

Luminescent copper(I) (pseudo)halide complexes with neocuproine and a novel bulky tris (aminomethyl) phosphine derived from 2-piperazinopyridine.

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Streszczenie

A novel bulky phosphine derived from 2-piperazinopyridine $P(CH_2N(CH_2CH_2)_2N-2-py)_3$ (**1**) and its chalcogenide derivatives (oxide, sulfide and selenide) have been synthesized and characterized by elemental analysis, NMR spectroscopy and mass spectrometry. Next, two new copper(I) iodide or isothiocyanate complexes with **1** and 2,9-dimethyl-1,10-phenanthroline (dmp): $[CuI(dmp)(\mathbf{1})]$ (**1I**) and $[CuNCS(dmp)(\mathbf{1})]$ (**1T**), have been also synthesized and characterized by elemental analysis and studied by NMR, UV-vis, IR and luminescence spectroscopies. The X-ray structure of the complex **1T**·1.81(CH_3COCH_3) was determined. The coordination geometry around the Cu(I) center is pseudo-tetrahedral with distortions resulting mostly from the molecular packing in the crystal cell. Both complexes exhibit orange photoluminescence in the solid state, which is much stronger for **1I** than for **1T**. The luminescence spectra of both complexes at room and 77 K temperatures show relatively large bands with a typical bathochromic shift accompanying the lowering of the temperature. On the basis of TDDFT calculations we interpreted these bands as of (MX,MPR₃)LCT type resulting mainly from the transitions from the copper-iodine (or isothiocyanate) bonds and a small admixture of copper-phosphine bonds to antibonding orbitals of dmp diimine.

Słowa kluczowe

Tris (aminomethyl) phosphine, 2-piperazinopyridine, Copper(I) complexes, Crystal structure, Luminescence, DFT calculations

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