Mariusz Radoń

Lista publikacji

- październik 2011

I. Prace oryginalne (rozdziały w książkach zbiorowych, artykuły w czasopismach):

1. **Radoń M.**, Brocławik E., 2011, ***Mono- and Dinitrosyls on Copper(I) Site in a Zeolite Model: Effects of Static Correlation***, *Journal of Physical Chemistry A* 115(42): 11761-11774.

2. **Radoń M.**, Brocławik E., Pierloot K., 2011, ***DFT and Ab Initio Study of Iron-Oxo Porphyrins: May They Have a Low-Lying Iron(V)-Oxo Electromer?***, *Journal of Chemical Theory and Computation* 7(4): 898-908.

3. Pietrzyk P., Srebro M., **Radoń M.**, Sojka Z., Michalak A., 2011, ***Spin Ground State and Magnetic Properties of Cobalt(II) — Relativistic DFT Calculations Guided by EPR Measurements of Bis(2,4-acetylacetonate)cobalt(II)-Based Complexes***, *Journal of Physical Chemistry A* 115(11): 2316-2324.

4. Borowski T., Noack H., **Radoń M.**, Zych K., Siegbahn P. E. M., 2010, ***Mechanism of Selective Halogenation by SyrB2: A Computational Study***, *Journal of the American Chemical Society* 132(37): 12887-12898.

5. **Radoń M.**, Brocławik E., Pierloot K., 2010, ***Electronic Structure of Selected {FeNO}^{7} Complexes in Heme and Non-Heme Architectures: A Density Functional and Multireference ab Initio Study***, *Journal of Physical Chemistry B* 114(3): 1518-1528.

6. Vancoillie S., Zhao H., **Radoń M.**, Pierloot K., 2010, ***Performance of CASPT2 and DFT for Relative Spin-State Energetics of Heme Models***, *Journal of Chemical Theory and Computation* 6(2): 576-572.

7. **Radoń M.**, Srebro M., Brocławik E., 2009, ***Conformational Stability and Spin States of Cobalt(II) Acetylacetonate: CASPT2 and DFT Study***, *Journal of Chemical Theory and Computation* 5(5): 1237-1244.

8. **Radoń M.**, Pierloot, K., 2008, ***Binding of CO, NO, and O2 to Heme by Density Functional and Multireference Ab Initio Calculations***, *Journal of Physical Chemistry A* 112(46): 11824-11832.

9. Rejmak P., Brocławik E., Góra-Marek K., **Radoń M.**, Datka J., 2008, ***Nitrogen monoxide interaction with Cu(I) sites in zeolites X and Y: quantum chemical calculations and IR studies***, *Journal of Physical Chemistry C* 112(46): 17998-18010.

10. **Radoń M.**, 2008, ***On the Properties of Natural Orbitals for Chemical Valence***, *Theoretical Chemistry Accounts* 120: 337-339.

11. **Radoń M.**, Brocławik E., 2007, ***Peculiarities of the Electronic Structure of Cytochrome P450 Compound I: CASPT2 and DFT Modeling***, *Journal of Chemical Theory and Computation* 3(3): 728-734.

II. Prace popularnonaukowe:

1. **Radoń M.**, 2000, ***Zastosowanie katalizatorów w reakcjach organicznych***, *Niedziałki* 4, Zakład Metodyki Nauczania Chemii Wydziału Chemii UJ.