

Crystal and molecular structure stabilized by weak interaction in unique 3,5-diiodo-L-tyrosinato copper(II) complex : synthesis, experimental and theoretical studies.

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Streszczenie

The ternary Cu(II)/amino-acid/diamine systems have large positive logK values than binary Cu/amino systems, suggesting stabilization due to the effective stacking interaction between aromatic diamine and the aromatic side group of the amino acid. Thus, a hybrid 3,5-diiodo-L-tyrosinato copper(II) complex with an aromatic diamine, of formula $[\text{Cu}(\text{L}-\text{I}_2\text{TyrO}^-)(\text{H}_2\text{O})(\text{phen})]\cdot 2\text{H}_2\text{O}$ (**1**) was characterized in depth by using X-ray, TG/DTG, DSC, FT-IR, Raman, Q-band EPR, NIR-Vis-UV, magnetic methods and the theoretical calculations. The crystal structure is stabilized by weak $\pi\cdots\pi$ stacking, metal $\cdots\pi$ and intra- and intermolecular $\pi\cdots\text{I}$ non-covalent interactions. The computed interaction energies of $\text{Cg}(1)\cdots\text{Cg}(2)$, $\text{Cg}(3)\cdots\text{I}$ and $\text{Cg}(1)\cdots\text{Cu}$ ranging from 0.69 kcal/mol– -2.20 kcal/mol. The weak interactions shift the bands assigned as $\nu(\text{C}-\text{I})$ to higher frequency in the FT-IR spectrum. The g tensor is axial with $g_{\parallel}$ (2.239) > $g_{\perp}$ (2.057) indicating that the unpaired electron resides in the $d_{x^2-y^2}$ orbital. The exchange pathway occurs in the zig-zag chain with $d(\text{Cu}\cdots\text{Cu}) = 9.429 \text{ \AA}$.

Słowa kluczowe

Diiodo-L-tyrosine, Copper(II), Weak interaction,
Spectroscopies (FT-IR, Raman, Q-band EPR, NIR-Vis-UV),
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