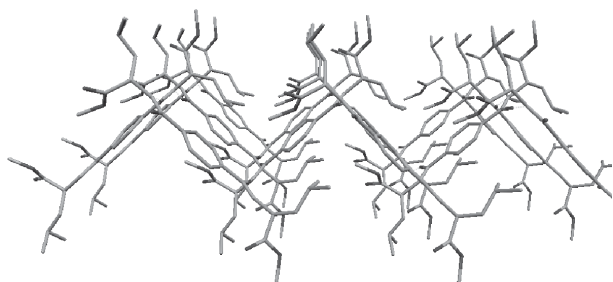


s13.m42.p19 **Hydrogen Bonding Organization in Crystal Structures of (S,S)-N,N'-phthaloyl-bis(amino acid) Derivatives.** Zoran Stefanic, Milan Jokic, Janja Makarevic, Mladen Zinic, Biserka Kojic-Prodic, Rudjer Boskovic Institute, POB 180, 10002 Zagreb, Croatia. E-mail: zoran.stefanic@irb.hr

Keywords: Hydrogen bonding; Aggregation; Gels

Understanding the role of hydrogen bonding and its overall topology in the formation of supramolecular assemblies is of great importance, both, in the theoretical and practical aspects. The organization of organic molecules into nano- or micro-dimensional assemblies can lead to design of new materials of versatile applications. Predicting the gelation on the basis of the constitutional and conformational characteristics of an organic molecule and the properties of liquid to be gelled is a challenge. Recently we have shown that chiral bis(amino acid) oxalamides represent a rare group of gelators capable to gel water and various lipophilic organic solvents, [1] whereas our new results are related to chiral bis(leucinol)oxalamides exhibiting gelating properties. [2] In continuation of this work the gelation properties of the series of (S,S)-N,N'-phthaloyl-bis(amino acid methyl ester) (ten compounds) and their free acids in connection to their hydrogen bonding pattern have been studied. To influence topology of hydrogen bond network the phthaloyl spacer with ortho-, meta- and para-substitutions was used. Modifications at the terminal side of the molecule by esterification reduce the number of donor sites. The derivative with ortho-substitution in the crystal packing develops one-dimensional hydrogen bond network. However, terephthaloyl derivatives organize in two-dimensional zigzag-networks.



A bulky terephthaloyl spacer forces molecules to be oriented in perpendicular fashion. In such an arrangement CH... π interactions are favoured. Due to the strong donor-acceptor abilities of carboxyl groups of amino-acids they exhibit much more intricate hydrogen bonded networks in the crystal structure.

- [1] Makarevic *et al.*, *Chem. Eur. J.* 2001, **7**, 3328.
 [2] Makarevic *et al.*, *Chem. Eur. J.* 2003, **9**, 5567.

s13.m42.p20 **Structural Changes in Crystals During Inter- and Intramolecular Photochemical Reactions.** Elzbieta Trzop and Ilona Turowska-Tyrk, Wroclaw University of Technology, Department of Chemistry, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw, Poland. E-mail: e.trzop@ch.pwr.wroc.pl

Keywords: Monitoring studies; Photoreactions in crystals; X-ray structure analysis

In the eighties and the nineties the crystallographic studies of the photochemical reaction course in crystals dealt with: (1) monitoring cell constants changes or (2) monitoring movements of an atom group inside a molecule. A couple of years ago we paid our attention to the step-by-step studies of movements of whole molecules in crystals during the photochemical reactions. Such movements and crystal structure changes accompanying them were monitored among others for the [4+4] photodimerization of 9-methlanthracene [1]. The unit cell volume in crystals of this compound increased slightly at the beginning of the photoreaction and afterwards gradually decreased. A very interesting phenomenon was observed for the adjacent reactant molecules. With the photoreaction progress the molecules smoothly come closer towards each other. The product molecules also change their position. We have carried out the studies on monitoring structural changes in crystals, and movements of whole molecules in particular, in the case of intramolecular photoreactions. The results will be also presented.

- [1] I. Turowska-Tyrk, E. Trzop, *Acta Cryst.*, **B56**, 779-786, 2003.