PS16.10.02 SOLVATES. CRYSTAL STRUCTURES, STATISTICS, EFFICIENCY OF CRYSTALLIZATION AND INTERACTIONS WITH DISSOLVED SUBSTANCES. Marek L. Glowka and Krystyna Kozlowska, Institute of General and Ecological Chemistry, Technical University of Lodz, ul. Zwirki 36, 90-924 Lodz, Poland

A good crystal is "to be or not to be" for an X-ray crystallographer. Getting a crystal from a friend (chemist, physicist or biologist) happens but usually we have to try hard ourselves to crystallize the "priceless" substance. As crystallization is still more art than science, it is very important to know not only solubilities of the compound but also scores of different solvents in question. Also interesting is the role of the solvent in formation of a crystal and frequency of solvate formation. The last problem is particularly important in case of active agents because solvent presence in the crystal may be dangerous for patients or makes the crystals unstable.

Is it possible to answer these important questions?

First we have looked at our crystallographic treasury, Cambridge Crystallographic Database. However, the Base is of limited help in this case, because:

-there is no information on crystallization trials from other solvents than the successful ones,

-there is no information on crystallization conditions at all (which is even worse),

-as solvates crystals often show disorder, they are frequently unpublished (crystallographic statistics is deformed),

-some groups of compounds are far more populated than others. We have also browsed through the crystallographic literature.

However laborious and tough, the task gave many practical information and surprising results, which will be presented.

PS16.10.03 THE ROLE OF MOBILE PHASES IN CRYSTALLIZATION OF POLYMERS: SIZE DEPENDANCE IN PHASE TRANSFORMATION. S. Rastogi, Centre for Polymers and Composites, Eindhoven University of Technology Den Dolech 2; P.O. Box 513 5600MB Eindhoven; Nederland

Solid phases may exist in a wide variety of forms such as polymorphs, solvates, liquid crystals and ampholytes. For a given set of experimental conditions such as temperature, pressure and composition only one solid phase will be consistent with a minimum free energy of the system. This will then be the most stable solid phase available and all other phases will be metastable with respect to this phase. However, the fact that these solids are metastable does not preclude their existence for long time periods. An extreme example of this is diamond which is metastable with respect to graphite at room temperature and pressure.

The appearance of polymorphs from a supersaturated and/or supercooled mother phase is, however, not only determined by the drive to minimise the free energy but also by the need for the system to do this by the kinetic route with the lowest activation energy. It is the balance between two processes-thermodynamic and kinetic that forms the basis of this colloquium. The importance of kinetics was recognised by Ostwald and is summarised in his 'Law of Stages' which simply states that when a system moves from an unstable to a stable state it does so by transformations to intermediate metastable states. Some of these effects will be demonstrated in polymers like polyethylene, trans-1,4 polybutadiene and poly di alkyl siloxanes.

PS16.10.04 THE DEVELOPMENT OF THE *IN SITU* OBSERVATION OF CRYSTAL GROWTH: THE RELATIONSHIP BETWEEN LINEAR AND MASS GROWTH RATES. L.V.Yashina, V.I.Dernovsky, V.P.Zlomanov, Moscow State University

This report is devoted to *in situ* control of crystal growth rate and habit in the case of $A(IV)B(VI)$ compounds grown from the vapor. Among different *in situ* methods the observation of linear crystal size is most attractive. It can be much more accurate then mass measurement, especially for small crystals. It is easy to control by computing. As a result of such measurement the kinetic curve $l(t)$ would be obtained. The statistical treatment of this curve can be in form $l=a+bt^c$, where c is the order of kinetic curve, a connected with error in the growth beginning moment, b expresss the growth rate. The order c is sensitive for limiting stage. If crystal shape is changed during experiment the determination of the limiting stage by order c can be incorrect.

To obtain the total information from the *in situ* experiment it is need to calculate the linear parameter to crystal mass. That is to calculate habit constants $q=Vd/l^3$, $q = S/l^2$, where V - crystal volume, d - density, S - crystal surface aria. We describe the total majority of polyhedral habits for *PbTe* and *GeTe* crystals. For *PbTe* habit is realized as parts of cube (12 types), the cross section coinciding with quartz surface. For *GeTe* crystal habit is realized as truncated cubooctahedron and rombohedron. If habit constants are known it is possible to evaluate condensation and diffusion coefficients from kinetic curve by equation. In our experiments with *PbTe* and *GeTe* the good agreement between parameters obtained from both integral measurements and kinetic curves take place. The deviation of final experimental habit constants from calculated connected with the instability of crystal shape. So detail analysis of kinetic curves $l(t)$ is attractive instrument for crystal growth study.

These results can be useful for small size (1-2 mm) crystals preparation.