

Lista publikacji

- październik 2011

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

1. Cukrowski I., Govender K. K., Mitoraj M. P., **Srebro M.**, 2011, ***QTAIM and ETS-NOCV Analyses of Intramolecular CH...HC Interactions in Metal Complexes***, *Journal of Physical Chemistry A* 115: 12746-12757.
2. **Srebro M.**, Govind N., de Jong W. A., Autschbach J., 2011, ***Optical Rotation Calculated with Time-Dependent Density Functional Theory: The OR45 Benchmark***, *Journal of Physical Chemistry A* 115: 10930-10949.
3. Babashkina M. G., Safin D. A., **Srebro M.**, Kubisiak P., Mitoraj M. P., Bolte M., Garcia Y., 2011, ***Solvent-induced 1,3-N,S- vs. 1,5-S,S'-coordination in the Ni^{II} complex [Ni(p-Me₂NC₆H₄NHC(S)NP(S)(OiPr)₂]₂***, *CrystEngComm* 13: 5321-5327.
4. Kamiński R., Herbaczyńska B., **Srebro M.**, Pietrzykowski A., Michalak A., Jerzykiewicz L. B., Woźniak K., 2011, ***On the nature of Ni...Ni interaction in a model dimeric Ni complex***, *Physical Chemistry Chemical Physics* 13: 10280-10284.
5. Pietrzyk P., **Srebro M.**, Radoń R., Sojka Z., Michalak A., 2011, ***Spin Ground State and Magnetic Properties of Cobalt(II) – Relativistic DFT Calculations Guided by EPR Measurement of Bis(2,4-acetylacetonate)cobalt(II)-Based Complexes***, *Journal of Physical Chemistry A* 115: 2316-2324.
6. Mitoraj M. P., Parafiniuk M., **Srebro M.**, Handzlik M., Buczek A., Michalak M., 2011, ***Applications of ETS-NOCV method in a description of chemical reactions***, *Journal of Molecular Modeling* 17: 2337-2352.
7. Babashkina M. G., Safin D. A., Bolte M., **Srebro M.**, Mitoraj M., Ute A., Klein A., Köckerling M., 2011, ***Intramolecular Hydrogen Bond Controls 1,3-N,S- vs. 1,5-S,S'-coordination in Ni(II) Complexes of N-thiophosphorylated thioureas RNHC(S)NHP(S)(OiPr)₂***, *Dalton Transactions* 40: 3142-3153.
8. Futera Z., Koval T., Leszczynski J., Gu J., Mitoraj M., **Srebro M.**, Burda J. V., 2011, ***Exploring a Reaction Mechanism for Acetato Ligand Replacement in Paddlewheel Tetrakisacetatodirhodium (II) Complex by Ammonia; Computational DFT Study***, *Journal of Physical Chemistry A* 115: 784-794.
9. **Srebro M.**, Piękoś Ł., Kim T. J., Cheong M., Ok M. A., Kang S. O., Michalak A., 2010, ***On Conformational Flexibility of Half-Titanocene Catalysts with Aryloxy Ligands for High-Temperature Olefin Polymerization Processes: Static and Dynamic Theoretical Studies***, *Organometallics* 29: 5341-5352.
10. **Srebro M.**, Piękoś Ł., Kim T. J., Cheong M., Ok M. A., Kang S. O., Michalak A., 2010, ***On Preference of Insertion Mechanism in the Ethylene Polymerization Catalyzed by Half-Titanocene Complexes with Aryloxy Ligands: Static and Dynamic Theoretical Studies***, *Macromolecular Research* 18: 960-966.

11. Kim T. J., Kim S. K., Kim B. J., Son H. J., Hahn J. S., Cheong M., Mitoraj M., **Srebro M.**, Piękoś Ł., Michalak A., Kang S. O., 2010, ***Sterically Less-Hindered Half-Titanocene(IV) Phenoxides: Ancillary-Ligand Effect on Mono-, Bis-, and Tris(2-Alkyl/arylphenoxy) Titanium(IV) Chloride Complexes***, *Chemistry – A European Journal* 16: 5630-5644.
12. **Srebro M.**, Michalak A., ***Computational Modeling of Polymerization Catalysts***, [w:] ***Handbook of Transition Metal Polymerization Catalysts***, Hoff R., Mathers R. T., John Wiley & Sons, New Jersey, 2010: 53-102.
13. Kim T. J., Kim S. K., Kim B. J., Hahn J. S., Ok M. A., Song J. H., Shin D. H., Ko J., Cheong M., Kim J., Won H., Mitoraj M., **Srebro M.**, Michalak A., Kang S. O., 2009, ***Half-Metallocene Titanium(IV) Phenyl Phenoxide for High Temperature Olefin Polymerization: Ortho-Substituent Effect At Ancillary o-Phenoxy Ligand for Enhanced Catalytic Performance***, *Macromolecules* 42: 6932-6943.
14. Radoń M., **Srebro M.**, Broclawik E., 2009, ***Conformational Stability and Spin States of Cobalt(II) Acetylacetonate: CASPT2 and DFT Study***, *Journal of Chemical Theory and Computation* 5: 1237-1244.
15. **Srebro M.**, Michalak A., 2009, ***Theoretical Analysis of Bonding in N-Heterocyclic Carbene–Rhodium Complexes***, *Inorganic Chemistry* 48: 5361-5369.
16. **Srebro M.**, Mitoraj M., 2009, ***The Role of Ancillary Ligands in a Description of the Copper(I) – Bis(trimethylsilyl)acetylene Bonding. A Theoretical Study***, *Organometallics* 28: 3650-3655.
17. **Srebro M.**, Mitoraj M., Michalak A., 2009, ***Binding of Polar Monomers in the Complexes with Organometallic Ethylene Polymerization Catalysts: Natural Orbitals for Chemical Valence and Energy Decomposition Analysis***, *Canadian Journal of Chemistry* 87: 1039-1054.
18. Jagoda-Cwiklik B., Vácha R., Lund M., **Srebro M.**, Jungwirth P., 2007, ***Ion Pairing as a Possible Clue for Discriminating between Sodium and Potassium in Biological and Other Complex Environments***, *Journal of Physical Chemistry B* 111: 14077-14079.