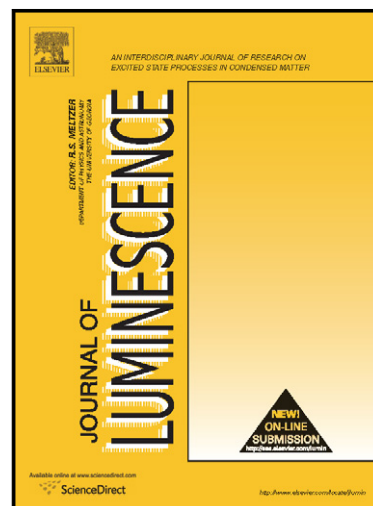


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Thiocyanate cadmium(II) complexes of 2,4,6-tri(2-pyridyl)-1,3,5-triazine - synthesis, structure and luminescence properties

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Abstract

Two new thiocyanate cadmium(II) complexes of 2,4,6-tri(2-pyridyl)-1,3,5-triazine were synthesized and characterised. The resulted complexes $[\text{Cd}(\text{SCN})(\text{NO}_3)(\text{tpz})(\text{H}_2\text{O})]$ (**1**) and $[\text{Cd}(\text{SCN})_2(\text{tpz})(\text{MeOH})]$ (**2**) were studied by IR, UV-Vis spectroscopy and single crystal X-Ray analysis. The luminescent properties of **1** and **2** were studied in solution and solid state and compared with the free ligand. To get detailed insight into the electronic structure and spectroscopic properties of $[\text{Cd}(\text{SCN})(\text{NO}_3)(\text{tpz})(\text{H}_2\text{O})]$ and $[\text{Cd}(\text{SCN})_2(\text{tpz})(\text{MeOH})]$, the density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations were performed.

Key words: luminescence; cadmium(II) complexes; 2,4,6-tri(2-pyridyl)-1,3,5-triazine; X-ray structure; supramolecular structure; DFT calculations.

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