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Experimental and Theoretical Studies on the Structural and Vibrational Spectra of Schiff Base and Their Complex

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ABSTRACT

The synthesis of 5,5 '- (ethane-1,2-diylbis (azaneylylidene)) bis (3-undecyl-1,5-dihydro-4H-1,2,4-triazol-4-amine) and its Co (II) complex was carried out, and their structural spectroscopic properties were determined. The mode of bonding for the complexes was accomplished based on the elemental analysis, IR, UV-Vis, and NMR spectroscopy. Electronic structures and spectroscopic properties of the title compound were investigated from the calculative point of view. DFT/B3LYP optimization was performed based on the 6–31++G(d,p) basis set. In addition, the vibrational frequency analysis was performed with the optimized geometry at the same level of theory.

KEYWORDS

Azo Compound, Co (II) Complex, DFT/B3LYP, IR Spectroscopy, Vibrational Analysis

INTRODUCTION

Over the last few years, the expansion of new structures of azo compounds has attracted great attention in the scientific community working on this topic (Al-Hamdani et al., 2010). Azo compounds are derived from heterocyclic diazo components; they form colored complexes involving metal ions (Kirkan and Gup, 2008). These compounds are important for industry and biological systems (Phatok et al., 2009). On the other hand, metal chelates have also attracted major interest and have been extensively investigated for their remarkable electronic and geometrical characteristics in connection with their applications in various fields (Kupradinun et al., 2008). These azo compounds contain (-acidic) azo imine (-N=N-C-N), and are quite interesting due to their great stability; they are very easy to purify and present distinguishable colors. These compounds show wavelength displacements that are consistent with metal ion transitions (Mehdi et al., 2005; Al-adely et al., 2010). The chelate complexes involving five-membered or six-membered chelate rings are the most stable complexes

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(Weaver et al., 1982). Moreover, some drugs including these complexes discourage the growth of a number of germs (Sharma et al., 2008; Majed, et al., 2008). In addition, these compounds can also be used as analytical reagents (Dmitrienko et al., 2005; Mirkhani et al., 2009; Bakhsh and Rufchahi, 2009) for solvent extraction for the purpose of determining some metal ions. The azo cyclazole compound plays an important role in spectral field determination to identify the amount of some elements, and particularly transition metal ions; this compound presents high sensitivity and selectivity (Gavali and Hankarep, 2007). In this research, it was possible to prepare a new ligand with its complex [Co (II)], while taking into account its spectral configuration in order to obtain optimal properties related to concentration and pH values; the metal to ligand ratio for the purpose of preparing the complex was also identified.

EXPERIMENTAL

Materials and Reagents

All reactions were monitored by thin layer chromatography (TLC) using silica gel F254 supplied by MERCK, and a mixture of different polar and nonpolar solvents in varying proportions. Several spots were observed using iodine as a visualizing agent.

All melting points were determined in open capillary tubes on a BÜCHI 540 melting point apparatus.

The infrared spectra of reactants and products were recorded by potassium bromide discs on a Shimadzu FTIR-8300 Fourier Transform infrared spectrophotometer in the range extending from 4000 to 400 cm-1.

The spectra of 1H and 13C NMR were measured in Chloroform-d (CDCl3) on a Bruker AM 300 MHZ Spectrometer at the University of Oran (Algeria), relative to the internal standard tetramethylsilane (TMS). The chemical shift values were expressed in parts per million (δ, ppm). The Ultraviolet spectra of reactants and products were identified by the Optizen spectrophotometer.

Preparation of Ethyl Laurate B

This ester was prepared according to the standard procedure reported in the literature (Becke, 1993). Lauric acid (5g, 0.025 mol) was dissolved in ethanol (200 mL) with 5 mL of concentrated sulfuric acid. The resulting mixture was refluxed at 80°C in an oil bath for 6 to 7 hours. The progress of the reaction was monitored by thin layer chromatography (TLC). The excess acid was neutralized with sodium bicarbonate then the solvent was evaporated; the final product was collected. The yield for compound B was 81.55%, and the resulting product was in liquid form with Rf=0.65 ($CHCl_3$/CH_3OH=8/2); IR (KBr, υ cm^{-1}): 1739.7 (C=O), 1016.4 (C-O-C). ^{1}H-NMR (δ ppm): 0.903 (3H,-O-CH2-C(H3)), 4.116 (2H, -O-C(H2)-CH3), 2.292 (2H, O=C-C(H2)-CH2-), 1.618 (2H, O=C-CH2-C(H2)-), 1.257 (2H, -CH2-C(H2)-C(H2)- C(H2)- C(H2)- C(H2)- C(H2)- C(H2)- C(H2)-CH3), 0.88 (3H, -CH2-CH2-C(H3)). 13C-NMR(δ ppm): 14.229 (-O-CH2-(C)H3, -CH2-CH2-(C)H3), 59.796 (-O-(C)H2-CH3), 174.068 (O=(C)-CH2-), 34.396 (O=C-(C)H2-CH2-), 24.987 (O=C-CH2-(C)H2-), 29.612 (-CH2-(C)H2-(C)H2-(C)H2-(C)H2-(C)H2-(C)H2-(C)H2-CH2-CH2-CH3), 31.918 (CH2-(C)H2-CH2-CH3), 22.695 (CH2-CH2-(C)H2-CH3).

Preparation of N'-Dodecanoylmethanedihydrazide C

Nalco (1.76g, 0.019mol) was added to a solution of lauric ethyl ester B (4.47 g, 0.019mol) in ethanol (100 mL). The mixture was heated for 10 hours in an oil bath. The progress of the reaction was monitored by TLC and the resulting yield was 81%, with Rf = 0.75 ($CHCl_3$/CH_3OH=8/2); IR (KBr, υ cm^{-1}): 3483.2 (NH-NH_2), 1737.7 (C=O). ^{1}H-NMR(δ ppm): 5.026 (3H, -N(H)-NH2, -N(H)-N(H)-), 4.135 (2H, -NH-N(H2)), 2.285 (2H, O=C-C(H2)-CH2-), 1.253 (2H, -CH2-C(H2)- C(H2)- C(H2)- C(H2)- C(H2)- C(H2)- C(H2)- C(H2)- C(H2)-CH3), 1.624(2H, O=C-CH2- C(H2)-), 0.854 (3H, -CH2-CH2-

Pretreatment of Lignocellulosic Biomass Feedstocks for Biofuel Production

Desikan Ramesh, Iniya Kumar Muniraj, Kiruthika Thangaveluand Subburamu Karthikeyan (2018). *Advanced Solid Catalysts for Renewable Energy Production (pp. 33-60).*

www.irma-international.org/chapter/pretreatment-of-lignocellulosic-biomass-feedstocks-for-biofuel-production/196144