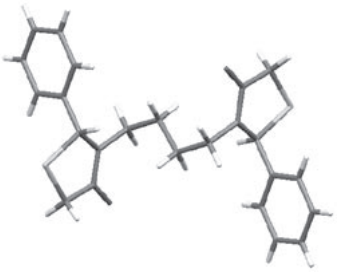
inflammatory, antihistaminic and analgesic activities. Moreover, recently, it was found that some bis-(2-aryl-4-oxothiazolidin-3-yl)ethanes act as good cyclooxygenase-2 inhibitory agents. The crystallographic characterization of the bis-heterocycle 1,4-bis-(2-phenyl-4-oxo-1,3-thiazolidin-3-yl)butane belonging to a family of compounds synthesized through a one pot three component condensation methodology, with acetonitrile as solvent are reported herein. This compound crystallizes in a monoclinic cell with the cell parameters *a*=5.7452A(11), *b*=27.065A(5) *c*=7.1157A(14) and β=105.53º(3), Space group $P2_1/c$ [No 14], *V* = 1066.05A3 and *Z*= 2.



Keywords: single-crystal, thiazolidinone, structural characterization

P06.09.42

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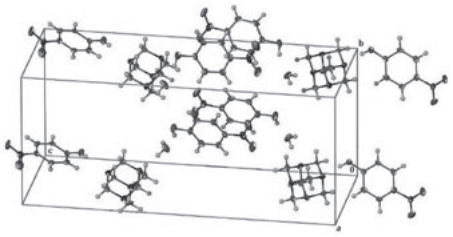
Hexamethylenetetramine bis(*p*-nitrophenol) monohydrate clathrate

Seik Weng Ng
University of Malaya, Department of Chemistry, Lembah Pantai, Kuala Lumpur, Kuala Lumpur, 50603, Malaysia, E-mail：seikweng@um.edu.my

Hexamethylenetetramine bis(p-nitrophenol) monohydrate, $(CH_2)_6N_4.2HO\text{-}C_6H_4\text{-}NO_2.H2O$, crystallizes as four independent formula units in the *P*1 space group [*a* 6.9325(1), *b* 11.6867(2), *c* 25.0826(5) Å; β 96.728(1), β 92.449(1), β 89.971(1)°]. The eight p-nitrophenol and four water molecules each function as a hydrogen-bond donor to two acceptor (nitrogen and oxygen) sites. Only two of the four nitrogen sites of each hexamine molecule are involved in hydrogen bonding. The hydrogen bonds connect the component molecules into a linear chain. Diffraction measurements were made at -173 ℃ . A previous room-temperature study has found a monoclinic *C*2 polymorph [*a* 49.989(4), *b* 5.901(1), *c* 7.056(1) Å; β 92.423(1)°]. The *p*-nitrophenol molecule is disordered about a two-fold axis; the p-nitrophenol, hexamine and water molecules are also linked by hydrogen bonds into a linear chain (Ng et al. (2001). J. Mol. Struct. 595, 189-194].



Keywords: clathrate, polymorph, *P*1 space group

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Structure of the anhydrous form of gossypol - Dianhydrogossypol

Azimjon Mamadrakhimov[1], Samat A.. Talipov[1],
Zavkibek G. Tiljakov[1], Michael K. Dowd[2], Bakhtiyar T. Ibragimov[1]
[1]Institute of Bioorganic Chemistry of Academy Sciences of Uzbekistan, Mirzo Ulugbek Str., 83, Tashkent, Mirzo Ulugbek district, 100143, Uzbekistan, [2]Southern Regional Research Center, ARS, USDA, 1100 Robert E. Lee Blvd., New Orleans, LA 70124, USA, E-mail：kimyogar@yahoo.com

Gossypol, $C_{30}H_{30}O_8$, is yellow pigment containing in glands of various species of cotton plants. By chemical modification of gossypol a great number of gossypol derivatives - its ethers, Schiff's bases, etc. - have been obtained. Dianhydrogossypol which is formed by dehydratation of gossypol is of a special interest for our studies. The crystals of dianhydrogossypol were obtained from saturated solution in dichloromethane. Data collection has been carried out on a Gemini R X-ray diffractometer equipped with an Oxford Cryosystems open-flow cryostat at 100 K. The crystallographic parameters are: *a*=33.8265(4), *b*=33.8265(4), *c*=9.1497(2)Å, *V*=4677Å3, Sp.gr.- $I4_1/a$. The results of the X-Ray studies show that molecular structure confirms anticipated one. The crystal structure has wide channels in the direction of c-axis and resembles the channel structure found earlier in one of gossypol polymorphs (zeolite-like structure). The packing factor of these crystals is very low and equal to 0.59. The volume of empty space of the an elementary cell is equal to 1641 Å3 or 15,7 % of the total volume. The dianhydrogossypol demonstrates good inclusion ability for molecules of many small volatile compounds which requires further detailed investigations in relation to potential new organic zeolite.
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Keywords: X-ray structural crystallography, inclusion compounds, zeolites

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A study on the effect of substitutions and intermolecular interactions in thiophene 3-carboxamides

M. K. Kokila[1], Dr. Puttaraja[1], G.N. Anil Kumar[2],
K. Chandra Kumar[3], S. Mohan[4], J. Saravanan[4], Manohar V. Kulkarni[5]
[1]Bangalore University, Physics, Department of Physics, Jnanabharathi campus, Bangalore, Karnataka, 560056, India, [2]Department of Physics, M.S. Ramaiah Institute of Technology, MSRIT Post, Bangalore, Karnataka, 560054, India., [3]Department of Engineering Physics, HKBK College of Engineering, Nagawara, Arabic College Post, Bangalore, Karnataka, 560045, India, [4]PES College of Pharmacy, Hanumanthanagar, Bangalore, Karnataka, 560050, India., [5]Department of Chemistry, Karnatak University, Dharwad, Karnataka, 580020, India, E-mail：prmkkgroup@gmail.com

The study of interactions involving halogens, particularly fluorine is a major interest in crystal engineering[1]. Conventional hydrogen bonding is the significant interaction in many crystal structures but a number of weak interactions have been also shown to play a role in stabilization of crystal structure. In view of these, as a part of our research on structural studies on biologically active molecules, we have reported intermolecular interactions in florinated compounds and some substituted thiophene 3-carboxamide derivatives[2]. These compounds were found to exhibit broad spectrum of biological activities such as antibacterial, antifungal and anti-inflammatory activities[3]. Our present research work describes the crystal structure and conformational studies of 2-amino thiophene 3-carboxamides and Schiff bases of thiophenes[4], which serve as starting material for a number of intermediate derivatives. It is noticed from the comparative study that the chloro substitution in the aryl amide group had a significant effect on crystal packing. 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 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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3. Mohan, S. et al, (2003). Asian J. Chem. 15, 67-70.
4. Anilkumar G.N. et al, Acta Cryst. (2007). E63, o2077-o2079.

Keywords: organic crystal structures, chemical crystallography, hydrogen bonds

P06.10.45

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

G. N. Anil Kumar[1], M. K. Kokila[2], Dr. Puttaraja[2], S. Mohan[3], J. Saravanan[3]
[1]M S Ramaiah Institute of Technology, Physics, Department of Physics, M S Ramaiah Institute of Technology, MSRIT Post, MSR Nagar, Bangalore, Karnataka, 560054, India, [2]Department of Physics,Bangalore University, Jnanabharathi campus, Bangalore, Karnataka, 560056, India, [3]PES College of Pharmacy, Hanumanthanagar, Bangalore, Karnataka 560050 India, E-mail：anilkumargn@gmail.com

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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2. George N. et al. / Bioorg. Med. Chem. 14 (2006) 2358-2365.
3. G. N. Anilkumar, et al, Acta Cryst. (2007). E63, o2077-o2079.

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

P06.10.47

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

K. Chandra Kumar[1], M.K. Kokila[2], Dr. Puttaraja[2], S. Mohan[3], J. Saravanan[3], Manohar V. Kulkarni[4]
[1]HKBK College of Engineering, Physics, Nagawara Arabic college Post, Bangalore, Karnataka, 560045, India, [2]Bangalore University,Department of physics, Jnanabharathi, Bangalore, Karnataka, 560056, India., [3]P.E.S. College of Pharmacy, Hanumanthanagar, Bangalore, Karnataka, 560050, India., [4]Department of Chemistry, Karnatak University,Dharwad 580 003, Karnataka, India., E-mail：prmkkgroup@gmail.com

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.
(2 George N. et al. / Bioorg. Med. Chem. 14 (2006) 2358-2365.

Keywords: hydrogen bonds, chemical crystallography, organic compounds

P06.10.48

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An experimental and theoretical approach to the 2-chloro-1-(3-methyl-3-phenylcyclobutyl) ethanone

Muharrem Dincer[1], Namik Ozdemir[2], Ibrahim Yilmaz[3]
[1]Ondokuz Mayis University, Physics, Arts and Sciences Faculty, SAMSUN, Kurupelit, 55139, Turkey, [2]Ondokuz Mayis University, Arts and Sciences Faculty, SAMSUN, Kurupelit, 55139, Turkey, [3]Firat University,Arts and Sciences Faculty, ELAZIG, 23119,Turkey., E-mail：mdincer@omu.edu.tr

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.