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2003, *68*, 423–446

Density Functional Study of the Electronic Structure and Related Properties of $Pt(NO)/Pt(NO_2)$ Redox Couples

Paraskevas Karipidis, Athanassios C. Tsipis and Constantinos A. Tsipis

$Pt(NO)/Pt(NO_2)$

Redox Couples

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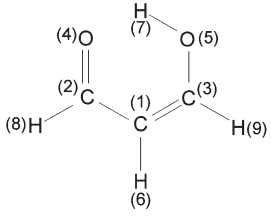
2003, *68*, 447–462

MR-CISD and MR-AQCC Calculation of Excited States of Malonaldehyde: Geometry Optimizations Using Analytical Energy Gradient Methods and a Systematic Investigation of Reference Configuration Sets

Silmar A. do Monte, Michal Dallos, Thomas Müller and Hans Lischka



ab initio calculations

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2003, *68*, 463–488

On the Performance of Bond Functions and Basis Set Extrapolation Techniques in High-Accuracy Calculations of Interatomic Potentials. A Helium Dimer Study

Małgorzata Jeziorska, Robert Bukowski, Wojciech Cencek, Michał Jaszuński, Bogumił Jeziorski and Krzysztof Szalewicz

He_2 interatomic potentials by CCSD and FCI

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2003, *68*, 489–508

A Comprehensive Computational Study on OCH^+–Rg (Rg = He, Ne, Ar, Kr, Xe) Complexes

Yinghong Sheng and Jerzy Leszczynski

OCH^+–Rg

(Rg = He, Ne, Ar, Kr, Xe)

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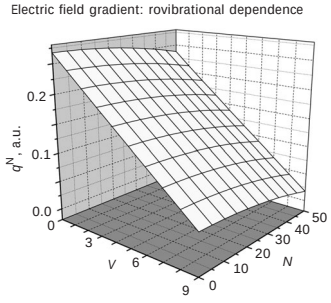
2003, *68*, 509–528

The Rovibrational Dependence of the ^{14}N Nuclear Quadrupole Coupling Constants in the $X^2\Sigma^+$ and $B^2\Sigma^+$ States of CN from the Multireference CI Approach

Rudolf Polák and Jiří Fišer



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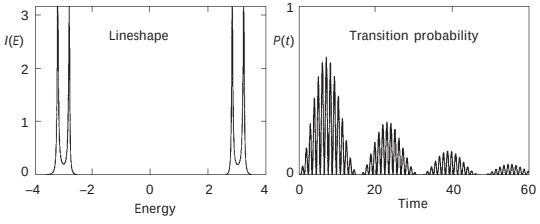
2003, *68*, 529–553

Quantum Resonances: Line Profiles and Dynamics

Ivana Paidarová and Philippe Durand



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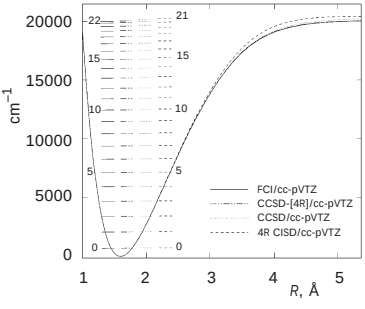
2003, *68*, 554–586

Externally Corrected Coupled-Cluster Approaches: Energy *versus* Amplitude Corrected CCSD

Josef Paldus and Xiangzhu Li



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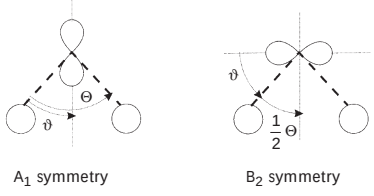
2003, *68*, 587–626

Modeling of the Three-Body Effects in the Neutral Trimers in the Quartet State by *ab initio* Calculations. H_3, Na_3, and Na_2B

Jacek Jakowski, Grzegorz Chałasiński, Malgorzata M. Szczęśniak and Slawomir M. Cybulski



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2003, *68*, 627–643

Calculation of Thermodynamical, Transport and Structural Properties of Neon in Liquid and Supercritical Phases by Molecular Dynamics Simulations Using an Accurate *ab initio* Pair Potential

- Global Simulation of Neon
- Bulk Properties

Muthusamy Venkatraj, Markus G. Müller, Hanspeter Huber and Robert J. Gdanitz

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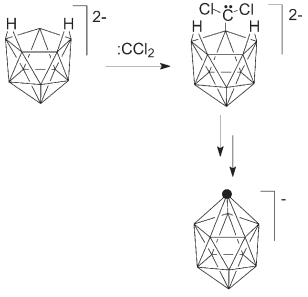
2003, *68*, 644–662

A Proposed Mechanism of [*closo*-$CB_{11}H_{12}$]$^-$ Formation by Dichlorocarbene Insertion Into [*nido*-$B_{11}H_{14}$]$^-$. A Computational Study by Density Functional Theory



Pawel Rempala and Josef Michl