substitution induced stabilizing effects via more number of inter molecular hydrogen bonds. The strong intramolecular N-H...N bond locks the molecular conformation and eliminates conformational flexibility in all derivatives. The comparative study on detailed structural features, intermolecular interactions and modes of packing will be presented.

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Keywords: organic crystal structures, chemical crystallography, hydrogen bonds

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Crystal and molecular structure of biologically active thiophene 3 -furfuryl carboxamide derivative

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The synthesis and design of the compounds possessing important pharmacological and biological properties is an important area of research. In this respect, Schiff bases and their related thiophene derivatives containing amino and carboxyl functions have been synthesized. They have been found to exhibit broad spectrum of biological activities such as antiviral, antiinflammatory and antimicrobial activities[1]. Specifically, 2-aminothiophene-3-carboxylates and carboxamides were recognized as allosteric enhancers for A1 adenosine receptors[2]. In view of the above and in continuation of our work on structural studies of thiophene 3-carboxamide derivatives [3], crystal structure of "2-{[(1*E*)-(2-chlorophenyl)methylene]amino}-N-(2-furylmethyl)-4,5-dimethylthiophene-3-carboxamide" was determined. The compound $C_{24}H_{25}N_3O_2S$, crystallizes under Orthorhombic system, $P2_12_12_1$ space group, a = 6.1105(19), b = 15.977(5) and c = 18.575(6) Å, V = 1813.5(10) Å^{-3}, Z= 4, & D= 1.366 Mgm^{-3}. The intensity data were collected using Bruker Smart CCD diffractometer using graphite monochromated MoKα radiation. The structure was solved using SIR92 program and refined using fullmatrix least squares on F^2 to an R value of 0.056 using SHELXL-97 for 2842 reflections with I>2 σ(I). In the non-planar molecule, the furan and chlorophenyl ring making dihedral angle of 89.1(2) and 15.8(7)° respectively with the thiophene ring. The crystal structure is stabilized by intramolecular N-H...N, C-H...Cl, C-H...S hydrogen bonds. The intermolecular C-H...O and C-H...π interactions link the molecules in a zigzag manner inside the unit cell.

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Keywords: small molecular crystallography, organic sulfur compounds, hydrogen bonds

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Crystal structure of 2-amino-4,5,6,7-tetrahydro-1-benzothiophene -3-carboxamide

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Thiophene derivates containing amino and carboxyl functions have been found to exhibit broad spectrum of biological activities like anti-viral, anti-inflammatory, antimicrobial activities. Specifically, the 2-amino-carboxylic acid esters were recognized as allosteric enhancers for A1 adenosine receptors. Recent Structure activity relation studies have shown that the amides also exhibit similar properties. Our earlier investigations on the structures of biologically active thiophene 3-carboxamides, has shown that the chloro substitution in the aryl amide group had a significant effect[1]. The ortho -chloro group reversed the orientation of the amide linkage and favoured the formation of more intra molecular hydrogen bonds. The para- chloro substitution induced stabilizing effects via more number of inter molecular hydrogen bonds. The titled compound in the present study bears a close structural relationship with the reported allosteric enhancers for adenosine[2] and hence its structure has been investigated. The compound $C_9H_{12}N_2OS$, crystallizes under Tetragonal system, $I\,4_1/a$ space group, a = b = 20.5807(16) Å and c = 8.9233(13) Å, V = 3779.6(7) Å^3, Z= 16, μ = 0.303 mm^{-1}, & D= 1.38 gm^{-3}.The three dimensional intensity data were collected using Bruker Smart CCD diffractometer using graphite monochromated MoKα radiation. The structure was solved using SIR92 program and refined till R value converges to 0.0576. The crystal structure stabilized by both intra and intermolecular N-H...O hydrogen bonds.

Reference:
(1)Acta Cryst. (2005). E61, o304-o306.
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An experimental and theoretical approach to the 2-chloro-1-(3-methyl-3-phenylcyclobutyl) ethanone

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The title compound, $C_{13}H_{15}ClO$, crystallize in orthorhombic space group $Pca2_1$, and has a nonplanar conformation. The phenyl ring and chloroacetaldehyde group are in cis positions. The cyclobutane ring is puckered, with a dihedral angle of 26.81 (13)º. Molecules are linked to one another by intermolecular C−H···O interactions, forming a C(4) chain running parallel to the [001] direction [1]. The molecular structure of the title compound in the ground state (in vacuo) is optimized by HF and DFT(B3LYP) with the 6-31G(d) basis set and then compared with that of experimentally obtained.