

s13.m42.o3 **Effect of hydrophilic-hydrophobic ratio in organic molecules on the crystal packing.** Gubaidullin Aidar, *Institute of Organic and Physical Chemistry of Russian Academy of Science, Kazan, Arbuzov str. 8, 420088, Russia. E-mail: aidar@iopc.knc.ru*

**Keywords: Crystal packing; Supramolecular structure; Amphiphilic properties**

The principles, describing formation of crystalline structures, are based on a various approaches which are taking into account such factors as intermolecular hydrogen bondings, weak interactions, steric factors, peculiarities of molecular structure. Recently it was found that the role of some factors was overestimated. However correlation and interdependence of these factors remain by the object of a research till now. As a result of our comparative analysis of molecular and supramolecular structure of extensive series of a new organic and elementoorganic compounds of different nature, we offer an additional principle of formation of crystalline packing based on manifestation amphiphilic properties of molecules. The hydrophobic and hydrophilic regions are found to be strongly localised in the crystals of compounds. This localization leads to various types of supramolecular structures, these types being connected with the symmetry of crystals formed. Calculations of the hydrophilicity degree of molecular fragments and their correlation with the type of packing of molecules in crystal show, that the thermodynamic incompatibility of pseudo-phases, exhibited in localization of hydrophilic and hydrophobic areas, results in the origination of supercrystalline structures at a subatomic level in crystals. In the considered compounds the superstructures spanning all possible types of superstructures - completely hydrophilic structure, packing of hydrophilic cylinders and spherical areas in hydrophobic matrix, lamellar type with alternation hydrophilic and hydrophobic layers and inverse structures down to completely hydrophobic structure, - are observed. The type of superstructure depends on the hydrophilic-hydrophobic volume ratio, calculated for molecular fragments. The analogy between superstructures, formed due to manifestation of amphiphilic properties of molecules in crystals, and superlattices in the block-copolymer systems is drawn. It was established, that the similar separation of areas is observed in crystals of different organic compounds irrespective of their nature. Thus, the theory, developed for the description of microphase separation in polymeric heterogeneous systems, can be used for analysis not only packing of molecules of organic compounds in crystal, but also for a prediction of type of molecular packing. The analysis of the distribution of formed structures in the compounds under investigation and similar compounds, being available in Cambridge crystallographic database, is carried out and the correlation between a type of formed structures and symmetry of crystals is analysed. The possibility of analysis of polymorphic, enantiopure and racemic structures in the framework of the offered model is shown.

**Acknowledgment.** This work is supported by Russian Foundation for Basic Research (Grant No. 02-03-32280).

s13.m42.o4 **Intermolecular interactions in Au(I) and Au(III) complexes.** Catharine Esterhuysen<sup>a</sup>, Stephanie Cronje<sup>a</sup>, Helgard G. Raubenheimer<sup>a</sup> and Gert J Kruger<sup>b</sup>, <sup>a</sup>*Department of Chemistry, University of Stellenbosch, Private Bag XI, Matieland 7602, Stellenbosch, South Africa, and* <sup>b</sup>*Department of Chemistry and Biochemistry, Rand Afrikaans University, PO Box 524, Auckland Park 2006, Johannesburg, South Africa. E-mail: ce@sun.ac.za*

**Keywords: Intermolecular interactions; Auophilic interactions; Au(I) and Au(III) complexes**

Au(I) complexes are well-known for forming auophilic interactions, which are inter- or intramolecular Au...Au interactions with Au...Au distances shorter than 3.6Å [1]. Interactions between Au(III) atoms in neighbouring molecules are however much weaker, if they exist at all, with Au...Au distances often considerably longer than the sum of the van der Waals radii. Au(III)...Au(III) interactions thus very rarely play as important a role in directing packing as that observed for their Au(I) counterparts. Nevertheless packing in crystals of Au(III) complexes can be directed by other weak intermolecular interactions such as Au...halide, Au...S and even Au... $\pi$  interactions. In this work the crystal structures of a series of Au(I) and Au(III) compounds illustrating these interactions are presented. A Cambridge Structural Database [2] analysis of similar structures is also included, which shows that although often much rarer than the auophilic Au...Au interactions these interactions nevertheless play a role in packing that could lead to their use in crystal engineering methodologies.

- [1] S. S. Pathaneni, G. R. Desiraju *J. Chem. Soc., Dalton Trans.*, 319-322, 1993.  
 [2] F. H. Allen, *Acta Crystallogr.*, **B58**, 380-388, 2002.