

Collect. Czech. Chem. Commun.
2003, 68, 1–22

The ^4He Trimer: Structure and Energetics of a Very Unusual Molecule

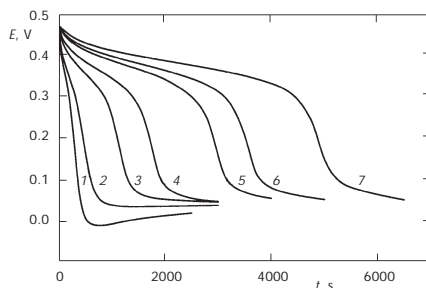
Cono Di Paola, Franco A. Gianturco,
Gerardo Delgado-Barrio,
Salvador Miret-Artés and
Pablo Villarreal

He_3 clusters
ab initio calculations

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2003, 68, 23–34

The Autocatalytic Reduction of Ferriin by Malonic Acid with Regard to the Ferriin-Catalyzed Belousov-Zhabotinsky Reaction

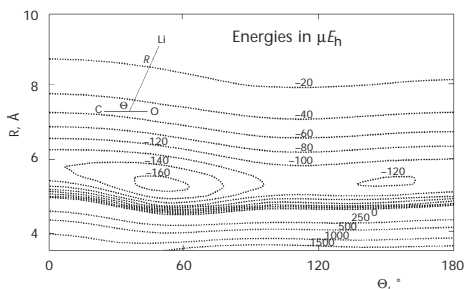
Marta Mrákavová, Milan Melicherčík,
Anna Olexová and Ludovít Treindl



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2003, 68, 35–46

***Ab initio* Study of the Li-CO van der Waals Complex**

Vladimír Lukeš, Viliam Laurinc,
Michal Ilčín and Stanislav Biskupič



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2003, 68, 47–60

Energies and Dipole Moments of Excited States of Ozone and Ozone Radical Cation Using Fock Space Multireference Coupled-Cluster Analytical Response Approach

Devarajan Ajitha, Kimihiko Hirao and
Sourav Pal

O_3 – dipole moments
– excited states
by FS-MRCC

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2003, 68, 61–74

Some Approximate Atomic and Molecular Energy Formulas

Peter Politzer, Abraham F. Jalbout and Ping Jin

$$V_0 = \alpha_0 + \alpha_1 Z + \alpha_2 Z^2 + \alpha_3 Z^3 + \alpha_4 Z^4$$

$$V_0 = \beta_1 Z^{1/3} + \beta_2 Z^{2/3} + \beta_3 Z^{3/3} + \beta_4 Z^{4/3}$$

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2003, 68, 75–88

Group IIIa Hydrides XH_2 and XH_2^- (X = B, Al, Ga): Electron Affinities and Singlet-Triplet Splittings Revisited

Ivan Černušák, Alena Zavažanová, Juraj Raab and Pavel Neogrady

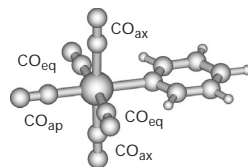
XH_2 and XH_2^-
(X = B, Al, Ga)

ab initio calculations

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2003, 68, 89–104

The Character of Low-Lying Excited States of Mixed-Ligand Metal Carbonyls. TD-DFT and CASSCF/CASPT2 Study of $[\text{W}(\text{CO})_4\text{L}]$ (L = ethylenediamine, N,N' -dialkyl-1,4-diazabutadiene) and $[\text{W}(\text{CO})_5\text{L}]$ (L = pyridine, 4-cyanopyridine)



Stanislav Záliš, Antonín Vlček, Jr. and Chantal Daniel

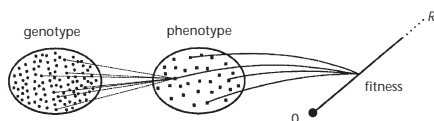
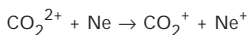
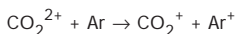
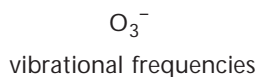
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2003, 68, 105–138

Effective Hamiltonian and Intermediate Hamiltonian Formulations of the Fock-Space Coupled-Cluster Method

Leszek Meissner and Jarosław Gryniaków

$$H_{\text{eff}} = PH(1 + X)P$$

*Collect. Czech. Chem. Commun.***2003, 68, 139–177****Artificial Chemistry and Molecular Darwinian Evolution *in silico***Vladimír Kvasnička and
Jiří Pospíchal*Collect. Czech. Chem. Commun.***2003, 68, 178–188****Charge Transfer Between CO_2^{2+} and Ar or Ne at Collision Energies 3–10 eV**Libor Mrázek, Ján Žabka,
Zdeněk Dolejšek and Zdeněk Herman*Collect. Czech. Chem. Commun.***2003, 68, 189–201****An Accurate Quartic Force Field and Fundamental Frequencies for the Ozonide Anion: A Rare Positive Anharmonicity for the Antisymmetric Stretch**Timothy J. Lee, Christopher E. Dateo,
Mercedes Rubio and Björn O. Roos*Collect. Czech. Chem. Commun.***2003, 68, 202–210****On the Concerted Ring Opening of Protonated Squalene Oxide and A-Ring Formation in the Biosynthesis of Lanosterol**

B. Andes Hess, Jr.

