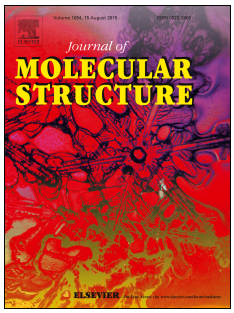
Accepted Manuscript



Synthesis, X-ray diffraction method, spectroscopic characterization (FT-IR, ^{1}H and ^{13}C NMR), antimicrobial activity, Hirshfeld surface analysis and DFT computations of novel sulfonamide derivatives

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PII: S0022-2860(18)30209-6

DOI: 10.1016/j.molstruc.2018.02.063

Reference: MOLSTR 24885

To appear in: *Journal of Molecular Structure*

Received Date: 5 December 2017

Revised Date: 13 February 2018

Accepted Date: 14 February 2018

Please cite this article as: Z. Demircioğlu, F.A. Özdemir, O. Dayan, Z. Şerbetçi, Namı. Özdemir, Synthesis, X-ray diffraction method, spectroscopic characterization (FT-IR, ^{1}H and ^{13}C NMR), antimicrobial activity, Hirshfeld surface analysis and DFT computations of novel sulfonamide derivatives, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.02.063.

Synthesis, X-ray Diffraction Method, Spectroscopic Characterization (FT-IR, ^{1}H- and ^{13}C-NMR), Antimicrobial Activity, Hirshfeld Surface Analysis and DFT Computations of Novel Sulfonamide Derivatives

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Abstract

Synthesized compounds of N-(2-aminophenyl)benzenesulfonamide **1** and (Z)-N-(2-((2-nitrobenzylidene)amino)phenyl)benzenesulfonamide **2** were characterized by antimicrobial activity, FT-IR, ^{1}H- and ^{13}C-NMR. Two new Schiff base ligands containing aromatic sulfonamide fragment of (Z)-N-(2-((3-nitrobenzylidene)amino)phenyl)benzenesulfonamide **3** and (Z)-N-(2-((4-nitrobenzylidene)amino)phenyl)benzenesulfonamide **4** were synthesized and investigated by spectroscopic techniques including ^{1}H- and ^{13}C-NMR, FT-IR, single crystal X-ray diffraction, Hirshfeld surface, theoretical method analyses and by antimicrobial activity. The molecular geometry obtained from the X-ray structure determination was optimized Density Functional Theory (DFT/B3LYP) method with the 6-311++G(d,p) basis set in ground state. From the optimized geometry of the molecules of **3** and **4**, the geometric parameters, vibrational wavenumbers and chemical shifts were computed. The optimized geometry results, which were well represented the X-ray data, were shown that the chosen of DFT/B3LYP 6-311G++(d,p) was a successful choice. After a successful optimization, frontier molecular orbitals, chemical activity, non-linear optical properties (NLO), molecular electrostatic mep (MEP), Mulliken population method, natural population analysis (NPA) and