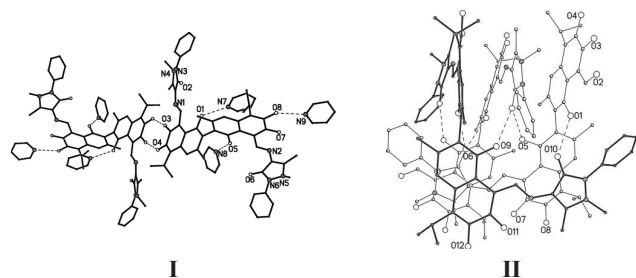


bonds with pyridine molecules (O1-H...N (2.755 Å), O5-H...N(2.740 Å), O8-H...N(2.782 Å)). So, two ragosin and six pyridine molecules form associate. The other 2 guest molecules do not have H-bonding with A molecule and their position is stabilized only by Van-der-Waals and  $\pi$ - $\pi$  (stacking) interactions.

The crystal structure of (II) is characterized by the presence of associates, consisting of two B molecules and one A molecule, formed by H-bonds of three types: with H-bonds O1-H...O10 and O9-H...O6 cross-linked molecule (B) with two molecules (A). In turn, two molecules of (A) are self associated by hydrogen bonds of the O5-H...O6. It should also be noted that the molecule of A, and associate in general has a symmetry axis of the second order.



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**Keywords:** clathrate, supramolecular assembly, hydrogen bonding

### MS53.P13

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#### Planarity and activity of aroyldithiocarbazoates

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The increasing resistance of *Mycobacterium tuberculosis* to existing agents and the resulting spread of the pathogen, in both developed and developing countries, makes the search for new tuberculostatics an important issue.

The studied compounds were obtained by Foks and coworkers from Department of Organic Chemistry, Medical University of Gdansk as derivatives of aroyldithiocarbazonic acids (Scheme), showing tuberculostatic activity [1,2]. It was suggested that general planarity of the molecules could be prerequisite for activity [3] in this chemical class.

	Compound	R <sup>1</sup>	R <sup>2</sup>	R <sup>3</sup>
	1	H		Me
	2	H		Bz
	3	Me		Me
	4	H	Me	Me
	5	H	Me	n-Bu

The planarity of molecules 1 and 2 is maintained by conjugations and intramolecular hydrogen contacts N-H...X(O,S). In structures 3, 4 and 5 substitution of hydrogen at any N atom by a methyl group unables formation of those attractive interactions through N-H...O. As a result, the molecules 3, 4 and 5 are not planar. In their crystals,

molecules 1, 4 and 5 form infinite chains C(4). Surprisingly, molecules 2 do not form any intermolecular hydrogen bonds (despite possessing unsubstituted amide group). Compound 1 showed the highest inhibition of *Mycobacterium tuberculosis* bacteria.

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**Keywords:** tuberculostatics, planarity-activity relationship, aroyldithiocarbazoates

### MS53.P14

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#### Polymorphism and co-crystal formation in the “glycine-carboxylic acid” systems

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SPolymorphism and co-crystal formation belong to “hot topics” in reactivity of organic solids. They are important for practical applications, in particular in pharmaceutical industry, because properties of different polymorphs differ, and the properties of co-crystals may also differ from those of a mixture of components.

Polymorphism is often related to the difference in hydrogen bond networks in the crystals. Crystallization of a desirable polymorph is known to be affected by pH. At the same time, pH is modified by adding acids, which can also act as co-crystal and/or salt co-formers. The aim of the present study was to compare the effect of a series of carboxylic acids on crystallization of glycine in a wide range of relative glycine : carboxylic acid concentrations. Crystallization from solutions was compared with the results of mechanochemical synthesis (co-grinding). The crystal structures of co-crystals were analyzed, with a special attention paid to the transfer of protons between amino acids and carboxylic acids in the solid state in relation to relative pKa values in solution. Examples of “true” co-crystals with no proton transfer between an amino acid and a carboxylic acid are given.

Depending on the carboxylic acid and relative glycine : carboxylic acid ratio the following results were obtained:

1. Recrystallization of glycine from alpha- to gamma- polymorph (at low concentration of most acids used), both in solution and in solid mixtures;
2. Formation of co-crystals and salts for some carboxylic acids (when the acid was added in a stoichiometric 1:1 ratio);
3. Crystallization of the two components in the mixture separately.

The results of the experiments are discussed in relation to the molecular structures of carboxylic acids, their pKa in solution, as well as relative solubility of glycine and a carboxylic acid in water.

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**Keywords:** crystallization, co-grinding, hydrogen bonds