

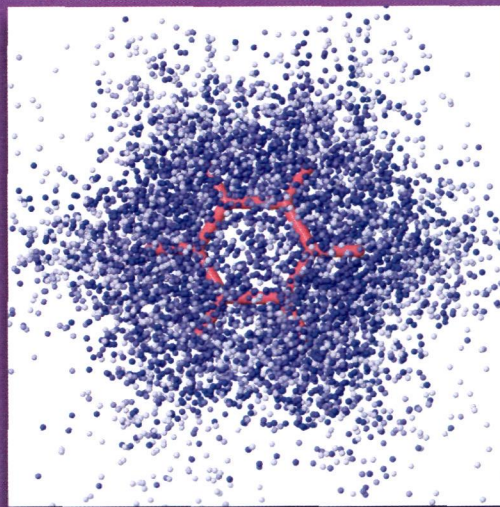
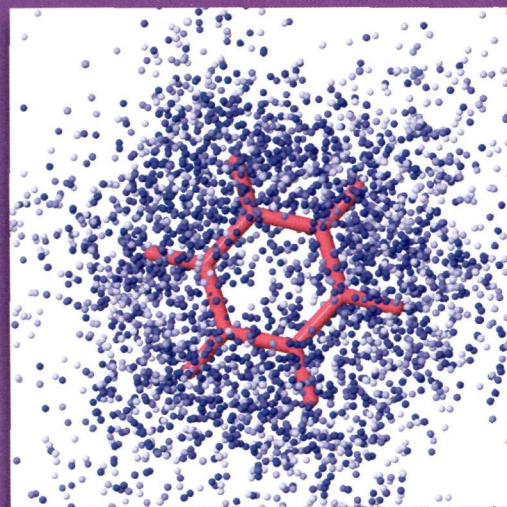
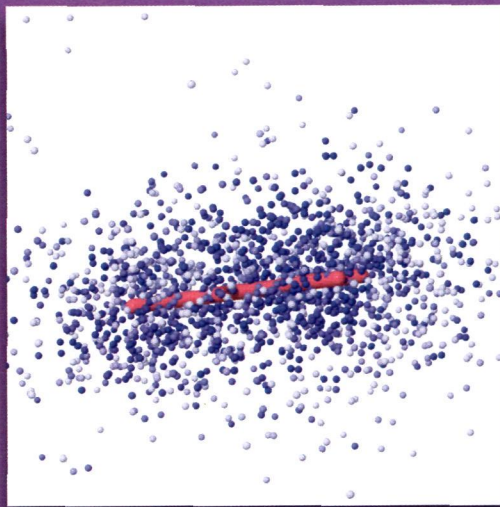
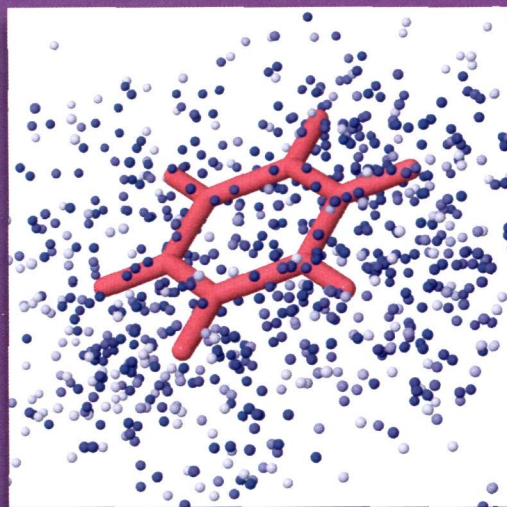
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# THE JOURNAL OF PHYSICAL CHEMISTRY

**A**

Electron–Electron  
Walker Pairs in  
Monte Carlo  
Second-Order  
Many-Body  
Perturbation Theory  
(see page 5A)

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



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**ON THE COVER:** Cover graphics show the distribution of electron coordinates in the first 1000 (top left), 2000 (top right), 4000 (bottom left), and 8000 (bottom right) electron–electron pairs generated by the Metropolis algorithm in a Monte Carlo second-order many-body perturbation calculation of benzene. The darker shade of blue means a shorter electron–electron distance, where the Coulomb repulsion is greater. See page 655.

## Feature Article

655 [dx.doi.org/10.1021/jp410587b](https://doi.org/10.1021/jp410587b)  
**Second-Order Many-Body Perturbation Theory: An Eternal Frontier**  
So Hirata,\* Xiao He, Matthew R. Hermes, and Soohaeng Y. Willow

## Articles

### Kinetics and Dynamics

673  [dx.doi.org/10.1021/jp4107102](https://doi.org/10.1021/jp4107102)  
**Products from the Oxidation of Linear Isomers of Hexene**  
Frédérique Battin-Leclerc,\* Anne Rodriguez, Benoit Husson, Olivier Herbinet, Pierre-Alexandre Glaude, Zhandong Wang, Zhanjun Cheng, and Fei Qi

684 [dx.doi.org/10.1021/jp5000655](https://doi.org/10.1021/jp5000655)  
**Mode-Specific Tunneling in the Unimolecular Dissociation of *cis*-HOCO to H + CO<sub>2</sub>**  
Xiaohong Wang and Joel M. Bowman\*

### Spectroscopy, Photochemistry, and Excited States

690 [dx.doi.org/10.1021/jp407997w](https://doi.org/10.1021/jp407997w)  
**New Fragmentation Pathways in K–THF Collisions As Studied by Electron-Transfer Experiments: Negative Ion Formation**  
D. Almeida, F. Ferreira da Silva, S. Eden, G. Garcia, and P. Limão-Vieira\*

697 [dx.doi.org/10.1021/jp4110085](https://doi.org/10.1021/jp4110085)  
**Matrix Photochemical Study and Conformational Analysis of CH<sub>3</sub>C(O)NCS and CF<sub>3</sub>C(O)NCS**  
Luis A. Ramos, Sonia E. Ulic, Rosana M. Romano, Helmut Beckers, Helge Willner, and Carlos O. Della Védova\*

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[dx.doi.org/10.1021/jp411257k](https://doi.org/10.1021/jp411257k)**Polarized Matrix Infrared Spectra of Cyclopentadienone: Observations, Calculations, and Assignment for an Important Intermediate in Combustion and Biomass Pyrolysis**

Thomas K. Ormond, Adam M. Scheer, Mark R. Nimlos, David J. Robichaud, John W. Daily, John F. Stanton, and G. Barney Ellison\*

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[dx.doi.org/10.1021/jp411415p](https://doi.org/10.1021/jp411415p)**High-Energy Chemistry of Formamide: A Simpler Way for Nucleobase Formation**

Martin Ferus, Regina Michalčíková, Violetta Shestivská, Jiří Šponer, Judit E. Šponer,\* and Svatopluk Civiš\*

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[dx.doi.org/10.1021/jp411893p](https://doi.org/10.1021/jp411893p)**Interaction between Freons and Amines: The C–H···N Weak Hydrogen Bond in Quinuclidine–Trifluoromethane**

Qian Gou, Gang Feng, Luca Evangelisti, and Walther Caminati\*

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

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[dx.doi.org/10.1021/jp407058b](https://doi.org/10.1021/jp407058b)**Measuring Rate Constants for Reactions of the Simplest Criegee Intermediate (CH<sub>2</sub>OO) by Monitoring the OH Radical**

Yingdi Liu, Kyle D. Bayes,\* and Stanley P. Sander

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

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[dx.doi.org/10.1021/jp408103y](https://doi.org/10.1021/jp408103y)**Analytic Density Functional Theory Calculations of Pure Vibrational Hyperpolarizabilities: The First Dipole Hyperpolarizability of Retinal and Related Molecules**

Bin Gao, Magnus Ringholm, Radovan Bast, Kenneth Ruud,\* Andreas J. Thorvaldsen, and Michał Jaszuński

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[dx.doi.org/10.1021/jp410407u](https://doi.org/10.1021/jp410407u)**Evaluating Charge Transfer in Epicocconone Analogues: Toward a Targeted Design of Fluorophores**

Olga A. Syzgantseva, Vincent Tognetti,\* Agathe Boulangé, Philippe A. Peixoto, Stéphane Leleu, Xavier Franck, and Laurent Joubert

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[dx.doi.org/10.1021/jp410496t](https://doi.org/10.1021/jp410496t)**Reaction Profiles and Energy Surfaces of Compressed Species**

Jacob Spooner, Brandon Yanciw, Brandon Wiebe, and Noham Weinberg\*

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[dx.doi.org/10.1021/jp411502u](https://doi.org/10.1021/jp411502u)**Phenol–Quinone Tautomerism in (Arylazo)naphthols and the Analogous Schiff Bases: Benchmark Calculations**

S. Tahir Ali, Liudmil Antonov, and Walter M. F. Fabian\*

**Additions and Corrections**

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[dx.doi.org/10.1021/jp500307r](https://doi.org/10.1021/jp500307r)**Correction to “Magnetic Circular Dichroism Spectroscopy of *N*-Confused Porphyrin and Its Ionized Forms”**

Christopher J. Ziegler,\* Nathan R. Erickson, Michael R. Dahlby, and Victor N. Nemykin\*

S Supporting Information available via online article