



Title

**Reactions of Group VIB metal carbonyls with two novel rigid macrocyclic Schiff base ligands incorporating acridine inter-crossing group**

### Abstract

Two acridine Schiff base ligand derivatives; 1,1'-(acridine-3,6-diylbis(azaneylylidene))bis(methaneylylidene))bis(naphthalen-2-ol);  $L^1$  and N,N'-(acridine-3,6-diyl)bis(1-(quinolin-2-yl)methanimine);  $L^2$ , were prepared and reacted with group VIB metal carbonyls ((M(CO)<sub>6</sub>) M= Cr, Mo, and W) to give the complexes of molecular formula;  $[Cr(L^1)(O)_2(DMF)](1)$ ,  $[Mo(L^1)(O)_3(DMF)](2)$ ,  $[W(L^1)(O)_3(DMF)](3)$ ,  $[Cr(L^2)(O)_2(DMF)](4)$ ,  $[Mo(L^2)(O)_3(DMF)](5)$ , and  $[W(L^2)(O)_3(DMF)](6)$ .

Several analytical and spectroscopic analyses characterized all formed compounds. Furthermore, ligand one was analyzed by X-ray crystallography. The L1 molecule crystallized in a monoclinic crystal system with a space group P21/c. It's interesting to note that L1 formed as a double zwitterion when the H<sup>+</sup> of hydroxynaphthalene's OH group moved to the nitrogen of the azomethine to produce NH<sup>+</sup> and O<sup>-</sup> moieties, with hydrogen bonding occurring between them. Additionally, the L1's Hirshfeld surface analysis was examined. The spectroscopic analysis revealed that all complexes formed as oxo complexes and coordinated to the ligands through two centers, in addition to a DMF molecule which was used as a solvent. Biological activity including antimicrobial and antioxidant activities of all compounds was investigated. In addition, DNA binding including UV-vis, fluorescence quenching, and viscosity evaluations was carried out. It was determined that the binding interaction with DNA was electrostatic binding mode rather than intercalative mode. The molecular docking of the compounds was also investigated with three large molecule receptors (PDB: 4BJP, 1BQB, and 1BNA). Docking studies demonstrated that the molybdenum derivative with ligand 1 showed the highest binding degree towards DNA with a value of -8.40 kcal/mol. This result is consistent with the biological studies mentioned above, such as DNA binding, fluorescence quenching, and viscosity tests.