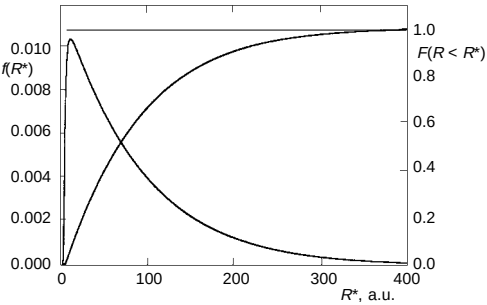
Collect. Czech. Chem. Commun.
1998, *63*, 1089–1093

Probing Weakly-Bound Species with Nonresonant Light: Dissociation of He_2 Induced by Rotational Hybridization

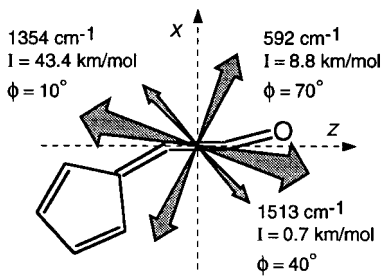
Bretislav Friedrich, Manish Gupta and Dudley Herschbach



Collect. Czech. Chem. Commun.
1998, *63*, 1094–1106

Bent Cyclopenta-2,4-dienylideneketene: Spectroscopic and *ab initio* Study of Reactive Intermediate

Juliusz G. Radziszewski, Piotr Kaszynski, Anders Friderichsen and Jens Abildgaard



Collect. Czech. Chem. Commun.
1998, *63*, 1107–1142

Full Configuration Interaction Energies, Geometries, and Quartic Force Fields of the Nitrenium Ion

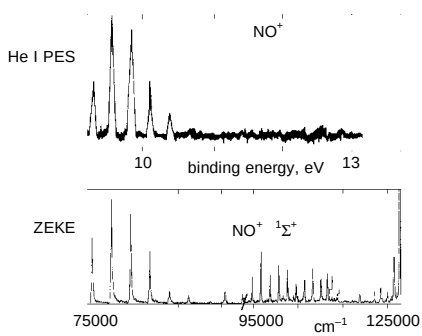
Timothy J. Van Huis, Matthew L. Leininger, C. David Sherrill and Henry F. Schaefer III

- NH_2^+ Properties and Force Fields at the DZP Full CI Level
- Examination of Trends in Ground and Excited States
- Effectiveness of Force Field Generation at Non-Stationary Point Geometries

Collect. Czech. Chem. Commun.
1998, *63*, 1143–1151

Two Classes of ZEKE Spectroscopy

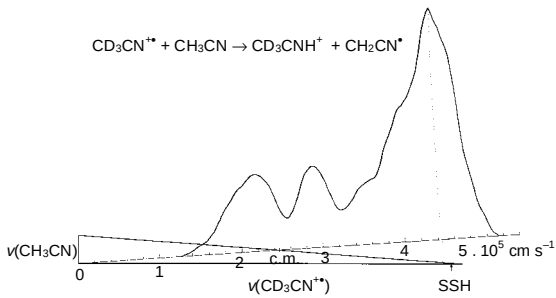
Heinrich L. Selzle, Edward W. Schlag, Francoise Remacle and Raphael D. Levine



Collect. Czech. Chem. Commun.
1998, *63*, 1152–1160

Dynamics of Protonated Acetonitrile Formation in $CD_3CN^{+\bullet}$ + CH_3CN Collisions: A Crossed-Beam Scattering Study

Jan Zabka, Zdenek Dolejsek, Inosuke Koyano and Zdenek Herman



Collect. Czech. Chem. Commun.
1998, *63*, 1161–1176

Analytical Solutions of the Schrödinger Equation. Ground State Energies and Wave Functions

Jan Dvorak and Lubomir Skala

- Standard Approach
- Two Generalizations

Collect. Czech. Chem. Commun.
1998, *63*, 1177–1186

***Ab initio* Calculation of Transport Properties of Supercritical Carbon Dioxide**

Gerold Steinebrunner, Anthony J. Dyson, Barbara Kirchner and Hanspeter Huber

A combination of quantum chemistry and molecular dynamics simulations allows the prediction of transport properties of supercritical CO_2 without any empirical calibration.

Collect. Czech. Chem. Commun.
1998, *63*, 1187–1201

New Approach to the Theory of Circular Dichroism

Jaroslav Zamastil, Lubomir Skala, Petr Pancoska and Oldrich Bilek

- CD Spectroscopy
- Quantum Chemistry

Collect. Czech. Chem. Commun.
1998, *63*, 1202–1212

Reliability of DFT Methods for Description of Cu Sites and Their Interaction with NO in Zeolites

Dana Nachtigallova, Marketa Davidova and Petr Nachtigall

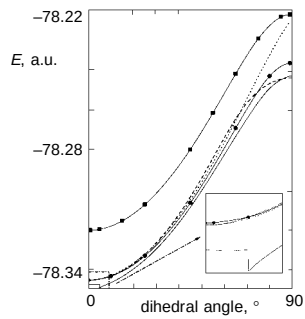
$$Cu^{n+}H_2O \rightarrow Cu^{n+} + H_2O$$

$$Cu^{n+}NO \rightarrow Cu^{n+} + NO$$

Collect. Czech. Chem. Commun.
1998, *63*, 1213–1222

Single-Root Multireference Brillouin–Wigner Coupled-Cluster Theory. Rotational Barrier of the Ethylene Molecule

Jozef Masik, Pavel Mach, Jan Urban, Martin Polasek, Peter Babinec and Ivan Hubac



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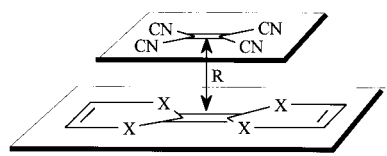
1998, *63*, 1223–1244

Binding Energies of Organic Charge-Transfer Complexes Calculated by First-Principles Methods

Cordula Rauwolf, Achim Mehlhorn and Jurgen Fabian



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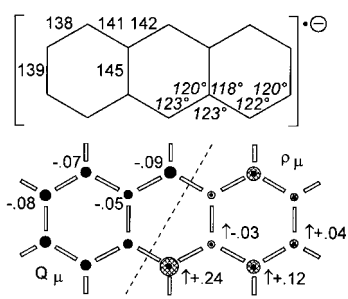
1998, *63*, 1245–1263

Bare Molecular Anions of Unsaturated Hydrocarbons: Density Functional Charge and Spin Distributions Based on Their Single Crystal Structures

Zdenek Havlas and Hans Bock



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1998, *63*, 1264–1284

Evaluation of Molecular Integrals in a Mixed Gaussian and Plane-Wave Basis by Means of the Faddeeva Function and Its Derivatives

Petr Carsky and Tomas Reschel

($gk|gk$) and ($gg|gk$) integrals

g's are Cartesian Gaussians

and $k = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})$

Collect. Czech. Chem. Commun.
1998, *63*, 1285–1294

Ultrafast Nonadiabatic Dynamics. Theoretical Study of Femtosecond Electron Transfer Processes

Joshua Jortner and Mordechai Bixon

- Correlations in the Franck–Condon Quasicontinuum
- Upper Bounds for Nonadiabatic Rates