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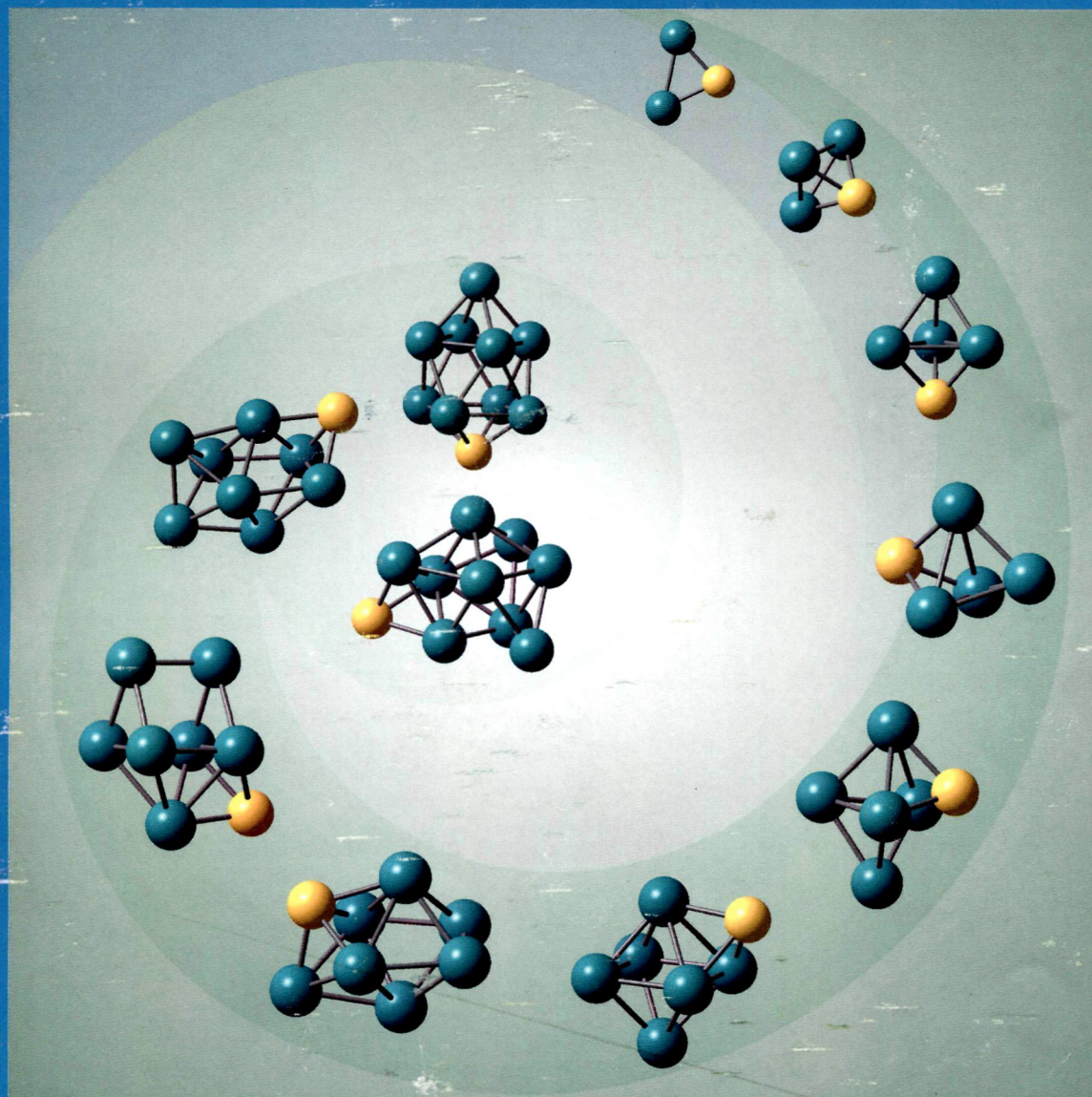
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A



Rhodium Sulfide
Cluster Structures
Obtained via
Basin-Hopping
with Subsequent
DFT Optimization
(see page 5A)

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



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ON THE COVER: Low-energy rhodium sulfide cluster geometries obtained using the basin-hopping search algorithm with subsequent geometry optimization at the density functional level of theory. See page 4278.


Articles


Kinetics and Dynamics

- 4235 [dx.doi.org/10.1021/jp504411j](https://doi.org/10.1021/jp504411j)
Quasiclassical Trajectory Study of the $C(^1D) + H_2 \rightarrow CH + H$ Reaction on a New Global *ab Initio* Potential Energy Surface
Ying Wu, Chunfang Zhang, Jianwei Cao,* and Wensheng Bian*


Spectroscopy, Photochemistry, and Excited States


- 4243  [dx.doi.org/10.1021/jp500572f](https://doi.org/10.1021/jp500572f)
Morphing the Internal Dynamics of Acetylacetone by $CH_3 \rightarrow CF_3$ Substitutions. The Rotational Spectrum of Trifluoroacetylacetone
Laura B. Favero, Luca Evangelisti, Andrea Velino, and Walther Caminati*

- 4249  [dx.doi.org/10.1021/jp5039283](https://doi.org/10.1021/jp5039283)
Spin Dynamics of Radical Pairs with Restricted Geometries and Strong Exchange Coupling: The Role of Hyperfine Coupling
Mehdi Zarea, Raanan Carmieli, Mark A. Ratner, and Michael R. Wasielewski*

- 4256  [dx.doi.org/10.1021/jp504153p](https://doi.org/10.1021/jp504153p)
Structures of Protonated Thymine and Uracil and Their Monohydrated Gas-Phase Ions from Ultraviolet Action Spectroscopy and Theory
Sara Øvad Pedersen, Camilla Skinnerup Byskov, Frantisek Turecek,* and Steen Brøndsted Nielsen*

Molecular Structure, Quantum Chemistry, and General Theory

- 4266  [dx.doi.org/10.1021/jp411520f](https://doi.org/10.1021/jp411520f)
Structural and Energetic Properties of Acetonitrile–Group IV (A & B) Halide Complexes
Heather M. Helminiak, Robin R. Knauf, Samuel J. Danforth, and James A. Phillips*

- 4278  [dx.doi.org/10.1021/jp412457m](https://doi.org/10.1021/jp412457m)
Density Functional Theory Study of $Rh_nS^{0,\pm}$ and $Rh_{n+1}^{0,\pm}$ ($n = 1-9$)
Michael J. Lecours, W. C. Theodore Chow, and W. Scott Hopkins*

DFT Study on the Mechanisms and Diastereoselectivities of Lewis Acid-Promoted Ketene–Alkene [2 + 2] Cycloadditions: What is the Role of Lewis Acid in the Ketene and C = X (X = O, CH₂, and NH) [2 + 2] Cycloaddition Reactions?
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Exciton Coupling Model for the Emergence of Second Harmonic Generation from Assemblies of Centrosymmetric Molecules

Gregory R. Snyder, Azhad U. Chowdhury, and Garth J. Simpson*

Doped Aluminum Cluster Anions: Size Matters

Elisa Jimenez-Izal,* Diego Moreno, Jose M. Mercero, Jon M. Matxain, Martha Audiffred, Gabriel Merino,* and Jesus M. Ugalde

Anion Receptors Based on Highly Fluorinated Aromatic Scaffolds

Neetha Mohan and Cherumuttathu H. Suresh*

Clar Theory Extended for Polyacenes and Beyond

Debojit Bhattacharya, Anirban Panda, Anirban Misra, and Douglas J. Klein*

Importance of C*–H Based Modes and Large Amplitude Motion Effects in Vibrational Circular Dichroism Spectra: The Case of the Chiral Adduct of Dimethyl Fumarate and Anthracene

Marco Passarello, Sergio Abbate,* Giovanna Longhi, Susan Lepri, Renzo Ruzziconi,* and Valentin Paul Nicu*

Fundamental Relation between Molecular Geometry and Real-Space Topology. Combined AIM, ELI-D, and ASF Analysis of Hapticities and Intramolecular Hydrogen–Hydrogen Bonds in Zircocene-Related Compounds

Stefan Mebs,* Maren Annika Chilleck, Kathrin Meindl, and Christian Bertram Hübschle