A rare diiodo-L-tyrosine copper(II) complexes – Crystal and molecular structure of materials stabilized by weak interactions

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Streszczenie

The problem in formation of 3,5-diiodo-L-tyrosinato (L-I_2Tyr) various metal ion complexes as a crystals is generated by the low solubility of iodo-L-tyrosinato derivatives (as ligands) in pure aqueous solution. However, two inorganic–organic hybrid l-I_2Tyr copper(II) complexes *i.e.* [CuCl(L-I_2TyrOH)(phen)]·2H_2O (**1**) and [Cu(l-I_2TyrOH)(H_2O)(phen)](NO_3) (**2**) with l-I_2TyrOH were isolated in acid aqueous/methanol medium. In crystals **1** and **2**, the monomeric distorted square planar pyramidal copper(II) coordination is stabilized by weak intramolecular π···π stacking, copper(II)···π and π···I non-covalent interactions. The connection of adjacent 2D layers into 3D supramolecular network is realised by weak π···π contacts in **1**, while in **2** the 3D architecture is stabilized by weak CH···π interaction as well as π···π contacts. The complexes are also characterized by infrared and Raman spectroscopies (FT-IR, FT-Raman), X- and Q-band electron paramagnetic resonance spectroscopy (EPR), electronic spectroscopy (NIR-Vis-UV), magnetic method, and theoretical calculation.

Słowa kluczowe

Diiodo-L-tyrosine, Copper(II), Weak interactions, Crystal structure, FT-IR, Raman, Q-band EPR, NIR-Vis-UV, Theoretical calculation, Magnetic

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