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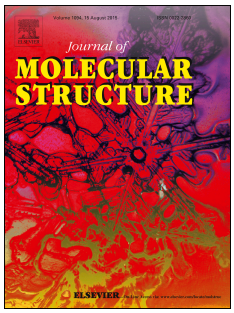

Synthesis, characterization, crystal structure and theoretical studies of 4-[(E)-(3-chloro-4-hydroxyphenyl) diazenyl]-1, 5-dimethyl-2-phenyl-1, 2-dihydro-3H-pyrazol-3-one

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SYNTHESIS, CHARACTERIZATION, CRYSTAL STRUCTURE AND THEORETICAL STUDIES OF 4-[(*E*)-(3-CHLORO-4-HYDROXYPHENYL) DIAZENYL]-1, 5-DIMETHYL-2-PHENYL-1, 2-DIHYDRO-3*H*-PYRAZOL-3-ONE.

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Abstract

Crystals of new heterocyclic azo compound of 4-aminoantipyrine, 4-[(*E*)-(3-chloro-4-hydroxyphenyl)diazenyl]-1,5-dimethyl-2-phenyl-1,2-dihydro-3*H*-pyrazol-3-one have been grown by slow evaporation method at room temperature and its structural characterization was performed by X- ray diffraction method. The spectroscopic characterization was also performed by FT-IR, UV-Vis, ^{13}C and ^{1}H NMR techniques. The compound crystallizes in the monoclinic C_C space group with cell dimensions a = 12.4842(13), b = 16.4492(16), c = 8.3389(8) and β = 102.698(3)^0. The phenyl ring attached to the pyrazolone moiety is disordered over two positions with an occupancy ratio 52:48. The components of the disorder were refined. DFT calculations have been performed by using B3LYP/6-311G(d,p) level basis set. The calculated vibrational frequency showed a red shift for C=O and OH stretching. The natural bond orbital analysis of monomer, dimer and trimer structures reveals the absence of intramolecular hydrogen bonding; however intermolecular hydrogen bonding is observed. The cationic and anionic reactive sites of compound have been visualized on MEP surface.

Keywords: azo dye, XRD study, DFT, MESP, NBO analysis.