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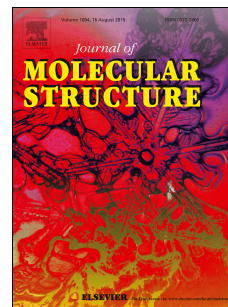
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Synthesis, X-Ray Diffraction, Theoretical and Anti-bacterial studies of Bis-Thiourea Secondary Amine

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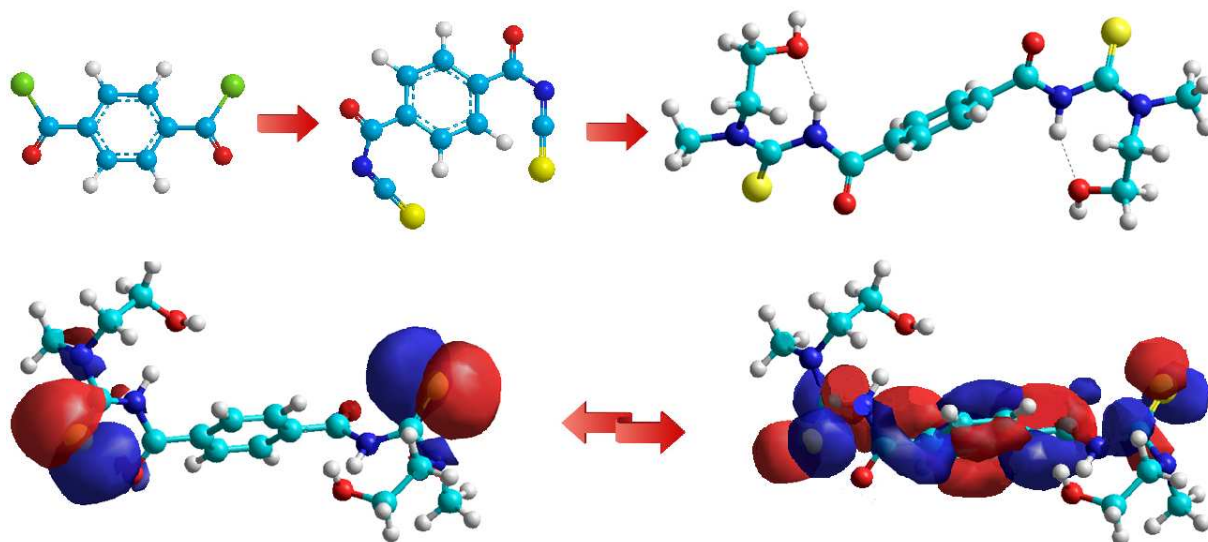
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Abstract: N¹,N⁴-Bis{(2-hydroxyethyl)(methyl)carbamothioyl}terephthalamide (1A) was synthesized by reacting terephthaloyl chloride and ammonium thiocyanate and the product was reacted with 2-Methyl amino ethanol to afford the final product. The product was characterized by Infra Red, Nuclear Magnetic Resonance and Electrospray Ionization mass Spectrometric techniques. The crystal was obtained by recrystallization from DMSO by slow evaporation technique. The X-ray studies reveal that (1A) is crystallized in monoclinic system with space group P 21/n, a = 6.9727(9), b = 17.649(2), c = 8.2629(11), $\alpha = 90$, $\beta = 112.329(4)$, $\gamma = 90$. Z = 2 and V = 940.6(2). In the crystal structure, the molecules are linked by O(1)...H(1)...S(1), and O(1)...H(1)...O(2) intermolecular H-bonds forming a 3-D network. In addition, the antibacterial activities against four different strains of bacteria and theoretical evaluation for the stable geometries for (1A) has been performed using semi-empirical calculations of PM3 method.

Graphical Abstract



Keywords: Bis-thiourea; anti-bacterial; PM3; crystallographic study

1. Introduction

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