

Zinc Barbiturate Complexes with Bidentate N-Donor Ligands: Syntheses, Crystal Structures, Spectroscopic, Thermal and Voltammetric Studies

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Two new bis(5,5–diethylbarbiturato) (barb) complexes of zinc, $[\text{Zn}(\text{barb})_2(\text{en})]$ (**1**) and $[\text{Zn}(\text{barb})_2(\text{bpy})] \cdot \text{H}_2\text{O}$ (**2**) [en = ethylenediamine, bpy = 2,2'–bipyridine], have been prepared and characterized by elemental analysis, IR spectroscopy, thermal analysis and single crystal X-ray diffraction. Complexes **1** and **2** crystallize in monoclinic space groups. The zinc(II) ions in complex **1** are tetrahedrally coordinated by two barb and an en ligand. The barb ligands are N-coordinated while the en ligand acts as a bidentate chelating ligand. One carbonyl oxygen atom of each barb ligands in complex **2** participates in the bonding with the zinc ion with remarkably long Zn–O bonds resulting in a highly distorted octahedral geometry. Molecules of complex **1** are connected *via* N–H...O hydrogen bonds, involving hydrogen atoms of both barb and en ligands, while molecules of complex **2** are linked by N–H...O and O–H...O hydrogen bonds and also aromatic $\pi(\text{bpy}) \cdots \pi(\text{bpy})$ stacking interactions. The voltammetric behavior of complexes **1** and **2** was investigated in aqueous solution by cyclic voltammetry using a $\text{NH}_3/\text{NH}_4\text{Cl}$ buffer. The cyclic voltammogram of **1** shows a cathodic peak at –1.260 V and an anodic peak at –1.068 V due to a quasi-reversible two-electron process. Complex **2** yields two reduction peaks at –1.312 and –1.412 V. The former corresponds to a quasi-reversible electrode process of the zinc(II) ions in complex **2**, while the latter is attributed to the reduction of the coordinated bpy ligands.

Key words: Barbiturate, Ethylenediamine, 2,2'–Dipyridyl, Zinc, Crystal Structure