Synthesis and characterization of copper(I) coordination compounds with (1-(2-pyridylazo)-2-naphthol) and (4-(2-pyridylazo)resorcinol).

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Streszczenie

Two cuprous complexes with 1-(2-pyridylazo)-2-naphthol (PAN) or 4-(2-pyridylazo)resorcinol (PAR) and triphenylphosphines, $[Cu(PAN)(PPh_3)_2]BF_4$ (**1**) and $[Cu(PAR)(PPh_3)_2]BF_4$ (**2**), are described in this work. The structures of both compounds were characterized by NMR and UV–Vis spectroscopies, mass spectrometry, IR-ATR measurements and DFT calculations. The single crystal diffraction of both complexes confirmed that the coordination polyhedrons around the copper centres are distorted tetrahedrons. Interestingly, the PAR and the PAN ligands are not planar in the synthesized complexes. The ligands coordinate to the central copper(I) ions by only two nitrogen atoms: one from pyridine and one from an azo group. The oxygen atoms from the hydroxyl groups do not form bonds with copper, but take part in strong intramolecular hydrogen bonds, which stabilize the conformations of the ligands. It is noteworthy that these bonds have different characters. In complex **2** we observed a typical O–H···N hydrogen bond, whereas in complex **1** proton transfer takes place, resulting in O···H–N bond formation. DFT data confirm the different characters of the H-bonds observed in the X-ray structures.

Słowa kluczowe

Copper(I) complexes, 1-(2-Pyridylazo)-2-naphthol, 4-(2-pyridylazo)resorcinol, DFT studies, Structural studies

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