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Laser induced multi-component luminescence of [CuNCS(1,10-phen)P($CH_2N(CH_2CH_2)_2O)_3$]–the first example of CuNCS complexes with diimines and tris(aminomethyl)phosphanes.

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Streszczenie

[CuNCS(phen)P($CH_2N(CH_2CH_2)_2O)_3$], a novel mixed-ligand complex of copper(I) isothiocyanate with 1,10-phenanthroline and tris(aminomethyl)phosphane derived from morpholine have been synthesized. It was characterized by elemental analysis, thermogravimetric and differential thermal analyses and studied by NMR, mass, UV–Vis, IR and luminescence spectroscopies. The X-ray structure of the complex was determined. The coordination geometry about the Cu(I) center is pseudo-tetrahedral. The complex exhibits a very weak photoluminescence in the solid state. Surprisingly, the luminescence spectra of the crystalline sample at room and LN temperatures show several bands similarly to absorption(reflectance) spectrum. On the basis of TDDFT calculations we interpreted these bands as of MLLCT type resulting mainly from two transitions: π^*(CuNCS)$\rightarrow\pi^*$(phen) and σ(CuP)$\rightarrow\pi^*$(phen). This strongly suggests that all the ligands are involved into absorption and PL spectra, however their complex character (several bands observed) does not allow the more precise interpretation.

Słowa kluczowe

Copper(I) complex, crystal structure, luminescence, DFT calculation, Tris(aminomethyl)phosphane

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