

Design and Synthesis of a New Photoluminescent 2D Coordination Polymer Employing a Ligand Derived from Quinoline and Pyridine

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Streszczenie

Application of organic ligand 2-(3-ethyl-pyrazin-2-yl)quinoline-4-carboxylate with N/O donor atoms enabled solvothermal synthesis of a 2D Cu(II) coordination polymer, $\{Cu(L)BF_4\}_n$ (L = deprotonated 2-(3-ethyl-pyrazin-2-yl)quinoline-4-carboxylate). Both the ligand and its coordination polymer have been characterized. The condensed ring system of the applied ligand promotes the formation of coordination polymers rather than mononuclear species. The obtained 2D coordination polymer is photoluminescent with bathochromic/hypsochromic shifts in ligand absorption bands leading to a single absorption band at 465 nm. Density Functional Theory was employed to provide a theoretical description of the possible conformational changes within the ligand, with emphasis on the difference between the ligand conformation in its hydrochloride salt and in the polymer. Two models of polymer fragments were constructed to describe the electronic structure and non-covalent interactions. The Quantum Theory of Atoms in Molecules (QTAIM) was applied for this purpose. Using the obtained results, we were able to develop potential energy profiles for various conformations of the ligand. For the set of the studied systems, we detected non-covalent interactions, which are responsible for the spatial conformation. Concerning the models of polymers, electron spin density distribution has been visualized and discussed.

Słowa kluczowe

crystal structure, photoluminescence, magnetic properties, coordination polymer, DFT, QTAIM

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