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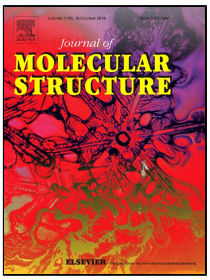

Synthesis, characterization, Thermal and DFT studies of S-methyl-β-N-(3-(2-nitrophenyl)allylidene)dithiocarbazate as anti-bacterial agent

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Synthesis, characterization, Thermal and DFT studies of S-methyl-β-N-(3-(2-nitrophenyl)allylidene)dithiocarbazate as anti-bacterial agent

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ABSTRACT

S-Methyl-β-N-(3-(2-nitrophenyl)allylidene)dithiocarbazate (HL), Schiff base of S-methyl dithiocarbazate, was synthesized by 1:1 condensation between S-methyl dithiocarbazate and trans-o-nitro cinnamaldehyde. It's in-vitro cytotoxicity is assayed against two habitually infection causing bacteria strains including gram-positive *Staphylococcus aureus* and gram-negative *Escherichia coli* for antibacterial activity. The results showed appreciable biological activity and the activity increased with increase in concentration. This nitrogen-sulfur based Schiff base (HL) was characterized by Mass, FT-IR, H^1-NMR, ^{13}C-NMR, Raman, and UV-Vis spectroscopic techniques. Theoretical quantum chemical calculation has been performed using DFT in combination with B3LYP exchange correlation functional and 6-311++ G (d, p) basis sets level. The computed parameters were: Chemical potential of compound (μ) -0.174 eV, HOMO-LUMO energy gap -0.11093 eV, chemical hardness (η) -0.055 eV, softness (S) 2.164 eV, ionization energy(IE) -0.23026 eV, electron affinity(EA) -0.11933eV, the electronegativity (EN) 0.174 eV, dipole moment (D) 1.3383 Debye and relative stabilization energy -1536.982 eV. In the theoretical FT-IR spectrum analysis 81 fundamental vibrational modes has be observed because of non-linear structure of HL, with potential energy distribution percentage (PED%) by using VEDA-4 package. Theoretically calculated parameters like H^1-NMR, ^{13}C-NMR, FT-IR, UV-VIS, Raman, electrostatic potential and HOMO-LUMO energy gap were in conformity with experimental results. Thermal reactivity of the ligand was studied by TGA decomposes completely to give gaseous products.

Key words:

Dithiocarbazate, DFT studies, thermal, chemical potential, antibacterial