

Synthesis, Characterization, and Bioactivity of Schiff Bases and Their Cd²⁺, Zn²⁺, Cu²⁺, and Ni²⁺ Complexes Derived from Chloroacetophenone Isomers with S-Benzylthiocarbamate and the X-Ray Crystal Structure of S-Benzyl-β-N-(4-chlorophenyl)methylenedithiocarbamate

ABSTRACT

Two bidentate Schiff base ligands having nitrogen sulphur donor sequence were derived from the condensation of S-benzylthiocarbamate (SBDTC) with 2-chloroacetophenone and 4-chloroacetophenone to give S-benzyl-β-N-(2-chlorophenyl)methylenedithiocarbamate (NS2) and S-benzyl-β-N-(4-chlorophenyl)methylenedithiocarbamate (NS4) isomers. Each of the ligands was then chelated with Cd²⁺, Zn²⁺, Cu²⁺, and Ni²⁺. The compounds were characterized via IR spectroscopy and melting point while the structure of NS4 was revealed via X-ray crystallography. Finally, the compounds were screened for antimicrobial activity to investigate the effect that is brought by the introduction of the chlorine atom to the benzene ring. X-ray crystallographic analysis showed that the structure of NS4 is planar with a phenyl ring that is nearly perpendicular to the rest of the molecules. The qualitative antimicrobial assay results showed that NS4 and its complexes lacked antifungal activity while Gram-positive bacteria were generally inhibited more strongly than Gram-negative bacteria. Furthermore, NS4 metal complexes were inhibited more strongly than the ligand while the opposite was seen with NS2 ligand and its complexes due to the partial solubility in dimethyl sulfoxide (DMSO). It was concluded that generally NS2 derivatives have higher bioactivity than that of NS4 derivatives and that the Cd complexes of both ligands have pronounced activity specifically on *K. rhizophila*.

Keyword: Schiff base; Chloroacetophenone; Dithiocarbamate; Antimicrobial.