1-D Framework L-arginine zinc(II) units bridged by oxalate: synthesis, structure, properties, and theoretical studies.

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Streszczenie

We synthesized a l-arginine containing Zn^{2+} complex and oxalate ions. $\{[Zn_2(l\text{-}Arg)_2(ox)_2]\cdot 8H_2O\}_n$ (**1**) (l-Arg =l-arginine, ox = oxalate) crystallize in the monoclinic space group $P2_1$ with a = 8.979(2), b = 9.840(2) (Å), c = 18.509(3) (Å), β = 95.58(3) (Å), V = 1627.6(6) $Å^3$, and Z = 2. The zinc centers are six-coordinate via one l-arginine zwitterion and two bridging oxalates. The binuclear $[Zn_2(l\text{-}Arg)_2(ox)_2]$ units are linked via oxalate and form 1-D “stair-like” linear chains. The complex was characterized using FT-IR, FT-Raman, UV–vis spectroscopy, and thermal analysis techniques, as well as DFT methods. Electronic bands above 31,000 cm^{-1} originate in $^{1,3}A_u$ ($n\rightarrow\pi^*$) transitions within oxalate ions. Theoretical studies were performed for the model compound $\{[Zn(l\text{-}Arg)(Hox)_2]\cdot 4H_2O\}$ using the fragment of the crystallographic structure of **1**. The interaction energy (ΔE) values for l-arginine and two oxalate ions are comparable at -145 kcal mol^{-1}. Natural bond orbital (NBO) analysis of the electronic structure and bonding is also discussed.

Słowa kluczowe

Zinc(II), l-arginine, crystal structure, density functional calculations, FT-IR spectra, FT-Raman spectra, electronic spectra

Adres publiczny

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