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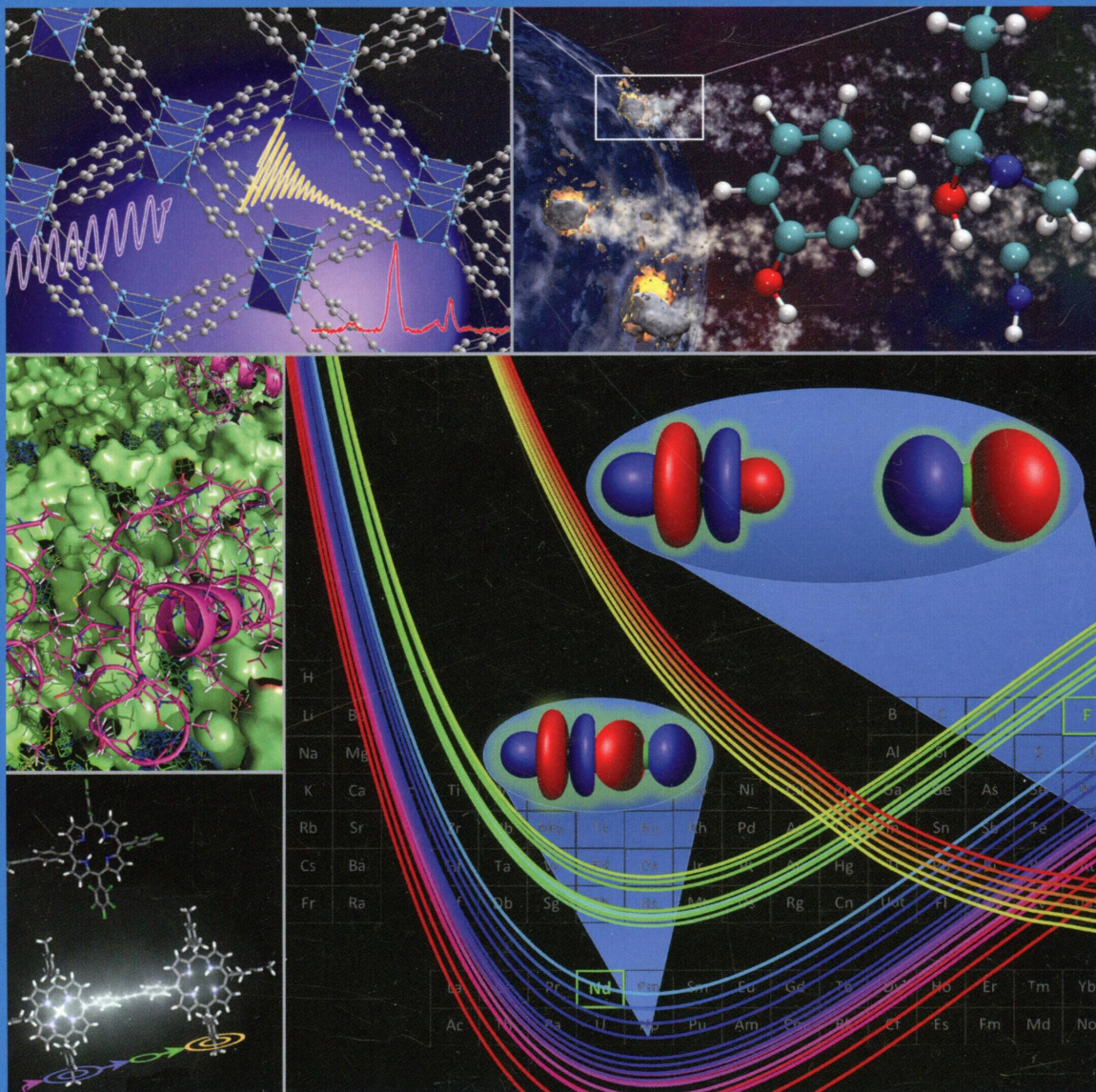
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ISOLATED MOLECULES, CLUSTERS, RADICALS, AND IONS; ENVIRONMENTAL CHEMISTRY,
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ON THE COVER: Collage of cover art from recent issues of *J. Phys. Chem.* Top Left: ^{17}O Solid-State NMR Spectra Provide Signatures of Various Oxygen Species in Metal-Organic Frameworks (*J. Phys. Chem. C* **2013**, *117* (33), 16953–16960). Center Left: Behavior of Amyloid β -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 NdF^{2+} (*J. Phys. Chem. A* **2013**, *117* (42), 10881–10888).

Articles

Kinetics and Dynamics

3211  [dx.doi.org/10.1021/jp4108987](https://doi.org/10.1021/jp4108987)

Radical Intermediates in the Addition of OH to Propene: Photolytic Precursors and Angular Momentum Effects

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3230  [dx.doi.org/10.1021/jp5014175](https://doi.org/10.1021/jp5014175)

Water-Accelerated OH Addition to Sulfur Dioxide SO_2 : Direct Ab Initio Molecular Dynamics (AIMD) Study

Hiroto Tachikawa*

3237 [dx.doi.org/10.1021/jp502023f](https://doi.org/10.1021/jp502023f)

Rate Constant and Mechanism of the Reaction $\text{Cl} + \text{CFCl}_2\text{H} \rightarrow \text{CFCl}_2 + \text{HCl}$ over the Temperature Range 298–670 K in N_2 or N_2/O_2 Diluent

E. W. Kaiser* and Khadija M. Jawad

3243 [dx.doi.org/10.1021/jp5028965](https://doi.org/10.1021/jp5028965)

Theoretical Kinetics Study of the $\text{O}(^3\text{P}) + \text{CH}_4/\text{CD}_4$ Hydrogen Abstraction Reaction: The Role of Anharmonicity, Recrossing Effects, and Quantum Mechanical Tunneling


Eloisa Gonzalez-Lavado, Jose C. Corchado, Yury V. Suleimanov,* William H. Green, and Joaquin Espinosa-Garcia*

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3253  [dx.doi.org/10.1021/jp500617n](https://doi.org/10.1021/jp500617n)

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3266 [dx.doi.org/10.1021/jp501763b](https://doi.org/10.1021/jp501763b)**Phenyl- vs Cyclohexyl-Substitution in Methanol: Implications for the OH Conformation and for Dispersion-Affected Aggregation from Vibrational Spectra in Supersonic Jets**

Jonas Altnöder, Sönke Oswald, and Martin A. Suhm*

3280 [dx.doi.org/10.1021/jp501784w](https://doi.org/10.1021/jp501784w)**Vaporization of Protic Ionic Liquids Studied by Matrix-Isolation Fourier Transform Infrared Spectroscopy**

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[dx.doi.org/10.1021/jp5019058](https://doi.org/10.1021/jp5019058)**Interplay between Temperature-Activated Vibrations and Nondipolar Effects in the Valence Excitations of the CO₂ Molecule**

Juho Inkinen, Johannes Niskanen,* Arto Sakko, Kari O. Ruotsalainen, Tuomas Pylkkänen, Szabolcs Galambosi, Mikko Hakala, Giulio Monaco, Keijo Hämläinen, and Simo Huotari*

Environmental and Atmospheric Chemistry, Aerosol Processes, Geochemistry, and Astrochemistry3295 [dx.doi.org/10.1021/jp411477e](https://doi.org/10.1021/jp411477e)**Mass Spectrometric and Computational Studies on the Reaction of Aromatic Peroxyl Radicals with Phenylacetylene Using the Distonic Radical Ion Approach**

George N. Khairallah, Richard A. J. O'Hair, and Uta Wille*

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[dx.doi.org/10.1021/jp501472s](https://doi.org/10.1021/jp501472s)**¹H NMR Diffusion Studies of Water Self-Diffusion in Supercooled Aqueous Sodium Chloride Solutions**


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Molecular Structure, Quantum Chemistry, and General Theory3313 [dx.doi.org/10.1021/jp410811m](https://doi.org/10.1021/jp410811m)**Theoretical Study on the Kinetics of the Reaction CH₂Br + NO₂**

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3319 [dx.doi.org/10.1021/jp411400m](https://doi.org/10.1021/jp411400m)**Thermodynamic Stability versus Kinetic Stability: Is the Planar Hexacoordinate Carbon Species D_{3h} CN₃Mg₃⁺ Viable?**

Chao-Feng Zhang, Shao-Jin Han, Yan-Bo Wu,* Hai-Gang Lu, and Gang Lu

3326 [dx.doi.org/10.1021/jp500518b](https://doi.org/10.1021/jp500518b)**Neutral Compounds with Xenon–Germanium Bonds: A Theoretical Investigation on FXeGeF and FXeGeF₃**

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Theoretical Design of n-Type Organic Semiconducting Materials Containing Thiazole and Oxazole Frameworks

Vu Thi Thu Huong, Truong Ba Tai, and Minh Tho Nguyen*

3344 dx.doi.org/10.1021/jp5014972

Tunable Fictitious Substituent Effects on the π - π Interactions of Substituted Sandwich Benzene Dimers

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3360  dx.doi.org/10.1021/jp502468s

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Tiago L.P. Galvão, Inês M. Rocha, Maria D.M.C. Ribeiro da Silva,* and Manuel A.V. Ribeiro da Silva

3367 dx.doi.org/10.1021/jp502491a

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Stefano Pelloni,* Guglielmo Monaco,* Paolo Della Porta, Riccardo Zanasi, and Paolo Lazzaretti

3376  dx.doi.org/10.1021/jp502588h

Homogeneous and Heterogeneous Noncovalent Dimers of Formaldehyde and Thioformaldehyde: Structures, Energetics, and Vibrational Frequencies

Eric Van Dornshuld, Christina M. Holy, and Gregory S. Tschumper*

3386  dx.doi.org/10.1021/jp502667k

Pnicogen-Bonded Anionic Complexes

Janet E. Del Bene,* Ibon Alkorta,* and José Elguero

Additions and Corrections

3393 dx.doi.org/10.1021/jp5039199

Correction to "Spiropyran to Merocyanine Conversion: Explicit versus Implicit Solvent Modeling"

Andrzej Eilmes*