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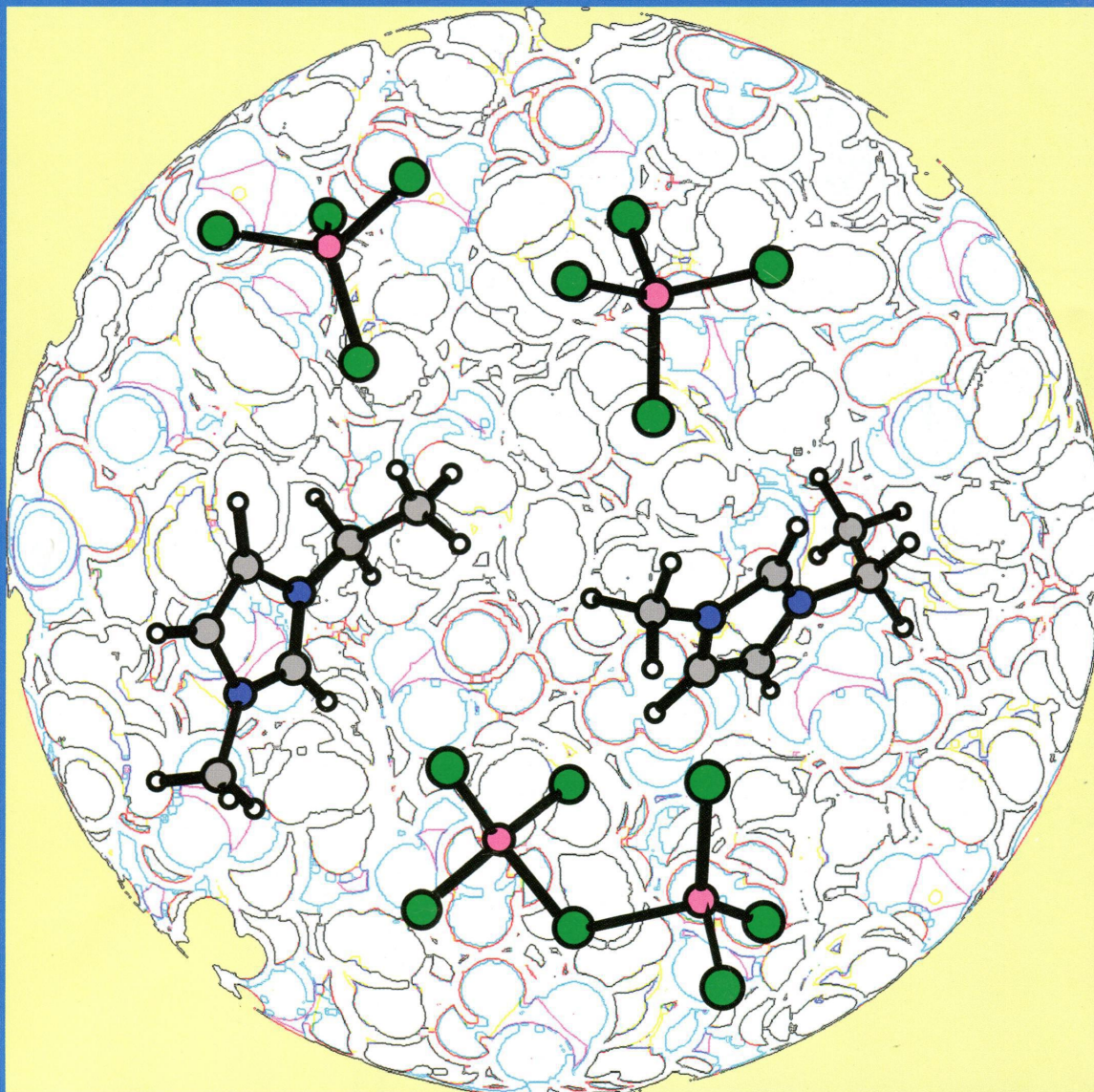
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THE JOURNAL OF PHYSICAL CHEMISTRY

A

Artistic Interpretation
of a 1-Ethyl-3-
methylimidazolium
Chloroaluminate
Ionic Liquid
(see page 11653)



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



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ON THE COVER: As a reaction medium, ionic liquids have been reported to enhance rates and stereoselectivities for numerous chemical reactions. In some extreme cases, these molten salts have been shown to induce mechanistic changes relative to conventional solvents. This feature article reviews our efforts developing and applying mixed quantum and molecular mechanical (QM/MM) methodology to elucidate the microscopic details of how these solvents operate on industrially and academically important reactions. Technical advances are also discussed. See page 11653.

Feature Article

11653

DOI: 10.1021/jp507967z

Simulating Chemical Reactions in Ionic Liquids Using QM/MM Methodology

Orlando Acevedo*

Articles

Kinetics and Dynamics

11667



DOI: 10.1021/jp5066874

Ion-Specific Solvation Water Dynamics: Single Water versus Collective Water Effects

Klaus F. Rinne, Stephan Gekle, and Roland R. Netz*

11678

DOI: 10.1021/jp509246s

Chemical Waves in Heterogeneous Media

Mahmoud M. Ayass, Mazen Al-Ghoul, and István Lagzi*

11683

DOI: 10.1021/jp509891w

Quasiclassical Trajectory Study of the Rotational Mode Specificity in the $O(^3P) + CHD_3(v_1 = 0, 1, JK) \rightarrow OH + CD_3$ Reactions

Gábor Czakó*

11688

DOI: 10.1021/jp510227k

Thermal Decomposition of 1,1,1-Trifluoroethane Revisited

Akira Matsugi,* Kenji Yasunaga, and Hiroumi Shiina

Spectroscopy, Photochemistry, and Excited States

11696 DOI: 10.1021/jp5099393

Chimeric Behavior of Excited Thioxanthone in Protic Solvents: I. Experiments

T. Villnow, G. Ryseck, V. Rai-Constapel, C. M. Marian, and P. Gilch*

11708 DOI: 10.1021/jp5099415

Chimeric Behavior of Excited Thioxanthone in Protic Solvents: II. Theory

Vidisha Rai-Constapel, Torben Villnow, Gerald Ryseck, Peter Gilch, and Christel M. Marian*

11718  DOI: 10.1021/jp508513p

Mechanism of Co–C Bond Photolysis in the Base-On Form of Methylcobalamin

Piotr Lodowski, Maria Jaworska, Tadeusz Andruniów, Brady D. Garabato, and Pawel M. Kozlowski*

11735  DOI: 10.1021/jp509987p

Photophysics of Organometallic Platinum(II) Derivatives of the Diketopyrrolopyrrole Chromophore

Subhadip Goswami, Russell W. Winkel, Erkki Alarousu, Ion Ghiviriga, Omar F. Mohammed, and Kirk S. Schanze*

11744  DOI: 10.1021/jp510119e

Fourier Transform Microwave and Millimeter-Wave Spectroscopy of Bromiodomethane, CH₂BrI

S. Bailleux,* D. Duflot, K. Taniguchi, S. Sakai, H. Ozeki, T. Okabayashi, and W. C. Bailey

11751  DOI: 10.1021/jp511428v

Short-Range Solvation Effects on Chiroptical Properties: A Time-Dependent Density Functional Theory and *ab Initio*

Molecular Dynamics Computational Case Study on Austdiol

Daniele Tedesco, Riccardo Zanasi, Barbara Kirchner, and Carlo Bertucci*

Molecular Structure, Quantum Chemistry, and General Theory

11758 DOI: 10.1021/jp505722y

Electronic Spectrum of the UO and UO⁺ Molecules

Rajni Tyagi, Zhiyong Zhang, and Russell M. Pitzer*

11768  DOI: 10.1021/jp507793v

Challenges in Predicting $\Delta_{\text{en}}G$ in Solution: The Mechanism of Ether-Catalyzed Hydroboration of Alkenes

Daniel J. S. Sandbeck, Colin M. Kuntz, Christine Luu, Rachele A. Mondor, John G. Ottaviano, Aravind V. Rayer, Kazi Z. Sumon, and Allan L. L. East*

11780 DOI: 10.1021/jp509526a

Ring-Puckering Effects on Electron Momentum Distributions of Valence Orbitals of Oxetane

Jing Yang, Xu Shan, Zhe Zhang, Yaguo Tang, Minfu Zhao, and XiangJun Chen*

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DOI: 10.1021/jp510062b

Can Short- and Middle-Range Hybrids Describe the Hyperpolarizabilities of Long-Range Charge-Transfer Compounds?

Alejandro J. Garza, Nuha A. Wazzan, Abdullah M. Asiri, and Gustavo E. Scuseria*

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DOI: 10.1021/jp5101126

Benchmarking the DFT+*U* Method for Thermochemical Calculations of Uranium Molecular Compounds and Solids

George Beridze and Piotr M. Kowalski*

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DOI: 10.1021/jp510249v

Simplified Wave Function Models in Thermochemical Protocols Based on Bond Separation Reactions

Dirk Bakowies*

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DOI: 10.1021/jp510362p

Probing the Radical and Base Dual Properties of Peptide Sulfinyl Radicals via Mass Spectrometry

Lei Tan, František Tureček, Joseph S. Francisco,* and Yu Xia*

5 Supporting Information available via online article