Title:	Ni(II) and Co(III) complexes of 5-methyl-1,3,4-thiadiazole-2-thiol: Syntheses, spectral, structural, thermal analysis, and DFT calculation
Authors:	Prashanth, B. (/jspui/browse?type=author&value=Prashanth%2C+B.) Singh, Sanjay (/jspui/browse?type=author&value=Singh%2C+Sanjay)
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Abstract:	Two new complexes, [Ni(en)2(mtt)2] (1) and [Co(en)2(mtt)2](mtt) (2) (Hmtt = 5-methyl-1,3,4-thiadiazole-2-thiol and en = ethylenediamine), have been synthesized and characterized by various physicochemical techniques. Complexes 1 and 2 crystallize in monoclinic and orthorhombic system with space groups P 21/n and P 21 21 21, respectively. The molecular structures of 1 and 2 show that the metal ions are six-coordinate bonded through four equatorial nitrogens of two en and two axial nitrogens of mtt ligands. The crystal structures of the complexes reveal that mtt is present in thione form and bound to the metal ion through the thiadiazole nitrogen. The crystal structures of the complexes are stabilized by various intermolecular hydrogen bonding providing supramolecular architecture. Complex 2 is also stabilized by weak π···π interactions occurring between two thiadiazole rings. The bioefficacies of the ligand and complexes have been examined against the growth of bacteria to evaluate their antimicrobial potential. The biological results suggest that 2 is more active than the ligand and 1 against the tested bacteria. The geometries of the ligand and the complexes have been optimized by the DFT method and the results are compared with the X-ray diffraction data. The Co(III) complex exhibits an irreversible Co(III)/Co(II) process while the Ni(II) complex displays quasi-reversible Ni(II)/Ni(III) redox processes with large peak separation as compared to that expected for a one electron process which is thought to be coupled with some chemical reaction
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