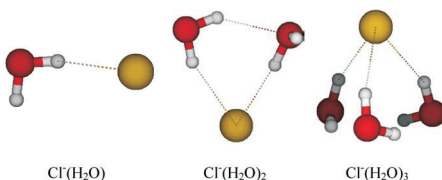


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### The Onset of Ion Solvation by *ab initio* Calculations: Comparison of Water and Methanol

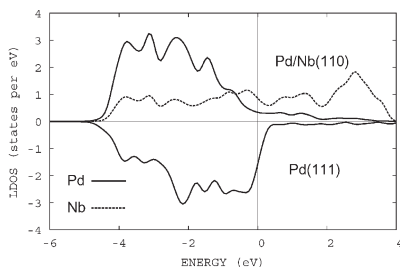
Eva Pluhařová and Pavel Jungwirth



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2008, 73, 745–754

### Tailoring the Surface Reactivity: Comparison of Pd/Nb(110) and Rh/Nb(110)

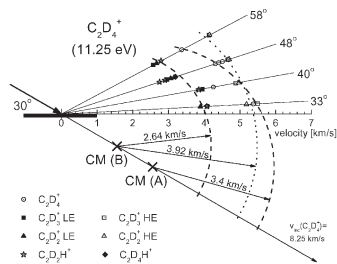
Štěpán Pick



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### Scattering of Low-Energy (5–12 eV) C<sub>2</sub>D<sub>4</sub><sup>++</sup> Ions from Room-Temperature Carbon Surfaces

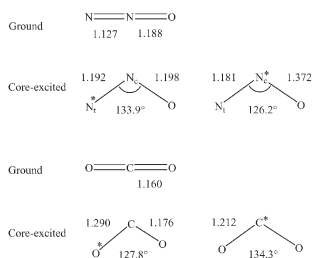
Andriy Pysanenko, Jan Žabka and Zdenek Herman



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### Geometry Relaxations After Inner-Shell Excitations and Ionizations

Masahiro Ehara and Hiroshi Nakatsuji

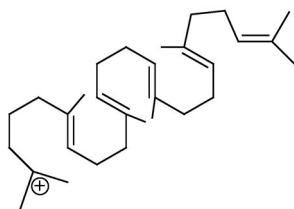


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**The Concerted Nature of the Enzymatic Cyclization of Rings A-D of Squalene to Hopene**

B. Andes Hess, Jr. and Lidia Smentek

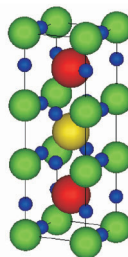


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**Aspects of Electronic Structure Instability in Search for New Superconductors: Superconducting Boride at Liquid Nitrogen Temperature?**

Pavol Baňacký

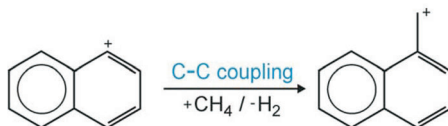


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**On the C–C Coupling of the Naphthylum Ion with Methane**

Jana Roithová, Claire L. Ricketts and Detlef Schröder

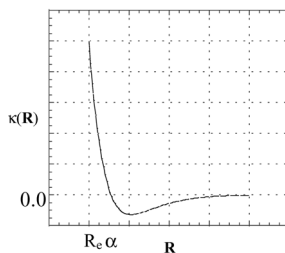


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**The Position-Dependent Reaction Force Constant in Bond Dissociation/Formation**

Peter Politzer and Jane S. Murray

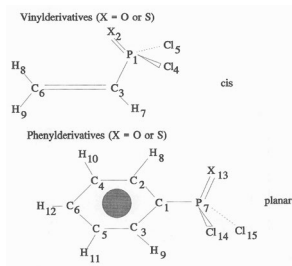


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### Absence of Conjugation in Vibrational Spectra and Assignments of Dichloro(vinyl)phosphine and Dichloro(phenyl)phosphine Oxides and Sulfides

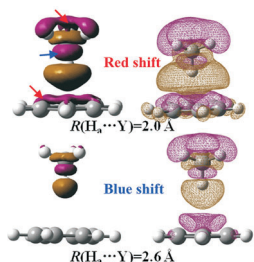
Wolfgang Förner and Hassan M. Badawi

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### Application of Berlin's Theorem to Bond-Length Changes in Isolated Molecules and Red- and Blue-Shifting H-Bonded Clusters

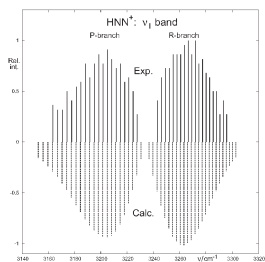
Weizhou Wang and Pavel Hobza

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### Energies and Electric Dipole Moments of the Bound Vibrational States of $\text{HN}_2^+$ and $\text{DN}_2^+$

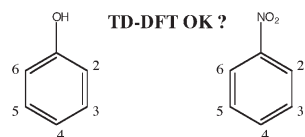
Vladimír Špirko, Ota Bludský and Wolfgang P. Kraemer

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### Assessment of the Accuracy of TD-DFT Absorption Spectra: Substituted Benzenes

Jean-Marie André, Denis Jacquemin, Eric A. Perpète, Daniel P. Vercauteren and Valérie Wathelet

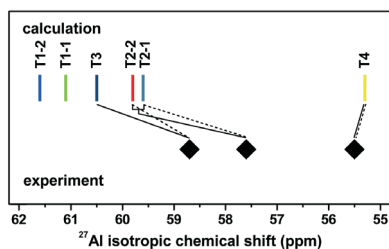


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**Aluminum Siting in the ZSM-22 and Theta-1 Zeolites Revisited: A QM/MM Study**

Stepan Sklenak, Jiří Dědeček, Chengbin Li, Fei Gao, Bavornpon Jansang, Bundet Boekfa, Blanka Wichterlová and Joachim Sauer

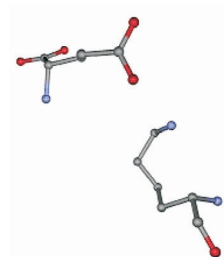


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**The Stabilization Energy of the GLU–LYS Salt Bridge in the Protein/Water Environment: Correlated Quantum Chemical *ab initio*, DFT and Empirical Potential Studies**

Jan Řezáč, Karel Berka, Dominik Horinek, Pavel Hobza and Jiří Vondrášek



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**A Note on the Symmetry Properties of Löwdin's Orthogonalization Schemes**

András T. Rokob, Ágnes Szabados and Péter R. Surján

