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Theoretical study of structure and intramolecular rearrangement of coordination compounds of transition metals: methods and models

© **Vitaliy V. Koval**,[1] and **Andrey G. Starikov**[2]*[+]
[1] *Institute of Physical and Organic Chemistry. Southern Federal Uiversity. Stachka St., 194/2. Rostov on Don, 344090. Russian Federation. Phone: +7 (863) 297-51-95. E-mail: smit@ipoc.rsu.ru*
[2] *Southern Scientific Center of Russian Academy of Sciences. Chehova St., 41. Rostov on Don, 344006. Russian Federation Phone: +7 (863) 243-44-88. E-mail: andr@ipoc.rsu.ru*

*Supervising author; [+]Corresponding author

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Abstract

The applicability of different calculations schemas (HF, MP2, DFT, CAS and CCSD) for quantum chemical study of transition metals coordination compounds structure and intramolecular rearrangement have been considered. It is found, that B3LYP and B3LYP* functionals with 6-311++G(d, p) basis are correct reproduces the characteristics of compounds with variable magnetic properties. It is shown that theoretical study of transition metals coordination compounds with sterically overloaded ligands must to be performed with full molecules geometry because bulk substituents may have essential influence on stereochemistry of coordination center and stabilization of spin states.