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“Physicochemical and structural studies of the complexes of chromium, molybdenum, and tungsten carbonyls with a molecularly designed bicompartmental Schiff base ligand”

By

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ABSTRACT

Two novel macrocyclic Schiff base ligands [1,1'-(acridine-3,6-diylbis(azaneylylidene))bis(methaneylylidene))bis(naphthalen-2-ol); L1 and N,N'-(acridine-3,6-diyl)bis(1-(quinolin-2-yl)methanimine); L2] were synthesized and their structures were confirmed with various spectroscopic analysis. The X-ray single crystal analysis was carried out on L1 and explored that the ligand was crystallized in a monoclinic crystal system with a space group P21/c. The compound was crystalized with five water molecules. Interestingly, L1 occurred as a double zwitterion, where the hydrogen of the OH group of the hydroxynaphthalene transferred to the azomethine nitrogen to form NH+ and O- moieties with the presence of hydrogen bonding between them. Hirshfeld surface analysis of the L1 was also investigated.

The reaction of these Schiff base ligands with metal carbonyls [Cr(CO)6, Mo(CO)6, and W(CO)6] produced novel six oxo complexes [Cr(L1)(O)2(DMF)] 1, [Mo(L1)(O)3(DMF)] 2, [W(L1)(O)3(DMF)] 3, .[Cr(L2)(O)2(DMF)] 4, [Mo(L2)(O)3(DMF)] 5, and [W(L2)(O)3(DMF)] 6

All complexes were synthesized by heating to reflux an equimolar of M(CO)6 and the ligands. The synthesized complexes were characterized by spectroscopic and elemental analysis. TGA and DTG studies were also used to assess the thermal stability of the oxo complexes. The two Schiff base ligands and their complexes were tested against microbial strains and some of the complexes outperformed the free ligands in terms of antibacterial activity. Furthermore, antioxidant activity and .CT-DNA binding of the compounds were studied by different techniques

Spectroscopic investigation of the synthesized compounds confirmed the proposed structure of each compound. Mass spectrometry and elemental analysis proved the metal complexes were structurally formulated in a 1:1 (metal: ligand) ratio. The IR spectroscopy showed that the metal coordinated with ligands through two coordination sites: azomethine group and oxygen of the phenolic-OH group. The IR of the Cr complexes (CrL1, CrL2) showed two asymmetric and symmetric stretching frequencies at 977 and 811 cm-1 due to cis Cr=O bonds. On the other hand, the Mo and W complexes' IR spectra displayed two asymmetric and symmetric stretching frequencies due to cis M=O bonds, in addition to another band at a higher wavenumber corresponding to a M=O gp in the apical position. Non-ligand stretching frequencies also appeared in the IR spectra of the complexes according to M-N and M-O .bonds

The magnetic measurements of the complexes revealed that the chromium complexes are paramagnetic. The effective magnetic moment (μeff) values of [Cr(L1)(O)2(DMF)] and [Cr(L2)(O)2(DMF)]at 298 k were 2.75 and 2.68 which are close to two unpaired electrons' spin-only value (2.83 BM). Therefore, the μeff values concluded that the chromium in the complex had a d2 .electronic configuration with a +4 formal oxidation state

On the other hand, the magnetic measurements of the Mo and W complexes of L1 and L2 confirmed the diamagnetic features of the complexes. Thus, the 1H NMR measurements of the molybdenum and tungsten complexes were conducted. The 1H NMR spectra confirmed the coordination of the ligands to metals through one azomethine group, hydroxyl group without deprotonation, in addition .to one molecule of dimethylformamide

Biological Activity

The ligands and complexes were investigated as antimicrobial, antioxidant, and CT-DNA binder agents. They showed superb biological activity, which will be discussed in the following lines. Thus, .they could be utilized as bio-inorganic agents in the medical field

Antimicrobial activity

Uv-Vis absorption titration

.Fluorescence quenching studies

Viscosity measurements

Molecular Docking studies