

Documents

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Quantum chemical insight into the molecular structure of L-chemosensor 1,3-dimethyl-5-(thien-2-ylmethylene)-pyrimidine-2,4,6-(1 H,3 H,5 H)-trione: Naked-eye colorimetric detection of copper(II) anions

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Abstract

A sensitive colorimetric L-chemosensor 1,3-dimethyl-5-(thien-2-ylmethylene)-pyrimidine-2,4,6-(1H,3H,5H)-trione was developed by Knoevenagel combination of barbituric acid with thiophene aldehyde chelating moiety. The sensor displayed a high colorimetric Cu(II)X₂ response; a dramatic methanol color change was recorded depending on anion type (X=Br⁻¹, Cl⁻¹, ClO₄⁻¹, NO₃⁻¹, OAc⁻¹, and SO₄⁻²). Off-on-off decolorized halochromism of the L-chemosensor/CuBr₂ was recorded in an acidic medium. The structure of the L-chemosensor was confirmed by single-crystal X-ray diffraction, elemental analysis, and molecular spectroscopic tools such as UV-Vis, Fourier transform infra-red, ¹H, and ¹³C nuclear magnetic resonance (NMR) spectroscopy. The thermal stability of the L-chemosensor was experimentally evaluated by thermogravimetric analysis. The structural optimized parameters of the ligand matched the crystallographic data, and the intermolecular forces were computed by Hirshfeld surface analysis. Electronic absorption in several solvents and ¹H NMR were correlated with the computed spectra in the gaseous state. The HOMO/LUMO, global reactivity descriptor quantum parameters, Mulliken charge population, and molecular electrostatic potential of the L-chemosensor were also computed. © 2018 World Scientific Publishing Company.

Author Keywords

colorimetric; Condensation; L-chemosensor; XRD

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