



Solid state luminescence of copper(I) (pseudo)halide complexes with neocuproine and aminomethylphosphanes derived from morpholine and thiomorpholine.

Autorzy

Radosław Starosta

Urszula K. Komarnicka

Małgorzata Puchalska

Maciej Barys

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Streszczenie

The copper(I) iodide or copper(I) isothiocyanate complexes with 2,9-dimethyl-1,10-phenanthroline (dmp) and two interesting aminomethylphosphanes: $P(CH_2N(CH_2CH_2)_2O)_3$ (**1**) and novel $P(CH_2N(CH_2CH_2)_2S)_3$ (**2**): $CuI(dmp)P(CH_2N(CH_2CH_2)_2O)_3$ (**1I**), which was presented in our previous papers, $CuI(dmp)P(CH_2N(CH_2CH_2)_2S)_3$ (**2I**), $CuNCS(dmp)P(CH_2N(CH_2CH_2)_2O)_3$ (**1T**) and $CuNCS(dmp)P(CH_2N(CH_2CH_2)_2S)_3$ (**2T**) are discussed in this work. The chemical structures of three new complexes were determined in solution by means of NMR spectroscopy and in solid state using X-ray measurements. For all presented complexes the coordination geometry about the Cu(I) centre is pseudo-tetrahedral showing the small flattening and large rocking distortions. All compounds crystallize as the discrete dimers bound by π -stacking interactions between dmp rings, which strongly depend on the phosphane ligand. Investigated complexes exhibit orange photoluminescence in the solid state of highly diversified intensity, position of the luminescence band and the lifetimes. On the basis of TDDFT calculations, the CT bands observed in UV-Vis spectra are assigned to the two mixed transitions from the CuX (X = I or NCS) bond with a small admixture of the CuP bond to π^* orbitals of the dmp ligand: (MX,MPR₃)LCT. However, emission bands can be interpreted to be of (MX)LCT type.

Adres publiczny

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