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Time resolved studies of lyotropic phase transitions using the pressure jump technique

Oscar Ces[1], Nicholas J Brooks[1], John M Seddon[1], Roland Winter[2], Charlotte Conn[3], Dora Tang[1], Richard H Templer[1]
[1]Imperial College, Department of Chemistry, Exhibition Road, London, London, SW7 2AY, UK, [2]Department of Chemistry, Physical Chemistry I, University of Dortmund, Otto-Hahn-Str. 6, D-44227 Dortmund, Germany, [3]CSIRO Molecular and Health Technologies, Ian Wark Laboratory, Bayview Ave, Clayton VIC 3169, Australia, E-mail：o.ces@imperial.ac.uk

Lyotropic liquid crystals of one-, two- or three-dimensional periodicity spontaneously assemble when biological amphiphiles are mixed with a solvent under various conditions of temperature, pressure and hydration. Mesophases formed by lipids include the fluid lamellar, inverse hexagonal and inverse bicontinuous cubic phases. Biologically, the fluid lamellar phase is ubiquitous, being the structure upon which cell membranes are based. The inverse bicontinuous cubic phases which consist of bilayers draped over the primitive (P), double diamond (D) and gyroid (G) periodic minimal surfaces are now also known to occur in-vivo. Although, a significant amount of work has been done to characterize the equilibrium behaviour of all these phases, kinetic and mechanistic studies of lyotropic phase transitions have been largely confined to transformations between lamellar structures and between lamellar to inverse hexagonal phases. This is surprising as the inverse bicontinuous cubic phases perform important biological functions and the mechanism of their formation from the lamellar phase has much in common with the mechanism of membrane fusion and fission during membrane trafficking. In order to further our understanding of their role in biological systems and to continue to exploit their biotechnological potential, a fundamental understanding of the kinetics and mechanisms involved in lamellar to inverse bicontinuous cubic transitions is a key area of study. To address this knowledge vacuum we have used the pressure jump technique to investigate phase transitions involving bicontinuous cubic phases and this has allowed us to gain valuable new insights into the mechanism of lamellar to inverse bicontinuous cubic phase transitions.

Keywords: high pressure, lipid polymorphism, phase transitions

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High-pressure macromolecular crystallography:Status, applications and prospects

Roger Fourme[1], Eric Girard[2], Richard Kahn[2], Anne-Claire Dhaussy[3], Isabella Ascone[1], Thierry Prange[4], Nathalie Colloc'h[5], Mohamed Mezouar[6]
[1]Synchrotron-Soleil, BP48 Saint Aubin, Gif sur Yvette, France, 91192, France, [2]IBS, 41 rue Jules Horowitz, 38027 Grenoble, France, [3]CRISMAT Ensicaen, 6 bd Marechal Juin, 14704 Caen, France, [4]UMR 8015 CNRS-Univ. Paris 5, 4 av. Observatoire, 75006 Paris, France, [5]CI-NAPS (CNRS), bd Becquerel, 14704 Caen, France, [6]ESRF, BP220, 38027 Grenoble, France, E-mail：roger.fourme@synchrotron-soleil.fr

High-pressure (HP) molecular biophysics is a developing field. Pressure is a mild and efficient method to explore the whole spectrum of conformers of proteins and other biomolecules, from the native folded state to unfolded states. On the basis of differences in partial specific volume, higher-energy conformers can be selectively promoted by pressure. A better understanding of fundamental mechanisms responsible for the effects of HP on biomolecules requires high-resolution information. Since a few years, such information became accessible with the implementation of pressure perturbation in both NMR and macromolecular crystallography (MX). We shall describe recent instrumental advances of HPMX on the ID27 beamline at the European Synchrotron Radiation Facility using x-rays of ultra-short wavelength and new large-aperture diamond-anvil cells. Resolution, completeness and quality of data collected at HP reach usual standards, in spite of crystals at room temperature. HPMX is now a full-fledged technique applicable to a variety of biomolecules in the pressure range from ambient up to 2-2.5 GPa (the limit in each case is not technical but depends on the system under study). This versatility will be illustrated by a survey of selected applications, including nucleic acid components, monomeric and oligomeric proteins, and a large assembly. HPMX has also impacts on conventional MX such as gas-binding, improving molecular and crystalline order, and data- collection methodology. HPMX will be implemented on PSICHE, a multipurpose HP beamline which is currently under construction at the French synchrotron radiation facility SOLEIL. Overall, the prospects of HPMX and short-wavelength MX are bright and arguably would justify the construction of dedicated high-energy beamlines.

Keywords: high pressure, macromolecular crystallography, synchrotron radiation

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Temperature and pressure effects on the re-orientational dynamics of amino acids

Heloisa N. Bordallo[1], Elena V. Boldyreva[2,3], Boris Kolesov[4], Sven Landsgesell[1], Alexandra Buchsteiner[1], Fanni Juranyi[5], Marek M. Koza[6], Thierry Straessle[5]
[1]Hahn-Meitner-Institut Berlin, SF6, GLIENICKER STRASSE 100, Berlin, Berlin, 14109, Germany, [2]REC-008 Novosibirsk State University, ul. Pirogova 2, Novosibirsk 630090, Russia, [3]Institute of Solid State Chemistry and Mechanochemistry, ul. Kutateladze, 18, Novosibirsk 630128 , Russia, [4]Institute of Inorganic Chemistry SB RAS, pr. Lavrenteva, 3, Novosibirsk 630090, Russia, [5]Laboratory for Neutron Scattering, Paul Scherrer Institut, Villigen, 5232, Switzerland, [6]Institut Laue-Langevin, BP 156, Grenoble Cedex 9, 38042, France, E-mail：bordallo@hmi.de

Since Bridgman's pioneering work, showing that a pressure of 7 kbar is able to denature proteins of egg in a similar but not identical way as temperature, pressure effects have been puzzling to biochemists. In order to comprehend complex systems such as proteins, it is especially important to follow in details the motions of the same functional groups in the simpler biomimetics; crystalline amino acids. Additionally, subtle volume changes that arise from changes in packing density due to the decrease in intermolecular distances in the H-bond network can be magnified by pressure. It should be noted, that alterations in the spatial distribution of charges will play a part in the electrostatic interactions resulting in specific evolution of the structural conformation. Neutrons with a 1 Å wavelength and energy close to 1 kcal/mol are a valuable technique to characterize thermal molecular motions and conformational changes in hydrogen bond systems. In particular information on the mean-square displacement in a given time-scale can be obtained by elastic scattering and on vibrational modes by inelastic scattering. The mean-square displacements obtained by such approach are dominated by hydrogen motions due to its large incoherent cross-section value. In this work results of elastic and inelastic neutron scattering experiments on crystalline glycine polymorphs and L- and DL-serine as a function