Collect. Czech. Chem. Commun.
2003, *68*, 211–239

Standardized Medium-Size Basis Sets for Calculations of Molecular Electric Properties: Group IIIA

Ivan Černušák, Vladimir Kellö and Andrzej J. Sadlej

GAF, InF, TlF } dipole moments by basis sets polarization approach

Collect. Czech. Chem. Commun.
2003, *68*, 240–252

Application of MP2 Results in Comparative Studies of Semiempirical Ground-State Energies of Large Atoms

Jesus R. Flores, Karol Jankowski and Romuald Słupski

MP2/CA
DFT comparison

Collect. Czech. Chem. Commun.
2003, *68*, 253–264

Magnetic Linear Birefringence in Rare Earth Systems. Second-Order Approach

Lidia Smentek

$$\alpha_{p_1 p_2} = \sum_{Xx} \left\{ \frac{\langle 4\,f^N \psi | D^{(1)}_{p_1} | Xx \rangle \langle Xx | D^{(1)}_{p_2} | 4\,f^N \psi \rangle}{(\hbar\omega - \Delta E_{4f^N, X})} - \frac{\langle 4\,f^N \psi | D^{(1)}_{p_2} | Xx \rangle \langle Xx | D^{(1)}_{p_1} | 4\,f^N \psi \rangle}{(\hbar\omega + \Delta E_{4f^N, X})} \right\}$$

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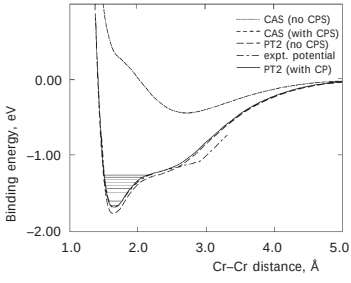
2003, *68*, 265–274

The Ground State Potential for the Chromium Dimer Revisited

Björn O. Roos



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2003, *68*, 275–294

Dirac–Coulomb Hamiltonian in *N*-Electron Model Spaces

Grzegorz Pestka and
Jacek Karwowski

$$\hat{H}_N(\rho) = \sum_{i=1}^{N} \hat{I}^{\otimes(i-1)} \otimes \hat{H}_1(\rho_i) \otimes \hat{I}^{\otimes(N-i)} + \hat{I}^{\otimes N} G$$

Collect. Czech. Chem. Commun.
2003, *68*, 295–306

New Version of the Rayleigh–Schrödinger Perturbation Theory

Miloš Kalhous, Lubomír Skála,
Jaroslav Zamastil and Jiří Čížek

$$E_n(H_0 - E_0)^{-1}\psi_0 = (H_0 - E_0)^{-1}\left(H_1\psi_{n-1} - \sum_{i=1}^{n-1} E_i\,\psi_{n-1}\right)$$

Collect. Czech. Chem. Commun.
2003, *68*, 307–330

A Nonorthogonal Coordinate Approach to Atom–Diatom Parallel Reactive Scattering Calculations

Antonio Laganà, Stefano Crocchianti,
Noelia Faginas Lago, Leonardo Pacifici and
Gianni Ferraro

$H + H_2$

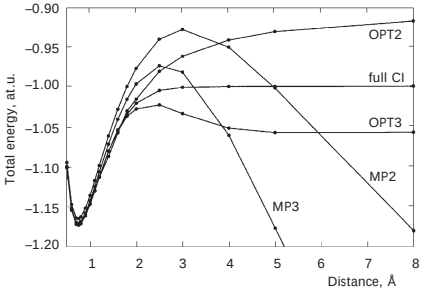
reactive scattering

calculations

Collect. Czech. Chem. Commun.
2003, *68*, 331–339

Optimized Quasiparticle Energies in Many-Body Perturbation Theory

Peter R. Surján, Dóra Kőhalmi and
Ágnes Szabados



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2003, *68*, 340–356

Towards Universal R12 Consistent Basis Sets

$$\Psi^{(1)} = \hat{R}^{(1)}\Phi + \chi^{(1)} = \sum_{\substack{l>j \\ k>l}} \left(c_{kl}^{ij}\right)^{(1)} \hat{R}_{ij}^{kl}\Phi + \chi^{(1)}$$

Jozef Noga and Pierre Valiron

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2003, *68*, 357–373

The Laplace Transform Perturbative Triples Correction Ansatz

$$E_{\mathrm{T}}^{[4]} = \frac{-1}{D_{\min}} \int_0^1 \sum_{\mathrm{v}} z_{\mathrm{v}} x^{\frac{D_{\mathrm{v}}}{D_{\min}}-1} \mathrm{d}x$$

Pere Constans and Gustavo E. Scuseria

Collect. Czech. Chem. Commun.
2003, *68*, 374–386

Similarity-Transformed Hamiltonians by Means of Gaussian-Damped Interelectronic Distances

$$\hat{H}^F = \exp(-F)\hat{H}\exp(F)$$

Henk J. A. Zweistra, Claire C. M. Samson and Wim Klopper

Collect. Czech. Chem. Commun.
2003, *68*, 387–404

Electronic Structure and Bonding Nature of the Ground State Monocarbide Cations, ScC^+, TiC^+, VC^+, and CrC^+

MC^+

M = Sc, Ti, V, Cr

ab initio calculations

Ioannis S. K. Kerkines and Aristides Mavridis

Collect. Czech. Chem. Commun.
2003, *68*, 405–422

Electronic States of $Fe_2S^{-/0/+}$

Olaf Hübner and Joachim Sauer