Biological Role of Water under Extreme Conditions

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There is a huge interest in the properties of water under extreme conditions of temperature, pressure and environment. This interest ranges from the water vapour jets that apparently emanate from the surface of Europa and Encedalus, fuelling speculation for the existence of vast liquid oceans beneath the icy exterior of these moons of Jupiter and Saturn. Somewhat closer to Earth, ice is found in the polar regions of Mars, and there is growing evidence for flows of salty water during the Martian summer the salt allowing the water to stay liquid at the sub-zero temperatures that are found there. Equally, water at the bottom of our own Earth's oceans, is under pressures of up to ~1000 atmospheres, is mostly cold, being at or below 4°C, but can also be very hot near undersea vents, and is briny, so presenting severe challenges to life. Yet many living organisms have adapted to thrive under these conditions. Whereas pure water and ice, both crystalline and amorphous, under pressure and over a range of temperatures, have been explored extensively using neutron scattering techniques, much less is known about the combined effects of salt content, confinement, pressure and temperature. The fact that water in living organisms is often in a highly confined and salty environment may be no coincidence. Perhaps it is the highly disruptive nature of these environments on water structure that is the primary reason why life occurs in the first place!

This project will be based in Leeds and will exploit neutron total and small angle scattering techniques at the ISIS Facility and will include the development of new sample environment equipment for neutron diffraction techniques to make the study of solutions as a function of pressure, temperature and concentration a routine tool for ISIS users. This will be achieved by means of a flow cell technology to allow sample composition to be modified without the time wasting process of removing the pressure cell from the neutron beam for each new composition studied, so allowing in situ sample changes. The student will make use of a computational modelling technique called Empirical Potential Structural Refinement (EPSR) which provides an ensemble of microscopic conformations compatible with the experimental data and provides access to pair-wise atomic interactions between all atoms in the system of interest. The student will also be trained in the preparation and characterisation of biomolecular solutions, making use of the extensive research facilities within the interdisciplinary Astbury Centre for Structural and Molecular Biology at Leeds. The project is highly interdisciplinary and innovative in nature.