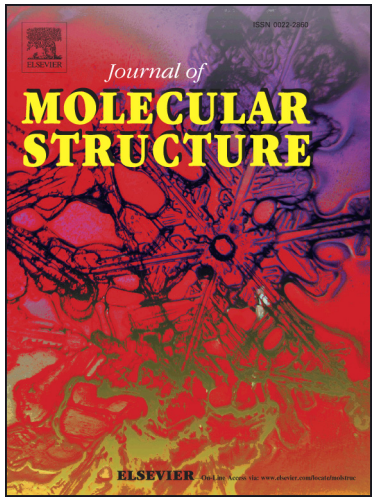

Synthesis, spectral characterization, molecular modeling, biological activity and potentiometric studies of 4-amino-5-mercapto-3-methyl-*S*-triazole Schiff's base complexes

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Revised manuscript

Synthesis, spectral characterization, molecular modeling, biological activity and potentiometric studies of 4-amino-5-mercapto-3-methyl-*S*-triazole Schiff's base complexes

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Abstract

The Schiff's base derived from condensation of *s*-triazole (4-amino-5-mercapto-3-methyl-*S*-triazole) with pyridine-2-aldehyde and their corresponding Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) complexes have been synthesized. The isolated solid complexes were characterized by elemental analyses, molar conductance, spectral (IR, UV–Vis, ^{1}H NMR, mass), magnetic moment and thermal measurements. The IR spectral data suggest that the ligand coordinate in a tridentate manner (SNN) via the one thiol (SH), one pyridine ring and the azomethine (C=N) groups. The data show that the complexes have composition of ML_2 type. The activation of thermodynamic parameters are calculated using Coast-Redfern, Horowitz–Metzger (HM), and Piloyan–Novikova (PN). The octahedral geometry of the complexes is confirmed using DFT method from DMOL3 calculations and ligand field parameters. Protonation constants of Schiff base and stability