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Organotin(IV) Complexes as Catalyst for Biodiesel Formation: Synthesis, Structural Elucidation and Computational Studie

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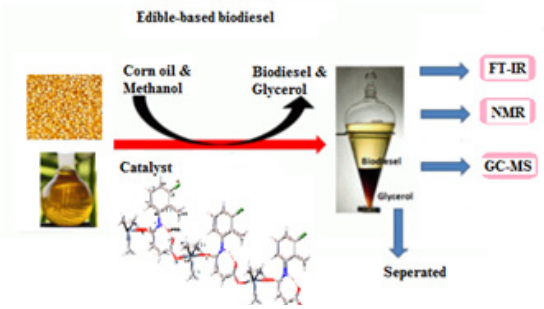
Abstract

Here we have presented the synthesis of three novel triorganotin(IV) complexes: trimethylstannyl 4-(3-chloro-2-methylphenylamino)-4-oxobut-2-enoate (1); tributylstannyl 4-(3-chloro-2-methylphenylamino)-4-oxobut-2-enoate (2) and triphenylstannyl 4-(3-chloro-2-methylphenylamino)-4-oxobut-2-enoate (3). The ligand and its three complexes were spectroscopically characterized by NMR (1H and 13C) in solution and by FT-IR in solid state. Complexes 1 and 2 were further characterized by single crystal X-ray diffraction analysis. The X-ray crystallographic data reveal that complexes 1 and 2 both are structurally trialkytin analogs with distorted trigonal bipyramidal geometry. The geometry around tin atom is constituted by three alkyl groups (methyl in complex 1 and butyl in complex 2) occupying the equatorial positions and two oxygen atoms of 4-(3-chloro-2-methylphenylamino)-4-oxobut-2-enoic acid ligand occupying the axial positions. The computational study was performed applying LANL2DZ (Los Alamos National Laboratory 2 Double-Zeta) functional with B3LYP (Lee, Yang and Parr) level of theory to obtain the optimized geometry, spectroscopic analysis, frontier molecular orbitals as well as global and local reactivity. A good correlation was found between the experimental and computational results. The homogeneous catalytic performance of synthesized compounds was evaluated for the transesterification of corn oil with methanol into biodiesel. The obtained corn oil biodiesel (COB) was confirmed by FT-IR, 1H NMR and GC-MS. The catalytic results revealed that the complexes were active at optimized conditions and therefore can be potential candidates for the development of new catalytic system for biodiesel production.

Biography



Biography

Muhammad Zubair attended Quaid-I-Azam University,Islamabad,Pakistan as a MPhil student in 2016 where I studied Natural Sciences, majoring in InorganicChemistry. I then continued my PhD in 2017 in Main Group Chemistry under the guidance of Prof Dr Saqib Ali. My research focused on Catalytic as well as Biological application of Organotin(IV) Carboxylate Complexes. I enjoy being outdoors and spending time with researcher

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