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Thermal properties, antimicrobial activity and DNA binding of Ni(II) complexes of azo dye compounds

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Abstract

A novel series of nickel(II) azo dye complexes of 5-(4-methoxyphenylazo)-2-thioxo-4-thiazolidinone (HL₁), 5-(4-methylphenylazo)-2-thioxo-4-thiazolidinone (HL₂), 5-(phenylazo)-2-thioxo-4-thiazolidinone (HL₃) and 5-(4-nitrophenylazo)-2-thioxo-4-thiazolidinone (HL₄) were prepared and characterized elemental analyses, IR, UV-Visible spectra, X-ray diffraction analysis and mass spectra as well as thermogravimetric analysis (TGA). The magnetic measurements of Ni(II) complexes (**1-4**) lie in 3.05-3.20 BM., as anticipated for octahedral geometry. Quantum chemical parameters and molecular structures of the complexes were theoretically computed and the results were studied. IR spectra show that HL_n ligands (n = 1-4) act a monobasic bidentate ligands by coordinating *via* the oxygen atom of the deprotonated -OH group moiety and nitrogen atom of azo group. The interaction between Ni(II) complexes and calf thymus DNA (CT-DNA) shows hyperchromism effect coupled with obvious bathochromism shift. The value of binding constant (K_b) obtained from the absorption spectral technique for Ni(II) complexes (**1-4**) was calculated and found to be 1.20×10^5 , 1.17×10^5 , 7.22×10^4 and 6.65×10^4 M⁻¹, respectively. The antimicrobial activities of Ni(II) complexes (**1-4**) were investigated. It was found that the Ni(II) complexes have low antibacterial activity against *Klebsiella pneumoniae*. Complex (**1**) has antifungal activity against *Penicillium italicum*. All the Ni(II) complexes have more antibacterial activity than the penicillin against *Klebsiella pneumoniae*. The thermodynamic parameters were calculated using Coats–Redfern and Horowitz–Metzger methods. From the values of the thermal activation energy for decomposition (E_a) of Ni(II) complexes (**1-4**), it was found that the E_a value for the complex (**4**) is higher compared to the other complexes. The positive value of Gibbs free energy change of the decomposition (ΔG^*) for the Ni(II) complexes is non-spontaneous processes.

Keywords: Ni(II) complexes; Calf thymus DNA; X-ray diffraction analysis; Thermal analysis; Thermodynamic parameters; Antimicrobial activity.

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