Supramolecular Arrangement of a Novel Asymmetric Azine: A C-H⋯H-C interaction?

Jean Marcos Custodio1, Ricardo R. Ternavisk1, Wesley F. Vaz1, Hamilton B. Napolitano1

1State University Of Goias, Anapolis, Brazil
E-mail: jean.custodio@ifgoiano.edu.br

Among the derivatives of hydrazones, the azines have been noted for its wide range of biological activities such as antibacterial and antifungal properties and the possibility of complexation with metals in the antitumor drugs complex due to the biological properties for hydrazones and their derivatives [1]. In addition, various compounds used in the pharmaceutical medium are synthesized from the azines, which act as intermediates in their synthetic route [2]. In this work, the structural study of a novel azine was proposed. Crystal data collection was performed on Bruker APEX II CCD diffractometer. Azine C15H12N3O4(AZN) crystallized in the P21/n monoclinic space group (R1 = 0.0451 and Goof = 1.098) with only one molecule in the asymmetric unit. Figure 1a shows the ORTEP diagram of ellipsoids at 50% probability level with the atomic numbering scheme for title compound. AZN is almost planar by analyzing the angle formed by its aromatic rings of 6.77°. Infinite chains of AZN along [010] with the C²2(12)[R²2(10)] motif are formed via C-H⋯O (d(D⋯A)=3.131Å and 3.400Å) interactions involving the nitro, methoxy and hydroxy groups. A zigzag layer parallel to (100) is formed by the association of these chains throughout C-H⋯O (d(D⋯A)=3.424Å) interaction in a C(6) chain motif (Figure 1b). The crystal packing of AZN is stabilized by one C-H⋯O interaction (d(D⋯A)=3.375Å) in C(6) motif involving the methoxy and hydroxyl groups, besides π⋯stacking interactions confirmed by shape index Hirshfeld surface analysis. Quantum Theory of Atoms in Molecules was performed to analyze the observed C-H⋯H-C interaction (Figure 1c). Additionally, DFT calculations [cam-b3lyp/6-311++g(d,p)] were performed to understanding the nature of hydrogen bonds involved in AZN.


Keywords: azine, structural analysis, theoretical calculations