

Recent advances in the structure elucidation of d^{10} transition metal complexes based on 16-membered ring macrolide drug

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Received 20 November 2023; accepted (revised) 22 March 2024

The present study outlines theoretical and spectroscopic investigations on a Tylan® ligand and some of its d^{10} transition metals complexes. Tylan interacts in a bidentate coordination manner through donor atoms of oxygen and nitrogen in its structure. Two essential Tylan metal complexes have been synthesized and characterized depending on their elemental analysis, molar conductivity and spectral studies (FT-IR and Mass spectra). The very low value of molar conductivity of complexes demonstrates their non-electrolytic nature. From experimental studies, general structures of these new complexes have been assumed as formula $[M(\text{TYS})\text{X}_2(\text{H}_2\text{O})_2]$, where TYS = Tylan ligand; $M = \text{Hg}(\text{II})$ and $\text{Cd}(\text{II})$; $\text{X} = \text{Cl}^-$. Based on spectroscopic studies, an octahedral geometry has been suggested for both complexes. Molecular modelling by Gaussian 09 software has been employed to give further light on bonding properties in addition to theoretically confirming binding sites of Tylan ligand and its new synthesized metal complexes. The quantum chemical reactivity parameters such as chemical hardness, chemical potential, electronegativity, electrophilicity index and HOMO-LUMO energy gap have been obtained theoretically. The thermal analysis by TG-DTA indicates that the complex has three consecutive phases of decomposition which ends by the formation of divalent metal oxide, CdO as a final product. While in case of Hg complex no metal oxide formation is observed due to Hg(II) sublimation. The kinetic and thermodynamic parameters have been calculated utilizing DTA curves. This study explains that Tylan ligand can form five-membered ring with metal ion Cd(II) and Hg(II) during formation of complexes which gives high stability to the synthesized complexes.

Keywords: Macrocyclic, Mass Spectra, Molecular Modelling, Mercury Complexes, Thermal Studies