

Unusual saccharin-N,O (carbonyl) coordination in mixed-ligand copper(II) complexes: synthesis, X-ray crystallography and biological activity

ABSTRACT

Three tridentate Schiff bases containing N and S donor atoms were synthesized via the condensation reaction between S-2-methylbenzylthiocarbamate with 2-acetyl-4-methylpyridine (S2APH); 4-methyl-3-thiosemicarbazide with 2-acetylpyridine (MT2APH) and 4-ethyl-3-thiosemicarbazide with 2-acetylpyridine (ET2APH). Three new, binuclear and mixed-ligand copper(II) complexes with the general formula, $[\text{Cu}(\text{sac})(\text{L})]_2$ (sac = saccharinate anion; L = anion of the Schiff base) were then synthesized, and subsequently characterized by IR and UV/Vis spectroscopy as well as by molar conductivity and magnetic susceptibility measurements. The Schiff bases were also spectroscopically characterized using NMR and MS to further confirm their structures. The spectroscopic data indicated that the Schiff bases behaved as a tridentate NNS donor ligands coordinating via the pyridyl-nitrogen, azomethine-nitrogen and thiolate-sulphur atoms. Magnetic data indicated a square pyramidal environment for the complexes and the conductivity values showed that the complexes were essentially non-electrolytes in DMSO. The X-ray crystallographic analysis of one complex, $[\text{Cu}(\text{sac})(\text{S2AP})]_2$ showed that the Cu(II) atom was coordinated to the thiolate-S, azomethine-N and pyridyl-N donors of the S2AP Schiff base and to the saccharinate-N from one anion, as well as to the carbonyl-O atom from a symmetry related saccharinate anion yielding a centrosymmetric binuclear complex with a penta-coordinate, square pyramidal geometry. All the copper(II) saccharinate complexes were found to display strong cytotoxic activity against the MCF-7 and MDA-MB-231 human breast cancer cell lines.

Keyword: Saccharin; Dithiocarbamic acid; Tridentate NNS Schiff bases; Pentacoordinate copper(II) complexes