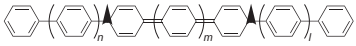
Collect. Czech. Chem. Commun.
2005, *70*, 689–730

Theoretical Study of Bipolaron Dynamics in Polyparaphenylene: II. Density Functional Theory (DFT) Calculations on Neutral Dimers and Semiempirical Hückel-Type Calculations on Neutral and Charged Model Chains

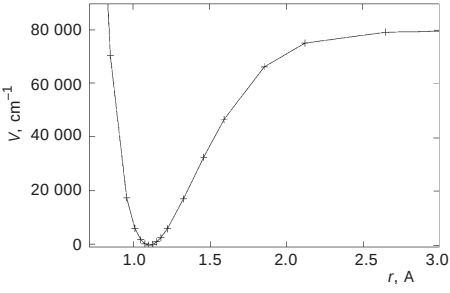


DFT calculations

Wolfgang Förner

Collect. Czech. Chem. Commun.
2005, *70*, 731–739

Potential Energy Curve of N_2 in Its Ground Electronic State



Vladimír Špirko

Collect. Czech. Chem. Commun.
2005, *70*, 740–754

On the Bidirectionality of the JWKB Connection Formula at a Linear Turning Point

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + kx - E\right)\psi(x) = 0 \quad (0 \le x \le x_1)$$

Hujun Shen, Harris J. Silverstone and Gabriel Álvarez

Collect. Czech. Chem. Commun.
2005, *70*, 755–770

General-Model-Space State-Universal Coupled-Cluster Method: Excited States of Ozone

B_2: $1a_2 \rightarrow 2b_1$, $1b_1 1a_2 \rightarrow 2b_1^2$

B_1: $6a_2 \rightarrow 2b_1$, $4b_2 1a_2 \rightarrow 2b_1^2$

A_2: $4b_2 \rightarrow 2b_1$, $6a_1 1a_2 \rightarrow 2b_1^2$

Xiangzhu Li

Collect. Czech. Chem. Commun.
2005, *70*, 771–796

Representation Theory and Wigner–Racah Algebra of the SU(2) Group in a Noncanonical Basis

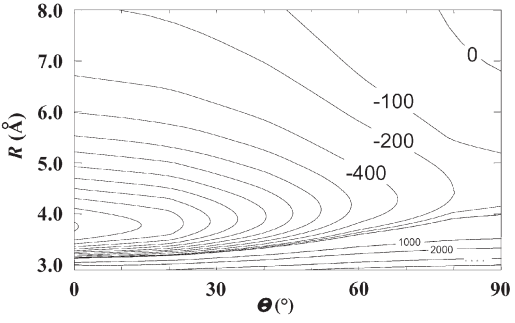
Maurice R. Kibler

$$|j\mu\rangle = \sum_{m=-j}^{j} |jm\rangle\langle jm|j\mu\rangle$$

Collect. Czech. Chem. Commun.
2005, *70*, 797–810

Theoretical Study of $H_2...I^-$ van der Waals Anion Complex

Michal Ilčin, Vladimír Lukeš, Viliam Laurinc and Stanislav Biskupič



Collect. Czech. Chem. Commun.
2005, *70*, 811–825

The Fock-Space Coupled-Cluster Method in the Calculation of Excited State Properties

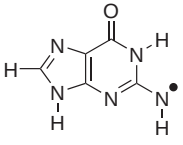
Monika Musiał and Leszek Meissner

CO, N_2 } excited states calculated by FS-CCSD

Collect. Czech. Chem. Commun.
2005, *70*, 826–836

Radicals Derived from Guanine: Structures and Energetics

Qiong Luo, Qian Shu Li, Yaoming Xie and Henry F. Schaefer



Collect. Czech. Chem. Commun.
2005, *70*, 837–850

Frozen Natural Orbitals: Systematic Basis Set Truncation for Coupled-Cluster Theory

Andrew G. Taube and Rodney J. Bartlett