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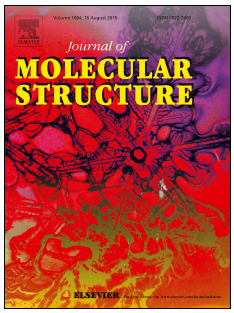


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# Facile synthesis of Co(II) and Cu(II) complexes of 2- hydroxybenzophenone: An efficient catalyst for oxidation of olefins and DFT study

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## Abstract

Two diketone complexes of Cu(II) and Co(II) were easily synthesized in reaction of M(CH3COO)2 with 2-Hydroxybenzophenone (bpoH). The complexes of $M(bpo)_2$ were characterized by UV-vis, IR spectroscopy, and elemental analysis. The complexes are active catalysts for the oxidation of styrene using TBHP as an oxidant. Under the optimized reaction conditions, 100% conversion of styrene with 63.5 % selectivity for Benzaldehyde and 36.5% for Styrene oxide were obtained by $Cu(bpo)_2$. Also, the effect of imidazole was investigated. Results confirmed that the addition of imidazole accelerates the oxidation of styrene. Our DFT results confirmed the necessity of diffuse functions in the basis set and including an accurate treatment of the dispersion energy for obtaining the most stable structure in these systems. Therefore, the geometry optimization and the vibrational frequencies were calculated at the M06-2X/6-311++G(d,p) level. The scaled theoretical frequencies and the structural parameters are in excellent agreement with the experimental data. The natural charge analysis indicated that an electron is transferred from $Cu(bpo)_2$ back to the TBHP to break the O−O bond and formation of tert-butoxyl radicals. Coordination of imidazole in the axial position of the $Cu(bpo)_2$ significantly assists in moving back of electron and increases the activity of the complex in oxidation.

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