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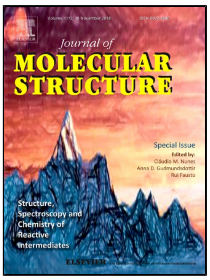

Structure, Spectroscopic Properties and Catalytic Activity for Epoxide Ring-Opening of Nickel Methylxanthate

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Structure, Spectroscopic Properties and Catalytic Activity for Epoxide Ring-Opening of Nickel Methylxanthate

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Abstract

The structure and spectroscopic properties of nickel methylxanthate, $Ni(S_2COCH_3)_2$, as isolated molecule and in crystalline phase, were investigated both experimentally and theoretically. Experimentally, single crystal X-ray diffraction, infrared and ultraviolet-visible spectroscopies have been used, while the applied theoretical approaches include density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations. The isolated molecule of the complex under study was found to exist in two nearly degenerated conformers (*cis* and *trans*, with the methyl groups of the ligand molecules positioned the same side or in opposite sides of the molecule, respectively). The *trans* conformer is selected upon crystallization. The crystal structure (at 100 K) was solved and discussed, with emphasis given to the characterization of the main intermolecular interactions. The infrared spectrum (in the 3500-300 cm^{-1} range) of the crystalline material was assigned in details, also taking into account the results of the normal coordinate analysis performed for the isolated molecule, which in turn was made using the data resulting from the DFT calculations. The UV-visible spectrum of the compound in $CHCl_3$ solution was also obtained and interpreted based on results of TD-DFT calculations, demonstrating the importance of the metal to ligand charge transfer in the studied complex. Finally, the catalytic activity of the complex for ring-opening reaction of styrene oxide resulting from nucleophilic attack of anilines was also evaluated, showing that the compound presents potential as catalyzer of this type of reactions.

Keywords: crystal structure, xanthate, DFT, Hirshfeld analysis, catalysis.

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