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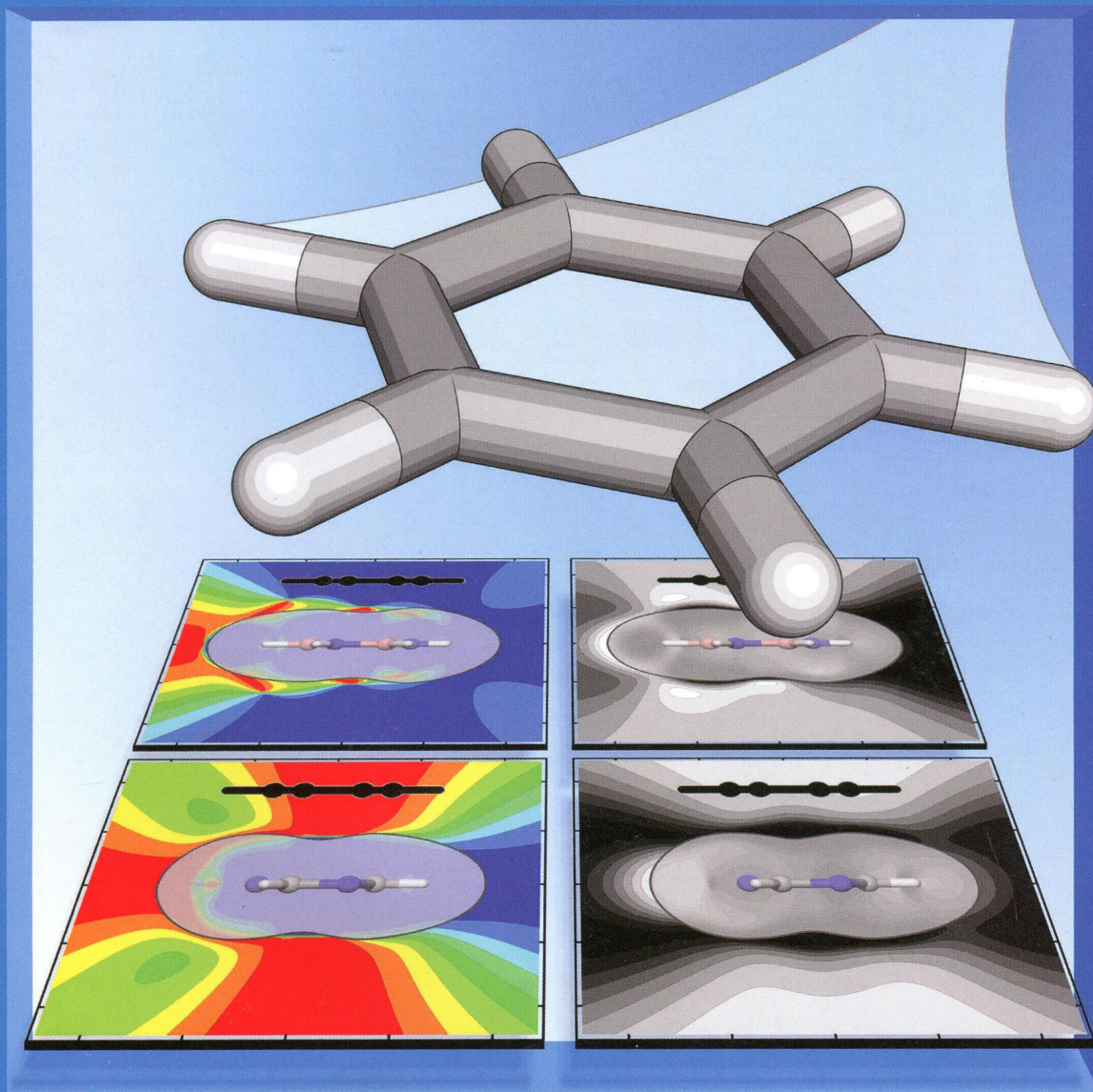
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THE JOURNAL OF PHYSICAL CHEMISTRY

A

Unraveling Substituent
Effects in π -Stacking
Interactions through
Examination of
Electric Fields
(see page 5A)



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



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ON THE COVER: Unraveling substituent effects in π -stacking interactions through examination of electric fields. Noncovalent interactions involving aromatic rings are central to many areas of physical chemistry. Recently, it has been revealed that substituent effects in π -stacking interactions are dominated by the interaction of the local dipole associated with the substituent and the electric field of the other ring. Consequently, comparing the strengths and direction of the electric fields surrounding unsubstituted arenes can explain trends in substituent effects in stacking interactions involving these systems. Bottom four figures adapted from: Raju, R. K.; Bloom, J. W. G.; Wheeler, S. E. Broad Transferability of Substituent Effects in π -Stacking Interactions Provides New Insights into Their Origin. *J. Chem. Theory Comput.* **2013**, *9*, 3479–3490. See page 6133.

Feature Article

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[dx.doi.org/10.1021/jp504415p](https://doi.org/10.1021/jp504415p)

Toward a More Complete Understanding of Noncovalent Interactions Involving Aromatic Rings

Steven E. Wheeler* and Jacob W. G. Bloom

Articles

Kinetics and Dynamics

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[dx.doi.org/10.1021/jp502891p](https://doi.org/10.1021/jp502891p)

Ultrafast Shock Compression of an Oxygen-Balanced Mixture of Nitromethane and Hydrogen Peroxide

Michael R. Armstrong,* Joseph M. Zaug, Christian D. Grant, Jonathan C. Crowhurst, and Sorin Bastea

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[dx.doi.org/10.1021/jp505346g](https://doi.org/10.1021/jp505346g)

EPR Line Shifts and Line Shape Changes Due to Heisenberg Spin Exchange and Dipole–Dipole Interactions of Nitroxide Free Radicals in Liquids: 9. An Alternative Method to Separate the Effects of the Two Interactions Employing ^{15}N and ^{14}N

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[dx.doi.org/10.1021/jp5054343](https://doi.org/10.1021/jp5054343)

Kinetics and Mechanism of the Tropospheric Reaction of 3-Hydroxy-3-methyl-2-butanone with Cl Atoms

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[dx.doi.org/10.1021/jp5057573](https://doi.org/10.1021/jp5057573)

A Possible Candidate to Be Classified as an Autocatalysis-Driven Clock Reaction: Kinetics of the Pentathionate–Iodate Reaction

Li Xu and Attila K. Horváth*

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[dx.doi.org/10.1021/jp505868q](https://doi.org/10.1021/jp505868q)

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

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[dx.doi.org/10.1021/jp503722m](https://doi.org/10.1021/jp503722m)

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[dx.doi.org/10.1021/jp505331s](https://doi.org/10.1021/jp505331s)

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[dx.doi.org/10.1021/jp504348f](https://doi.org/10.1021/jp504348f)

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[dx.doi.org/10.1021/jp505590g](https://doi.org/10.1021/jp505590g)

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[dx.doi.org/10.1021/jp505764k](https://doi.org/10.1021/jp505764k)

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Anissa Amar, Hacène Meghezzi, Julien Boixel, Hubert Le Bozec, Véronique Guerchais,* Denis Jacquemin, and Abdou Boucekkine*

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A Unified Perspective on the Nature of Bonding in Pairwise Interatomic Interactions

R. R. Lucchese, C. K. Rosales, L. A. Rivera-Rivera, B. A. McElmurry, J. W. Bevan,* and J. R. Walton

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