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Metal-based biologically active azoles and β-lactams derived from sulfa drugs

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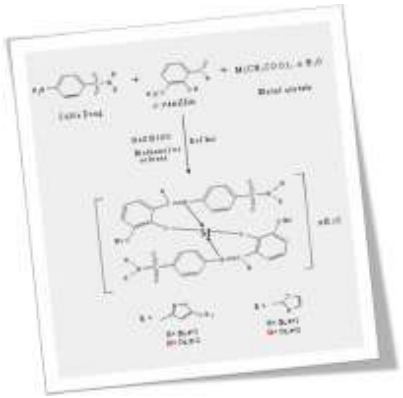
Abstract

Metal complexes of Schiff bases derived from sulfamethoxazole (SMZ) and sulfathiazole (STZ), converted to their β-lactam derivatives have been synthesized and experimentally characterized by elemental analysis, spectral (IR, ^{1}H NMR, ^{13}C NMR, and EI-mass), molar conductance measurements and thermal analysis techniques. The structural and electronic properties of the studied molecules were investigated theoretically by performing density functional theory (DFT) to access reliable results to the experimental values. The spectral and thermal analysis reveals that the Schiff bases act as bidentate ligands via the coordination of azomethine nitrogen to metal ions as well as the proton displacement from the phenolic group through the metal ions; therefore, Cu complexes can attain the square planner arrangement and Zn complexes have a distorted tetrahedral structure. The thermogravimetric (TG/DTG) analyses confirm high stability for all complexes followed by thermal decomposition in different steps. In addition, the antibacterial activities of synthesized compounds have been screened in vitro against various pathogenic bacterial species. Inspection of the results revealed that all newly synthesized complexes individually exhibit varying degrees of inhibitory effects on the growth of the tested bacterial species, therefore, they may be considered as drug candidates for bacterial pathogens. The free Schiff base ligands (**1–2**) exhibited a broad spectrum antibacterial activity against Gram negative *Escherichia coli*, *Pseudomonas aeruginosa*, and *Proteus* spp., and Gram positive *Staphylococcus aureus* bacterial strains. The results also indicated that the β-lactam derivatives (**3–4**) have high antibacterial activities on Gram positive bacteria as well as the metal complexes (**5–8**), particularly Zn complexes, have a significant activity against all Gram negative bacterial strains. It has been shown that the metal complexes have significantly higher activity than

corresponding ligands due to chelation process which reduces the polarity of metal ion by coordinating with ligands.

Graphical abstract



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Keywords

Metal Schiff base; β-Lactam; Sulfamethoxazole; Sulfathiazole; Antibacterial activity; NMR

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