antiaggregating drug reveals that phase relationships should be investigated. Knowing the solid state properties of ticlopidine hydrochloride polymorphs would avoid unexpected bioavailability resulted from solubility and stability changes. Since ticlopidine hydrochloride is not well studied in terms of solid state structures and properties, this study means an advance in its characterization and understanding of conformational features and crystal packing patterns.
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Keywords: polymorphism, drug, pharmaceutical

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Diversity of gossypol clathrates with pyrazine

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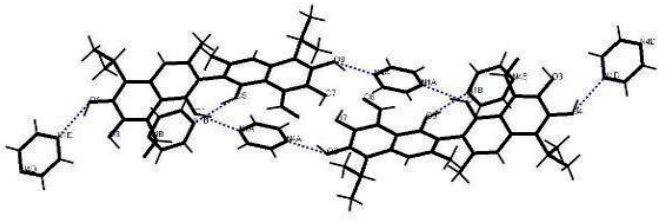
Gossypol, a yellow polyphenolic pigment of the cotton plant, has a wide range of biological action and is a surprisingly versatile host compound [1]. Single crystals of gossypol complex with pyrazine (1:4) have been obtained in the pyrazine solution of gossypol (t=56°C) and characterized by following crystallographic data: $C_{30}H_{30}O_8 \cdot 4(C_4H_4N_2)$, M=838.91, T=130 (2)K, MoK_a=0.71073Å, a=7.5230(3), b=13.9185(6), c=19.8328(8) Å, α=88.789(4), β=87.255(3), γ=86.683(4)°, V=2070.46(15) Å^3, Z=2, $D_{calc.}$=1.346 g/cm^3, crystal system triclinic, space group P-1. Pair of gossypol and pyrazine molecules are formed centrosymmetric tetramers untypical for gossypol type structures. Crystal structure is characterized with the presence of wide channels for guest molecules. Other gossypol inclusion complexes with pyrazine have been obtained from guest-free gossypol polymorphs P2, P3 and P4 by sorption of pyrazine vapors at room temperature and 50°C. When pyrazine vapors are absorbed at 50°C all three polymorphs of gossypol turn to one crystal form – a new clathrate of gossypol with pyrazine (1:4). Thus, when pyrazine vapors are absorbed at low temperatures, probably, formation of the new clathrate is limited on matrixes of corresponding polymorphs while at higher temperatures the crystal structure of polymorphs has a more tendency to form a clathrate.



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Keywords: clathrate, polymorphism, thermoanalysis

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Formation of gossypol clathrates by vapor sorption

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Gossypol obtained from cotton seeds has valuable biological properties [1]. It is known that gossypol is a versatile host compound forming clathrates with any small molecule substances. The other specific feature of this compound is unusual polymorphism of gossypol's guest-free crystals [2]. We present here the results of gossypol clathrates decomposition and vapor sorption by its polymorphic apohosts. The clathrates considered are obtained with following five solvents - acetic acid (**I**), acetone (**II**), 1,4-dioxane(**III**), chloroform (**IV**) and benzene (**V**). Depending on the crystal structure guest molecules of studied clathrates are freed at different temperatures. TG-DSC curves show that H-clatrates are more stabile comparatively to that of gossypol clatrates. For the studied clatrates the stability decreases in the following order: **I→II→ IV → V → III**.

Gossypol polymorphs P2, P3 and P4 are obtained by desolvatation of clathrates. We have studied the formation of clathrates by gossypol polymorphs in result of vapor sorption. For this purpose vapors of easily sublimating naphthalene and benzoquinone are used. Sorption was performed at room temperature and at 50ºC. In both cases the sorption of naphthalene vapors by appropriate polymorphs shows some increasing in masses of initial polymorphs. On example of 3 polymorphs the mass increasing at room temperature was insignificant and inconsiderable on XRD-pattern but at 50ºC the essential sorption of naphthalene by all of 3 polymorphs has been observed. The formation of new phase was not observed by exposure of benzoquinone vapors on 3 gossypol polymorphs at temperatures given above.

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Keywords: clathrate, polymorphism, sorption

MS53.P12

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The crystal structures of gossypol reaction products with 4-aminoantipyrine

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Gossypol is a yellow pigment of cottonseed possessing antiviral, antitumor, anticancer, antifertile, immunosuppressive and other types of biological activity [1]. A chemical modification of its structure in many cases leads to low toxic derivatives. For this purpose the gossypol derivatives with 4-aminoantipyrine were obtained. Symmetrical bis-derivative of gossypol with 4-aminoantipyrine is named ragosin (**A**) and unsymmetrical mono-derivative – monoragosin (**B**). In this report the crystal structures of (**A**)/pyridine(**I**) (1:5) and (**A**)/(**B**)/ethylacetate (**II**) (1:2:5) will be discussed. Crystal data (**I**): triclinic, P-1, a=15.2331(10)Å, b=15.4459(10)Å, c=16.2360(15)Å, α=111.902(7)°, β=101.386(7)°, γ=91.788(5)°, V=3451.5(5)Å^3, Z=2, $D_{cal.}$=1.236 g/cm^3; (**II**): monoclinic, C2/c, a=20.5152(5)Å, b=25.6725(7)Å, c=30.9163(7)Å, β=92.558(2)°, V=16266.7(7) Å^3, Z=2, $D_{cal.}$=1.258 g/cm^3.

In the structure of (**I**), two ragosin molecules form dimers via the pair of centro symmetrical H-bonds O4-H…O3 (2.764 Å). Other three hydroxyl groups of ragosin molecule are involved in the formation of H-