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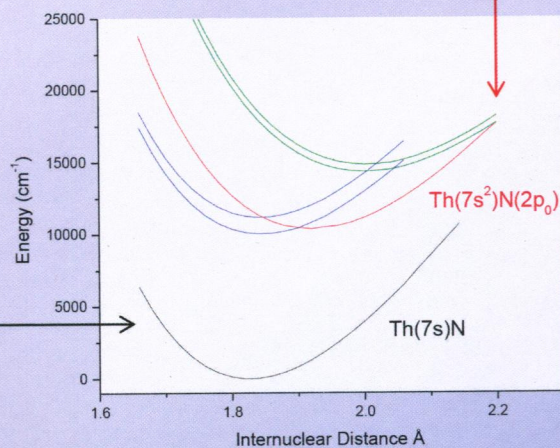
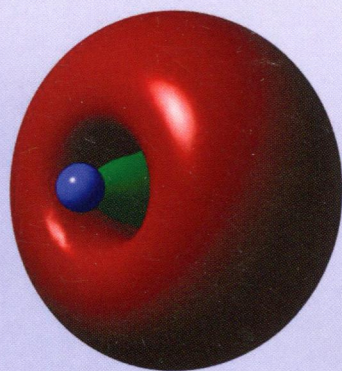
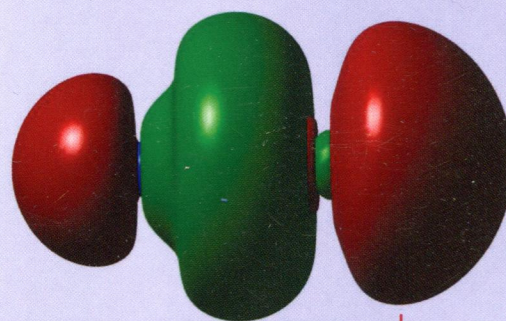
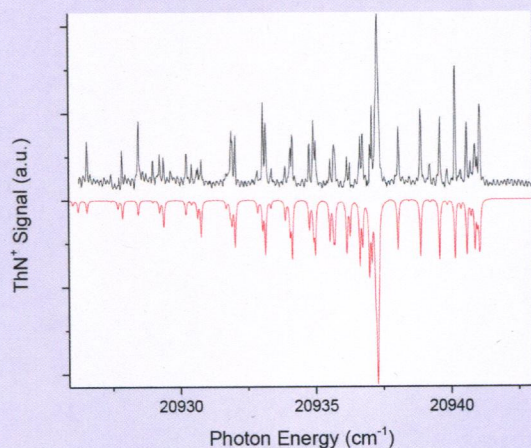
NUMBER 46

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# THE JOURNAL OF PHYSICAL CHEMISTRY

A

Probing the Nature of  
Actinide Bonds Using  
Electronic Spectroscopy  
and Multiphoton  
Ionization  
(see page 10867)



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



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**ON THE COVER:** The cover shows the essential components of the method used to investigate actinide bonding characteristics. The key experimental data are rotationally resolved spectra for gas phase molecules and ions recorded under low temperature conditions (upper right). Molecular constants derived from the spectra yield potential energy curves (lower left) and insights concerning electronic configurations. Electronic structure calculations, validated using the experimental observations, then provide information concerning the relative roles of the metal 5f, 6d, and 7s orbitals in bond formation. As examples, the orbitals for the HOMO and the first excited charge transfer state of ThN are shown. See page 10867.

## Feature Article

10867

DOI: 10.1021/jp507283n

### Spectroscopy and Structure of the Simplest Actinide Bonds

Michael C. Heaven,\* Beau J. Barker, and Ivan O. Antonov

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DOI: 10.1021/jp5076059

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DOI: 10.1021/jp507632z

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DOI: 10.1021/jp508242j

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DOI: 10.1021/jp508919s

### Ultrafast Excited-State Dynamics of 2,4-Dimethylpyrrole

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DOI: 10.1021/jp509203a

State-Specific Reactions of  $\text{Cu}^+(\text{}^1\text{S}, \text{}^3\text{D}, \text{}^1\text{D})$  with the Super Greenhouse Gas  $\text{SF}_2\text{CF}_2$ 

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DOI: 10.1021/jp506045q

Molecular Recognition and Interaction between Uracil and Urea in Solid-State Studied by Terahertz Time-Domain Spectroscopy

Jingqi Yang, Shaoxian Li, Hongwei Zhao,\* Bo Song, Guoxin Zhang, Jianbing Zhang, Yiming Zhu, and Jiaguang Han\*

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DOI: 10.1021/jp507397x

Experimental and Theoretical Investigation of the Pyrolysis Products of Iminodiacetonitrile,  $(\text{N}\equiv\text{CCH}_2)_2\text{NH}$ 

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DOI: 10.1021/jp5087784

The Limits of Rovibrational Analysis: The Severely Entangled  $\nu_1$  Polyad Vibration of Dichlorodifluoromethane in the Greenhouse IR Window

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DOI: 10.1021/jp509375y

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DOI: 10.1021/jp506123z

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DOI: 10.1021/jp506283y

Precipitates of Al(III), Sc(III), and La(III) at the Muscovite–Water Interface

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DOI: 10.1021/jp506436g

Hydroxyalkoxy Radicals: Importance of Intramolecular Hydrogen Bonding on Chain Branching Reactions in the Combustion and Atmospheric Decomposition of Hydrocarbons

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DOI: 10.1021/jp508516c

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DOI: 10.1021/jp509127h

**OH + (E)- and (Z)-1-Chloro-3,3,3-trifluoropropene-1 (CF<sub>3</sub>CH=CHCl) Reaction Rate Coefficients: Stereoisomer-Dependent Reactivity**

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DOI: 10.1021/jp5080835

**Hydroxyl Migration in Heterotrimetallic Clusters: An Assessment of Fluxionality Pathways**

Debashis Adhikari\* and Krishnan Raghavachari\*

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DOI: 10.1021/jp5082438

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DOI: 10.1021/jp5086679

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DOI: 10.1021/jp508968z

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DOI: 10.1021/jp509100u

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Devis Di Tommaso\* and Ken L. Watson

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DOI: 10.1021/jp5092448

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Qinghua Ren,\* Jinyu Wan, and Yanfeng Gao