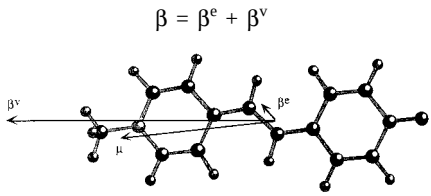
Collect. Czech. Chem. Commun.
1998, *63*, 1295–1308

Ab initio Hartree–Fock Investigation of π-Conjugated Compounds Presenting Large β^v/β^e Ratio: Merocyanines

Benoit Champagne, Thierry Legrand, Eric A. Perpete, Olivier Quinet and Jean-Marie Andre



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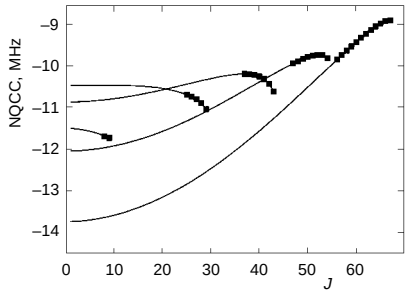
1998, *63*, 1309–1320

Expectation Values of Quasibound States: Nuclear Quadrupole Coupling Constants of BH in the $\tilde{X}^1\Sigma^+$ and $\tilde{B}^1\Sigma^+$ States

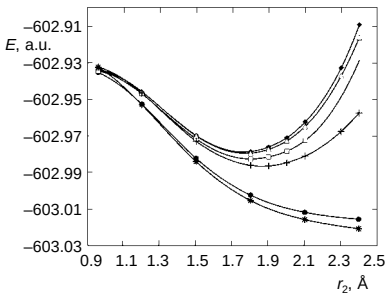
Michal Jurek, Vladimir Spirko and Wolfgang P. Kraemer



Collect. Czech. Chem. Commun.
1998, *63*, 1321–1328

Water Photolysis in Rare Gas Environment: The CASPT2 Excited State $H_2O(\tilde{A})$–Ar Potential

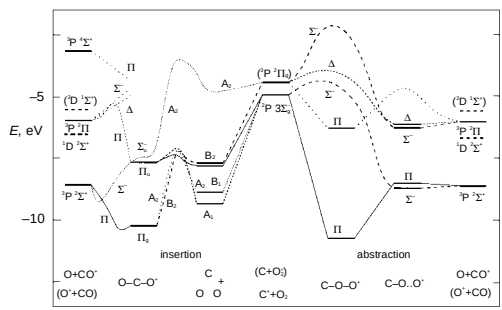
Dana Nachtigallova, Petr Slavicek, Petr Nachtigall and Pavel Jungwirth



Collect. Czech. Chem. Commun.
1998, *63*, 1329–1342

The Diatomics-in-Molecules Method as a Means for Predicting Potential-Energy-Surface Topolology. A Case Study for the Reaction of C^+ with O_2

Rudolf Polak



Collect. Czech. Chem. Commun.
1998, *63*, 1343–1354

Counterpoise-Corrected Potential Energy Surfaces of Simple Hydrogen-Bonded Systems

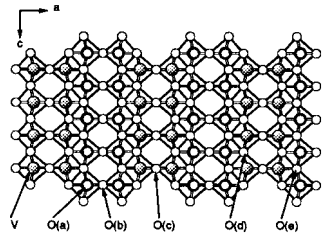
Pavel Hobza and Zdenek Havlas

● CP-corrected PES and standard PES may differ considerably, see, *e.g.*, the $(HF)_2$

Collect. Czech. Chem. Commun.
1998, *63*, 1355–1367

Surface Cluster Models for V_2O_5 – Studies of the Importance of Local Geometry

Malgorzata Witko, Renata Tokarz and Klaus Hermann



Collect. Czech. Chem. Commun.
1998, *63*, 1368–1380

Search for the Most Stable Structures on Potential Energy Surfaces

Lucjan Piela

$$\frac{dx_0}{d\alpha} = -A\left(\frac{d}{dx}\langle V\rangle(x,t)\right)_{x=x_0}$$

$$\frac{\partial\sigma}{\partial\alpha} = C - B\left(\frac{d^2}{dx^2}\langle V\rangle(x,t)\right)_{x=x_0}$$

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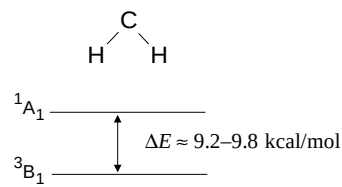
1998, *63*, 1381–1393

Singlet–Triplet Splitting in Methylene: An Accurate Description of Dynamic and Nondynamic Correlation by Reduced Multireference Coupled Cluster Method

Xiangzhu Li and Josef Paldus



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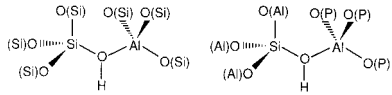
1998, *63*, 1394–1408

Comparing the Acidities of Microporous Aluminosilicate and Silico-Aluminophosphate Catalysts: A Combined Quantum Mechanics-Interatomic Potential Function Study



Joachim Sauer, Klaus-Peter Schroder
and Volker Termath

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1998, *63*, 1409–1430

Accuracy Assessment of the ROHF-CCSD(T) Calculations of Dipole Moments of Small Radicals

- Highly accurate theoretical calculations of dipole momenta
- Ways of internal controling of the accuracy of predictions
- Analysis of the "complicated cases"

Miroslav Urban, Pavel Neogrady, Juraj Raab
and Geerd H. F. Diercksen

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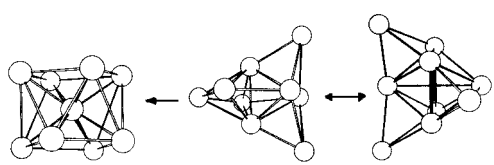
1998, *63*, 1431–1446

***Ab initio* Molecular Dynamics for Determination of Structures of Alkali Metal Clusters and Their Temperatures Behavior; An Example of Li_9^+**



Vlasta Bonacic-Koutecky, Detlef Reichardt,
Jiri Pittner, Piercarlo Fantucci
and Jaroslav Koutecky

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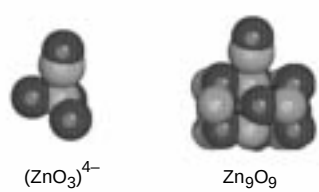
1998, *63*, 1447–1459

Theoretical Study of the Physisorption of CO on Metal Oxide Surfaces Using the KSCED-DFT Approach



Nathalie Vulliermet, Tomasz A. Wesolowski
and Jacques Weber

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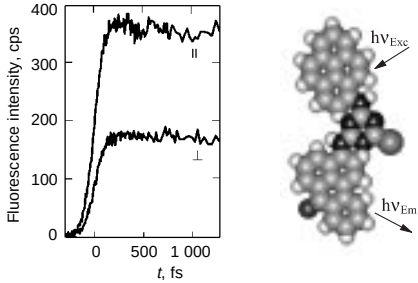
1998, *63*, 1460–1472

Ultrafast Electronic Energy Flow in a Bichromophoric Molecule

Vlastimil Fidler, Peter Kapusta, Milos Nepras, Jorg Schroeder, Igor V. Rubtsov and Keitaro Yoshihara



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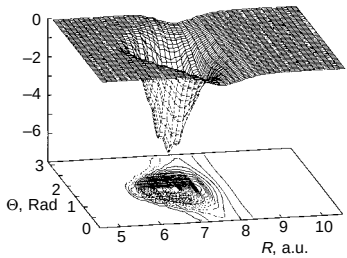
1998, *63*, 1473–1484

From Intermolecular Interactions to Incipient Chemical Bond

Grzegorz Chalasinski, Jacek Klos, Slawomir M. Cybulski and Malgorzata M. Szczesniak



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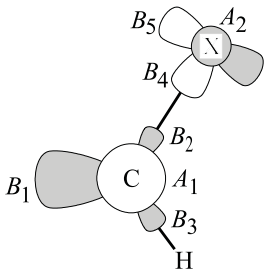
1998, *63*, 1485–1497

Spin–Orbit Coupling in Biradicals. 3. Heavy Atom Effects in Carbenes

Zdenek Havlas and Josef Michl



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1998, *63*, 1498–1512

Generation and Reactivity of Chromium Fluoride Cations (CrF_n^+, n = 0–4) in the Gas Phase

Ulf Mazurek, Detlef Schroder and Helmut Schwarz