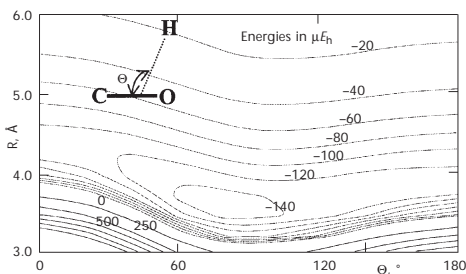


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2004, 69, 1–12

On the Structure and Physical Origin of the Weak Interaction Between H and CO

Vladimír Lukeš, Viliam Laurinc,
Michal Ilčín and Stanislav Biskupič

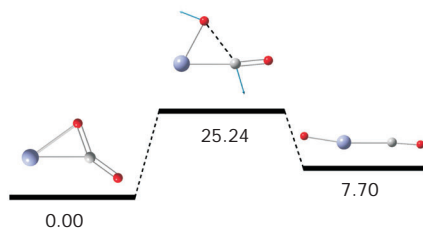


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2004, 69, 13–33

Theoretical Study on the Mechanism of Reaction of Ground-State Fe Atoms with Carbon Dioxide

Dimitrios A. Pantazis,
Athanasios C. Tsipis and
Constantinos A. Tsipis



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2004, 69, 34–46

Magnetic Linear Birefringence in Rare Earth Systems. II. Third-Order Approach

Lidia Smentek

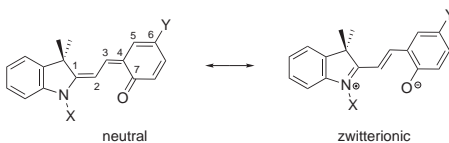
Ce^{3+} , Eu^{3+} , Gd^{3+} , Tb^{3+} , Yb^{3+}
magnetic anisotropy

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2004, 69, 47–62

Theoretical Study of the Substituent and Solvent Effects on the Molecular Structures, Absorption and Emission Spectra of Open-Form Spiroprans

Yinghong Sheng and Jerzy Leszczynski

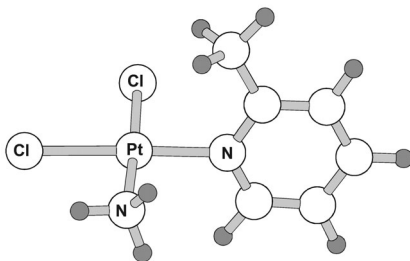


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2004, 69, 63–72

**Molecular Structure and Bonding
in Platinum–Picoline Anticancer
Complex: Density Functional Study**

Danuta Michalska and Rafał Wysokiński

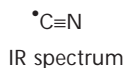


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2004, 69, 73–89

**The Infrared Spectrum of CN in Its
Ground Electronic State**

Veronika Horká, Svatopluk Civiš,
Vladimír Špirko and Kentarou Kawaguchi



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2004, 69, 90–104

**Can We Avoid the Intruder-State
Problems in the State-Universal
Coupled-Cluster Approaches While
Preserving Size Extensivity?**

Josef Paldus and Xiangzhu Li

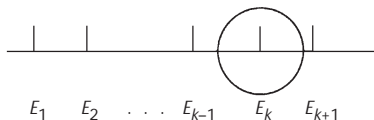
$$t_{p_1 \dots p_k}^{Q_1 \dots Q_k}(i) = - \sum_{p_k} \prod_{c=1}^p \langle \Phi_j | (n_c!)^{-1} [T_c(i)]^{n_c} | \Phi_i \rangle$$

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2004, 69, 105–120

**Convergence Enhancement
in Perturbation Theory**

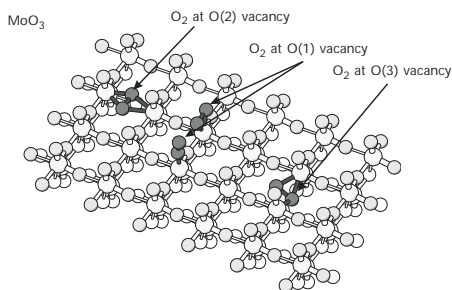
Péter R. Surján and Ágnes Szabados



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2004, 69, 121–140

Oxygen Sites at Molybdena and Vanadia Surfaces: Energetics of the Re-Oxidation Process

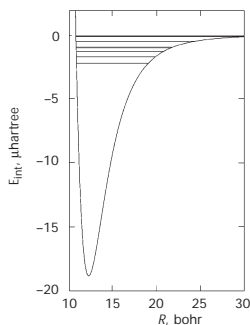
Renata Tokarz-Sobieraj, Robert Grybos,
 Małgorzata Witko and Klaus Hermann



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2004, 69, 141–176

Convergence Behavior of Symmetry-Adapted Perturbation Expansions for Excited States. A Model Study of Interactions Involving a Triplet Helium Atom

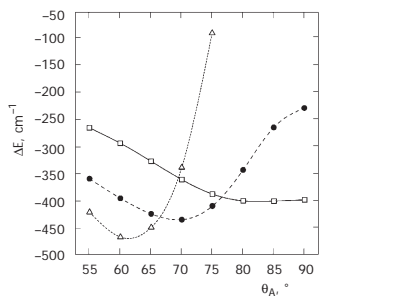
Michał Przybytek, Konrad Patkowski and
 Bogumil Jeziorski



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2004, 69, 177–188

Intermolecular Interactions in the (CO₂)₂, N₂-CO₂ and CO-CO₂ Complexes

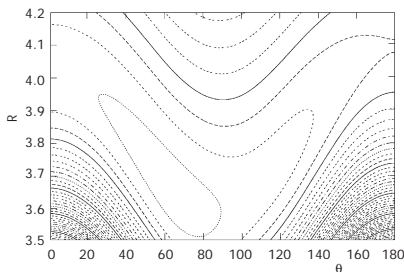
Jiří Fišer, Tomáš Boublík and
 Rudolf Polák



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2004, 69, 189–212

A Coupled Cluster Study of van der Waals Interactions of the He Atom with CN, NO and O₂ Radicals

Juraj Raab, Andrej Antušek,
 Stanislav Biskupič and Miroslav Urban

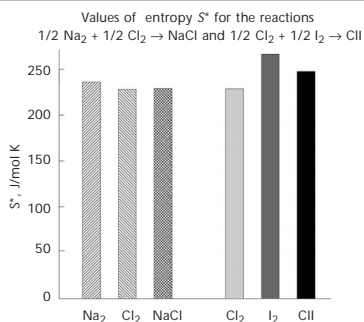


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2004, 69, 213–230

Additivity of Absolute Entropies

Ivan Černušák, Susan K. Gregurick,
Marjorie Roswell, Carol A. Deakyne,
H. Donald Brooke Jenkins and
Joel F. Liebman

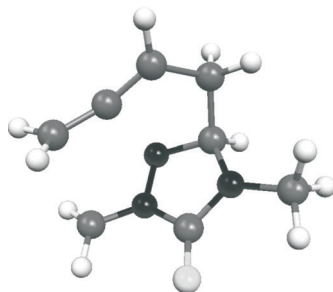


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2004, 69, 231–241

Quantum-Chemical Insight Into Mechanism of Combined Intra-Intermolecular Cycloaddition

Petr Kulhánek, Milan Potáček and
Jaroslav Koča

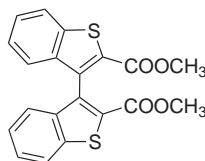


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2004, 69, 242–260

Synthesis and Electrochemical Reduction of Methyl 3-Halo-1-benzothiophene-2-carboxylates

Michal Rejňák, Jiří Klíma,
Jiří Svoboda and Jiří Ludvík



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2004, 69, 261–266

Formation of Ring A in the Biosynthesis of Hopanoids from Squalene. A Density Functional Study

B. Andes Hess, Jr.

