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Dicarboxylic acids, HOOC–(CH2)_n–COOH, are interesting compounds from the structural point of view [1]. A very long one-dimensional chain can be obtained through hydrogen bond formation at both ends of the molecule. These compounds configure layered structures in the solid state, as well as most of the polymorphic phases of long-chain compounds, such as *n*-alkanes, *n*-alcohols, and *n*-fatty acids. Dicarboxylic acids exhibit interesting thermal properties and a high enthalpy of melting that make them potential candidates for their use in the field of thermal protection and energy storage.

Dimorphism was prevalent in odd carbon members of dicarboxylic acids while one form is only present for even members: α form P2₁/c with Z=4 and β form C2/c with Z=4. High-quality x-ray powder diffraction analyses of pentadecanedioic acid (C₁₅H₂₈O₄) have been carried as a function of temperature. A new form, called γ has been observed just before melting: γ form C2/c with Z=4 at 383K.

The packing arrangement of the carboxyl groups at both end of the chain is different in the three forms. From the structural point of view for γ form the distance interlayer is intermediate between α and β distances. Crystal structure of the pentadecanedioic acid is presented.

The carboxyl's group in α form shows two different angles with middle plain of the chain. The packing arrangement of α and γ forms are radically different even if the molecular conformation are *cis* in both cases.

A reversible transition from β form to γ form was observed before melting. Slurry experiments indicate that β is the most stable form at room temperature.

[1]V.R.Thalladi, M. Nüsse and R. Boese, J. Am. Chem. Soc., 122, 9227-9236 (2000).

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FA4-MS35-P08

Polymorphism as an Obstacle for the Applicability of Methoxy-substituted Distyrylpyrazines. <u>Alain</u>

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Distyrylpyrazines (DSPs) are a promising class of organic semiconductors because of their superior electronic properties, such as a highly efficient emission of light and a high electron affinity [1]. Since the supramolecular structure is of great importance when rationalizing and tuning these interesting properties for the materials' use in devices such as organic LEDs, five methoxy-substituted distyrylpyrazines were synthesized and their solid-state structures were investigated; (E,E)-2,5-bis[2-(4-methoxyphenyl)ethenyl]pyrazine has already been subjected to a synchrotron study by Scaccianoce *et al.* [2]. For (E,E)-2,5-bis[2-(3,4-dimethoxyphenyl)ethenyl]pyrazine, (E,E)-2,5-bis[2-(2,4,6-methoxyphenyl)ethenyl]pyrazine and (E,E)-2,5-bis[2-(2,4,6-methoxyphenyl)ethenyl]

azine suitable crystals were grown and their supramolecular structures were analyzed. The methoxy groups are responsible for the majority of the interactions that determine the crystal packing – mostly through mutual weak hydrogen bonds and CH... π interactions – although the pyrazine moiety also acts as an acceptor of weak hydrogen bonds and is involved in π ... π interactions. The structures are compared mutually as well as to their distyrylbenzene counterparts. For each of the two former compounds, two polymorphs have been found. One polymorph of (*E*,*E*)-2,5-bis[2-(3,4,5-methoxyphenyl)-ethenyl]pyrazine proved to be light sensitive and turned out to be a good candidate for a solid-state polymerization reaction.

[1] Grimsdale A.C., Cervini R., Friend R.H., Holmes A.B., Kim S.T., Moratti S.C., *Synth. Met.*, 1997, 85, 1257. [2] Scaccianoce L., Feeder N., Teat S.J., Marseglia E.A., Grimsdale A.C., Holmes A.B., *Acta Cryst.*, 2000, C56, 1277.

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FA4-MS35-P09

Conformational flexibility of chlorpropamide molecule can generate new polymorph. <u>T.N.</u> <u>Drebushchak</u>^{a,b}, V.A. Drebushchak ^{a,c}, E.V. Boldyreva^{a,b}, ^a Novosibirsk State University, Russia, ^bInstitute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia ^cInstitute of Geology and Mineralogy SB RAS, Novosibirsk, Russia E-mail: tanya@xray.nsu.ru

Polimorphism of drugs is of utmost importance both for pharmaceutical industry and medicine. Various molecules behave in polymorphs in different ways. For example, polymorphs of sulphathiazole differ in the framework of hydrogen bonds between molecules with similar conformations [1]. In chlorpropamide polymorphs, on the contrary, the hydrogen bonds are very similar, but the molecules have different conformations [2, 3]. There is a correlation between conformation of of chlorpropamide molecule in a polymorph and its density.

We found a new phase transition of the high-temperature ε chlorpropamide (metastable under normal conditions) into a new polymorph on cooling [4]. The transition is reversible. Structure of the new polymorph was solved from the singlecrystal X-ray diffraction data. Space group symmetry of the polymorphs is the same, but the conformation of the molecule changes, resulting in the step-wise change in the density of chlorpropamide. Surprisingly, X-ray powder diffraction pattern of the new polymorph turned out to be nearly identical to that of stable α -chlorpropamide in the range of small angles.

Comparing the structures of chlorpropamide polymorphs, we came to the conclusion that the new polymorph is a transient point in the irreversible transition $\varepsilon \rightarrow \alpha$. The state is frozen because at low temperatures molecules cannot change their conformation completely, so that every second molecular ribbon would be inverted, to give the α -form. Only the alkyl tails of the molecules turn at about 180°, but the molecular packing of the initial ε -form is preserved. Probably, this is an example of a new general mechanism, when the freezing of one or several degrees of freedom in conformational