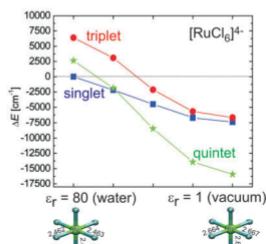


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2008, 73, 1231–1244

## Are Octahedral Ruthenium(II/III) and Osmium(II/III) Complexes Always Low-Spin?

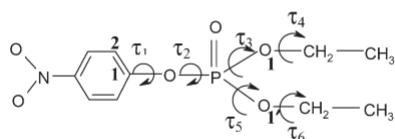
Martin Srnec, Jakub Chalupský and Lubomír Rulíšek



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2008, 73, 1245–1260

## Probing the Active Conformers of Paraoxon Through Theoretical Conformational Studies

Jason Ford-Green, Devashis Majumdar and Jerzy Leszczynski



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2008, 73, 1261–1270

## Quantum Chemical Benchmark Energy and Geometry Database for Molecular Clusters and Complex Molecular Systems ([www.begdb.com](http://www.begdb.com)): A Users Manual and Examples

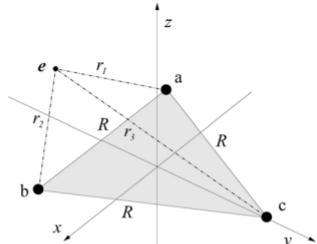
Jan Řezáč, Petr Jurečka, Kevin E. Riley, Jiří Černý, Haydee Valdes, Kristýna Pluháčková, Karel Berka, Tomáš Řezáč, Michal Pitoňák, Jiří Vondrášek and Pavel Hobza

BEGDB BENCHMARK ENERGY AND GEOMETRY DATA BASE					
Benchmark DataSets: <input checked="" type="checkbox"/> atomic <input type="checkbox"/> molecular <input type="checkbox"/> interatomic. Columns in table are sorted alphabetically <a href="#">see also CSD file</a>					
Benchmark DataSets: <input checked="" type="checkbox"/> atomic <input type="checkbox"/> molecular <input type="checkbox"/> interatomic. Columns in table are sorted alphabetically <a href="#">see also CSD file</a>					
System name	Optimization level	A/T	A/T	A/T	A/T
		COREL/CP	COREL/CP	MP2/CP	MP2/CP
2-chloro-2-(propynyl)cyclohexane	MP2/loc-pVTZ CP	-16.71	-17.37		
Acetone thinnest pentamer	MP2/loc-pVTZ CP	12.23	14.93		
Acetone thinnest trinuclear cluster	MP2/loc-pVTZ CP	14.29	14.54		
Acetone/thinnest trinuclear cluster	MP2/loc-pVTZ CP	13.17	13.20		
Acetone/thinnest trinuclear cluster	MP2/loc-pVTZ CP	13.17	13.20		
Benzene + Methanol complex	MP2/loc-pVTZ CP	-1.50	-1.86		
Benzene/acetone complex	MP2/loc-pVTZ CP	-2.89	-3.72		
Benzene/acetone dimer	MP2/loc-pVTZ CP	-0.73	-0.80		
Benzene dimer 2-substituted	MP2/loc-pVTZ CP	-0.74	-0.82		
Benzene/ethanol complex	MP2/loc-pVTZ CP	-1.46	-1.16		
Benzene/water complex	MP2/loc-pVTZ CP	-0.48	-0.43		
Boron cluster	CCSD(T)/loc-pVTZ MP2/loc-pVTZ	-1.53	-1.61		
Boron cluster	CCSD(T)/loc-pVTZ MP2/loc-pVTZ	-1.53	-1.69		

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2008, 73, 1271–1280

## About Non-Existence of the Molecular Ion

Héctor Medel-Cobaxin, Alexander Alijah and Alexander V. Turbiner



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2008, 73, 1281–1298

### Generalized Spin Bases for Quantum Chemistry and Quantum Information

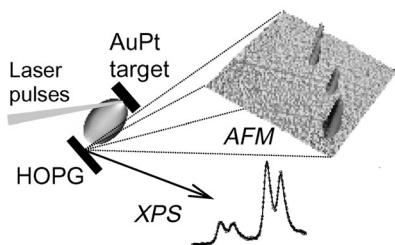
Maurice R. Kibler

$$|\langle j\alpha;ra|j\beta;rb\rangle = \delta_{\alpha,\beta}\delta_{a,b} + \frac{1}{\sqrt{2j+1}}(1-\delta_{a,b})$$

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2008, 73, 1299–1313

### Preparation of Au-Pt Nanostructures on Highly Oriented Pyrolytic Graphite Surfaces by Pulsed Laser Deposition and Their Characterization by XPS and AFM Methods

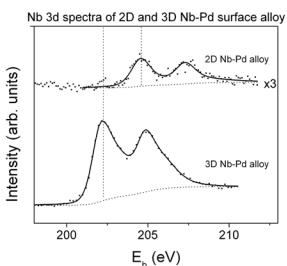
Jan Plšek, Pavel Janda and Zdeněk Bastl



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2008, 73, 1314–1326

### Interaction of Niobium with Polycrystalline Palladium Surface. X-ray Photoemission Study

Ivan Jirka and Zdeněk Bastl



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2008, 73, 1327–1339

### Analytic Energies and Wave Functions of Two-Dimensional Schrödinger Equation: Two-Dimensional Fourth-Order Polynomial Potential

Vladimír Tichý and Lubomír Skála

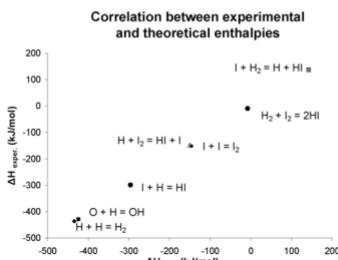
$$H\Psi = E\Psi$$

$$V = W_{40}^2 x^4 + W_{04}^2 y^4 + V_{31} x^3 y + V_{13} x y^3 + V_{22} x^2 y^2 + \dots$$

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2008, 73, 1340–1356

### Thermodynamic Data of Iodine Reactions Calculated by Quantum Chemistry. Training Set of Molecules

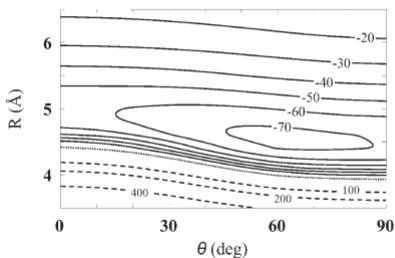
Katarína Mečiarová, Laurent Cantrel and Ivan Černušák



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2008, 73, 1357–1371

### Theoretical Study of the vdW Complex Cd...N<sub>2</sub>

Michal Ilčin, Vladimír Lukeš,  
Viliam Laurinc and Stanislav Biskupič



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2008, 73, 1372–1390

### Quasi-Exactly Solvable Models in Quantum Chemistry

Jacek Karwowski and Kamil Szewc

