Coordination studies of 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine towards Cu^{2+} cation. X-ray studies, spectroscopic characterization and DFT calculations.

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Streszczenie

The reactions of 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine with $CuCl_2 \cdot 2H_2O$, $Cu(NO_3)_2 \cdot 3H_2O$ and $CuSO_4 \cdot 5H_2O$ have been examined, and four $[CuCl_2(dppt)]$ (**1**), $[CuCl_2(dppt)_2] \cdot 2MeOH$ (**2**), $[Cu(dppt)_2(H_2O)_2](NO_3)_2$ (**3**) and $[Cu(SO_4)(dppt)(H_2O)]_n \cdot nH_2O$ (**4**) complexes have been obtained. All the complexes have been structurally and spectroscopically characterized, and compound **4** has been additionally studied by magnetic measurements. The electronic structure of **1** has been calculated with the density functional theory (DFT) method, and the time-dependent DFT calculations have been employed to calculate the electronic spectrum of **1**.

Słowa kluczowe

Copper complexes, photoluminescence, 6-Diphenyl-3-(2-pyridyl)-1, molecule, 4-triazine, X-ray and electronic structure, DFT calculations

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