Chlorpropamide, 4-chloro-N-((propylaminocarbonyl)-benzenesulfonamide, is an antidiabetic drug. Although the existence of several polymorphs of this compound was reported, by 2006, the crystal structure was solved only for one of them [1]. In 2006, we have initiated a systematic study of the crystallization of chlorpropamide from different solvents and from the same solvent under different conditions. Up to now, five polymorphs were obtained as single crystals, and for three of them crystal structures were solved [2-4]. The structures can serve as a very beautiful example of the polymorphism in a system with similar intermolecular hydrogen-bonds pattern, but different packing of molecules in different conformations. Different structures result in the pronounced differences in density (up to 5 %), IR-spectra, melting temperatures (several °C) and melting enthalpy (up to 15 %).

This work was supported by a 05-03-32468 grant from RFBR, the grants from BRHE (RUX0-008-NO-06, Y3-C-08-01), a grant from the Russian Ministry of Education and Science (2.2.2.3.2007) and #49 and #110 Integration Projects of SB RAS.

[1] Koo, C.H., Cho, S.I. & Yeon, Y.H. *Arch. Pharmacol. Res*. 1980, 3, 37-49.
[2] Drebushchak, T.N., Chukanov, N.V. & Boldyreva, E.V. *Acta Cryst.* 2006, E 62, o4393-o4395.
[3] Chukanov, N.V., Drebushchak, T.N., Drebushchak, V.A., Chesalov, Yu.A., Boldyreva, E.V. (2007) Crystal Growth & Design, in the press.
[4] Drebushchak, T.N., Chukanov, N.V. & Boldyreva, E.V. *Acta Cryst. C*. 2007, in the press.

MS20 P05

2-Nitro-3,4,4-trichloro-1-mono(ethylthio)-1-mono[1-(diphenylmethyl)-piperazine]-1,3-butadiene Compound

N.Gulsah Deniz[a], Cemil Ibis,[a] [a]*Department of Chemistry, Istanbul University.Istanbul,Turkey*
E-mail: yurdakul@istanbul.edu.tr

Keywords: crystal structure of organic compounds, organic sulfur compounds, chemical crystallography

It is known that monoaryl- and diarylpiperazines are important for clinical chemistry [1]. Some piperazine compounds were used in gen transfer reactions[2]. The piperidinyl derivatives show an excellent biological activity and chemical effects and according to the an US-patent, some thiosubstituted dienes exhibit high biological activity also [3].
2-Nitro-3,4,4-trichloro-1-mono(ethylthio)-1-mono[1-(diphenylmethyl)-piperazine]-1,3-butadiene was synthesized and crystal structure was determined. The compound crystallizes in the Orthorhombic crystal system (space group $P2_12_12_1$) with the unit cell parameters a=9.4240(2) Å, b=14.4007(2) Å, c=18.1891(2) Å, $\alpha\beta$, $\gamma=90^o$, V=2468.48(7) $Å^3$, Z=4. The structure has been solved by direct methods (SIR92) [4] and refined to the residul index R_1= 0.078.

[1] Solodin, I. and T. D. Heath, *Synlett.,* 1996, 7, 619.
[2] Diamond Alkali Company (Ert. H. Bluestone), U.S. Pat 3021370 (13 Feb. 1962); Chem. Abstr., 57,3293c (1962).
[3] Ceccletti, V.; Fravolini, A. *J.Med.Chem.*,1996, 39, 4952.
[4] Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., Camalli, M., SIR92, *J.Appl.Cryst,*, 1994, 27, 435.

MS20 P06

Structural proof for synergetic behaviour in organogels: Stearicacid/Octadecanol

Daniel Kalnin[a], Kees van Malssen[b], Henny Schaink[a], Erik van der Linden[a], Food Physics Laboratory, Wageningen University, P.O. Box 8129, 6700 EV Wageningen, The Netherlands. [b]Foods Structural Design, UFHRI, Unilever R&D, Vlaardingen, The Netherlands;
E-mail: daniel.kalnin@web.de

Keywords: lipid polymorphism, lipid crystallization, polymorphic structures

The structural properties of oils and fats are of interest for different sectors of the technological and scientific community. The mineral oil industry is interested in methods preventing gelation of (crude) oil in pipe lines [1, 2]. On the other hand novel materials based on structured oil matrices are desired as well in food technology [3-5] for structured products as in pharmaceutical technology for controlled release properties [6] or in material science for tuning hardness of materials.
Here we present the structural properties of organogels made from mixtures of stearic acid (Ac) and 1-octadecanol (Ol) in vegetable oil and a rheological evaluation of the resulting texture. Oscillating strain measurements are performed as a function of the temperature on the ternary system Ac/Ol/liquid vegetable oil. The total mass concentration of Ac/Ol was kept constant at 5 wt% in the ternary systems. Rheology experiments reveal a strong increase of the elastic modulus at temperatures under 30^oC. It is shown that the 1 to 2 mixture of Ac/Ol has an elastic modulus that is significantly larger than that of the other ternary samples. Using microscopy it is found that the shape of the crystals in the samples depends strongly on the composition of the mixture. The cause of the observed behavior of the elastic modulus lies in the crystal morphology due to the molecular structure of the self assembled lipid crystals. X-ray diffraction at small and wide angles revealed that at a 2/1 ratio a compound crystal is formed. The resulting crystal form is vey likely to the β modification of the StStSt. However no esterification could be noticed. The understanding of this synergetic effect in a very narrow concentration range of 1-octadecanol, and stearic acid in the organogels provides the possibility to tune the hardness of the lipid matrix.

[1] Visintin R.F.G., Lapasin R., Vignati E., Dántona P., Lockhart T.P. Langmuir, 2005, 21, 6240.
[2] Stachowiak C., Viguié J.-R., Grolier J.-P. E., Rogalski M. Langmuir 2005, 21, 4824.
[3] Ojijo N.K.O., Kesselman E., Shuster V., Eichler S., Eger S., Neeman I., Shimoni E. Food. Res. Int. 2004, 37, 385.
[4] Ojijo N.K.O., Neeman I., Eger S., Shimoni E. J. Sci. Food Agric., 2004, 84, 1585.
[5] Gandolfo F.G., Bot A., Flöter E. J Am. Oil Chem. Soc., 2004, 81,1.
[6] Realdon N., Regazzi. E. Drug development and Industrial Pharmacy, 2001, 27(2), 165.