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Quantum-chemical simulation of the magnetic sub-lattice of bifunctional compounds

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Abstract

On the basis of quantum-chemical calculations of magnetic properties of complex anions of various sizes we have described the procedure for modeling the magnetic sub-lattice of bifunctional compounds. Calculations of geometrical structure of various complexes in approximation B3LYP/LANL2DZ and of the constant exchange interaction (J) in approximation B3LYP/TZV have shown that complex anions $[L_2M1^{III}LM2^{II}L_2]$ n-, (L – ligand, M1 and M2 – three- and bivalent 3d-metals of transition series, n-a charge of anion) are optimal, only nine structural parameters being optimized.