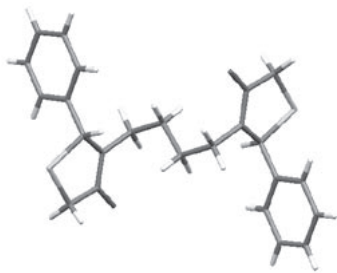


inflammatory, antihistaminic and analgesic activities. Moreover, recently, it was found that some bis-(2-aryl-4-oxothiazolidin-3-yl)ethanes act as good cyclooxygenase-2 inhibitory agents. The crystallographic characterization of the bis-heterocycle 1,4-bis-(2-phenyl-4-oxo-1,3-thiazolidin-3-yl)butane 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  $a=5.7452\text{\AA}(11)$ ,  $b=27.065\text{\AA}(5)$   $c=7.1157\text{\AA}(14)$  and  $\beta=105.53^\circ(3)$ , Space group  $P2_1/c$  [No 14],  $V = 1066.05\text{\AA}^3$  and  $Z=2$ .



Keywords: single-crystal, thiazolidinone, structural characterization

### P06.09.42

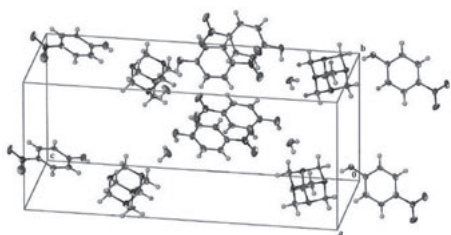
*Acta Cryst.* (2008). A64, C395

#### 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,  $(\text{CH}_2)_6\text{N}_4 \cdot 2\text{HO}-\text{C}_6\text{H}_4-\text{NO}_2 \cdot \text{H}_2\text{O}$ , crystallizes as four independent formula units in the  $P1$  space group [ $a$  6.9325(1),  $b$  11.6867(2),  $c$  25.0826(5) Å;  $\beta$  96.728(1),  $\beta$  92.449(1),  $\beta$  89.971(1) $^\circ$ ]. 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  $-173^\circ\text{C}$ . A previous room-temperature study has found a monoclinic  $C2$  polymorph [ $a$  49.989(4),  $b$  5.901(1),  $c$  7.056(1) Å;  $\beta$  92.423(1) $^\circ$ ]. 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,  $P1$  space group

### P06.09.43

*Acta Cryst.* (2008). A64, C395

#### Structure of the anhydrous form of gossypol - Dianhydrogossypol

Azimjon Mamadrakhimov<sup>1</sup>, Samat A. Talipov<sup>1</sup>,  
Zavkibek G. Tiljakov<sup>1</sup>, Michael K. Dowd<sup>2</sup>, Bakhtiyar T. Ibragimov<sup>1</sup>

<sup>1</sup>Institute of Bioorganic Chemistry of Academy Sciences of Uzbekistan, Mirzo Ulugbek Str., 83, Tashkent, Mirzo Ulugbek district, 100143,

Uzbekistan, <sup>2</sup>Southern Regional Research Center, ARS, USDA, 1100 Robert E. Lee Blvd., New Orleans, LA 70124, USA, E-mail: kimyogar@yahoo.com

Gossypol,  $\text{C}_{30}\text{H}_{30}\text{O}_8$ , 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 dehydration 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:  $a=33.8265(4)$ ,  $b=33.8265(4)$ ,  $c=9.1497(2)\text{\AA}$ ,  $V=4677\text{\AA}^3$ , 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 Å<sup>3</sup> 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.

Acknowledgements. This work was supported by STCU/ARS USDA grant - P181

Keywords: X-ray structural crystallography, inclusion compounds, zeolites

### P06.10.44

*Acta Cryst.* (2008). A64, C395-396

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

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

The study of interactions involving halogens, particularly fluorine is a major interest in crystal engineering<sup>1</sup>. 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 fluorinated compounds and some substituted thiophene 3-carboxamide derivatives<sup>2</sup>. These compounds were found to exhibit broad spectrum of biological activities such as antibacterial, antifungal and anti-inflammatory activities<sup>3</sup>. Our present research work describes the crystal structure and conformational studies of 2-amino thiophene 3-carboxamides and Schiff bases of thiophenes<sup>4</sup>, 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