. McCamant\*

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