

importance in understanding the polymorphic behaviour of APIs and so employs polymorph screening techniques in an attempt to sample a variety of different crystallization conditions. The large diversity of crystallization conditions provides the pharmaceutical industry with the confidence that all possible polymorphs of an API have been isolated. High-pressure techniques can provide a complementary method for exploring polymorphism and solvate formation in molecular solids. They are particularly useful for the identification and characterization of new forms that do not appear through standard crystallisation techniques such as those employed in conventional polymorph screens performed under ambient conditions. High-pressure methodologies are well-suited for obtaining so-called “disappearing” or elusive polymorphs in a reproducible manner. This presentation will highlight a number of different examples of polymorphism exhibited by pharmaceutical materials when subjected to high pressures.

Keywords: high-pressure crystallography, pharmaceuticals, polymorphism

## P20.05.28

*Acta Cryst.* (2008). A64, C614

### Kinetics and mechanisms of pressure-induced phase transitions of ternary model biomembrane systems

Christoph G. Jeworrek, Roland Winter

Dortmund University of Technology, Physical Chemistry I - Biophysical Chemistry, christoph.jeworrek@uni-dortmund.de, Dortmund, NRW, 44221, Germany, E-mail: christoph.jeworrek@uni-dortmund.de

Lipid bilayers, which provide valuable model systems for biomembranes, display a variety of polymorphic phases, depending on their molecular structure and environmental conditions, such as pH, ionic strength, temperature and pressure. By using calorimetric, spectroscopic and diffraction techniques, the temperature and pressure dependent structure and phase behavior of one- and two-component lipid systems, differing in chain configuration and headgroup structure, have been studied in recent years [1-3]. Very little is known about the phase behavior of the biologically more relevant heterogeneous three-component lipid systems, in particular about their kinetic and non-equilibrium behavior. We present data on structural and kinetic aspects of lamellar-to-lamellar lipid bilayer phase transitions of a three-component lipid mixture DOPC:DPPC:cholesterol, which serves as a canonical model raft mixture taking into account the heterogeneity of natural membranes. Applying static synchrotron small-angle x-ray scattering measurements and the pressure-jump relaxation technique in combination with time-resolved measurements (TRSAXS), the various temperature and pressure dependent phases and the kinetics of the lipid phase transformations have been investigated over a temperature range from 10 to 80 °C at pressures from ambient up to 3 kbar (300 MPa). Transitions in both the forward and reverse directions have been measured. The results are discussed in the light of possible kinetic mechanisms and are compared with the results of other lipid mesophase transitions.

[1] R. Winter and R. Köhling, *J. Phys.: Condens. Matter* 16 (2004) 327-352

[2] R. Winter and W. Dzwolak, *Phil. Trans. R. Soc. A* 363 (2005) 537-563

[3] I. Daniel, P. Oger, and R. Winter, *Chem. Soc. Rev.* 35 (2006) 858-875

Keywords: lipid phase transitions, TRSAXS, pressure perturbation

## P20.09.29

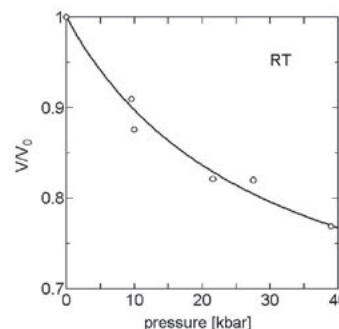
*Acta Cryst.* (2008). A64, C614

### Equation of state for the low-pressure crystalline phase of tin tetraiodide

Takahiro Sakagami<sup>1</sup>, Arata Miyauchi<sup>1</sup>, Takaki Hase<sup>2</sup>, Kazuhiro Fuchizaki<sup>1</sup>

<sup>1</sup>Ehime University, Department of Physics, Bunkyo-cho 2-5, Matsuyama, Ehime, 790-8577, Japan, <sup>2</sup>Altekna, nisi-ku usizima-cho 6-1, nagoya, aichi, 451-6004, Japan, E-mail: sakagami@cmt.phys.sci.ehime-u.ac.jp

A series of experimental studies on determination of the melting curve of the low-pressure crystalline phase (CP-I) of a molecular crystal tin tetraiodide and its polyamorphism (presented in this congress) has been performed since 2001 onward, utilizing the beam line BL14B1 of SPring-8 in Japan. A multi-anvil press consisted of 6 tungsten carbide anvils with a center flat of 10mm or 6mm was employed to cover a pressure range up to about 6GPa. In situ energy-dispersive synchrotron x-ray diffraction measurements were carried out (refer to Fuchizaki et al., 2004, for details as to the experimental setup). During this period of research sufficient diffraction data for the CP-I structure have been accumulated to construct the equation of state (EOS). In fact, the compression data obtained at room temperature were fitted to corrected second-order Murnaghan's EOS (Fuchizaki, 2006) as depicted in the figure. The bulk modulus and its pressure derivative at ambient conditions turned out to be 7.31GPa and 3.91, respectively. Contribution from the thermal pressure to the EOS will be discussed, together with the results obtained through molecular dynamics simulations.



Keywords: equations of state, high pressure, molecular crystals

## P20.09.30

*Acta Cryst.* (2008). A64, C614-615

### Molecular dynamics simulation study on liquid tin tetraiodide

Takaki Hase<sup>1</sup>, Kazuhiro Fuchizaki<sup>2</sup>

<sup>1</sup>Altekna, nisi-ku usizima-cho 6-1, nagoya, aichi, 451-6004, Japan, <sup>2</sup>Ehime University, Bunkyo-cho 2-5, Ehime, 790-8577, Japan, E-mail: takakihase@gmail.com

Recently, a pressure-induced liquid-to-liquid phase transition has been found in tin tetraiodide (Fuchizaki, presented in this congress). The polyamorphism in this substance, including two solid amorphous states found previously, can be understood in a unified way based on the pseudo-binary regular solution model. The high-pressure amorphous state, which forms beyond ~15GPa on compression at room temperature, was shown to be attained by molecular dissociation, whereas the low-pressure amorphous state consists of randomly oriented molecules. In this context, the high-pressure liquid phase may be attained by polymerization of molecules from the low-pressure molecular liquid state. In order to understand the mechanism of the transition, molecular dynamics simulations were carried out. The molecule was regarded as a rigid tetrahedron. The intermolecular interaction was modeled by van der Waals interactions between