Novel enaminone derived from thieno [2,3-b] thiene: Synthesis, X-ray crystal structure, HOMO, LUMO, NBO analyses and biological activity

Abstract

Background: Due to their structural and therapeutic diversity, thienothiophene derivatives have attracted much synthetic interest because of their reactivity and biological activity. The thieno [2,3-b] thiophene moiety has been used in the design of a novel pharmaceutical therapies. Additionally, its enaminones derivatives are versatile synthons and have a lot of synthetic applications such as N-heterocycles, wide variety of naturally occurring alkaloids and pharmaceutical drugs. Results: Synthesis of (2E,2'E)-1,1'-(3,4-diphenylthieno [2,3-b] thiophene-2,5-diyl) bis (3-(dimethylamino) prop-2-en-1-one) 5 was reported. The structure of compound 5 was deduced by spectroscopic techniques. The compound was crystallizes in the monoclinic system with space group P-1 with cell coordinates a=9.9685 (8) Å, b=10.1382 (8) Å, c=13.3220 (11) Å, α=101.018 (2) °, ß=94.480 (2) °, γ=107.207 (1) °, V=1249.3 (1) Å3, and Z=2. In the crystal molecules are packed in chains formed via weak intermolecular C21-H21A... O1, C22-H22A...O2 and C27-H27A...O2 hydrogen bondings. Theoretical quantum chemical calculations have been performed on the studied compound using the DFT B3LYP/6-311G (d, p) method. The geometric parameters of the optimized structure are in good agreement with the experimental data obtained from our reported X-ray structure. The two benzene rings and the two side chains are not coplanar with the fused thiophene rings. The electronic spectra of the studied compound have been calculated using the TD-DFT method at the same level of theory. The transition bands at 352.9 nm (f=0.5549) and 332.1 nm (f=0.2190) are due to the H-1→L (72%) and H→L + 1 (82%) excitations respectively. The NBO calculations were performed to predict the natural atomic charges at the different atomic sites and to study the different intramolecular charge transfer (ICT) interactions occurring in the studied system. It is found that the O and N-atoms have the highest negative charge densities while the S-atoms are the most electropositive. These results give idea about how our molecule could react with the receptor active sites. Compound 5 was evaluated against ant-microbial activity. Conclusions: Synthesis, molecular structure and spectroscopic invesitgation of (2E,2'E)-1,1'-(3,4-diphenylthieno [2,3-b] thiophene-2,5-diyl) bis (3- (dimethylamino) prop-2-en-1-one) 5 was studied.