

# TBAB semi-clathrates studied by Quasi Elastic Neutron Scattering (QENS) using Emu, the high resolution backscattering spectrometer at ANSTO

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Potential applications for gas hydrates include gas purification, water desalination, and CO<sub>2</sub> capture that is possibly combined with methane extraction. All of these rely on the high selectivity of the guest gas molecules in hydrates. It has been shown, that the addition of TBAB (i.e. Tetra-n-butyl ammonium bromide) softens the thermodynamic conditions of gas hydrate formation without compromising the CO<sub>2</sub> selectivity, a substantial benefit in reducing the carbon output from existing fossil-fuel power plants.

The hydrate structure formed using TBAB is known as a semi-clathrate which differs from the more common clathrate structures that are formed from pure water and gas. For common clathrate structures (sI, sII, or sH) only the gas molecules are entrapped in the cavities of the water structure. Semi-clathrates generally crystallize into two structure types known as type A and B. The Br-anion of TBAB participates to the water molecule framework, while the tetra n-butyl cation is located at the center of 4 large cages. Additional smaller cavities are available for the enclathration of gas molecules. It has been shown recently that these cavities are distorted by the inclusion of guest molecules like CO<sub>2</sub> (Muromachi et al., 2014).

We present here our first quasi-elastic neutron scattering (QENS) results for TBAB semi-clathrates formed with type A and B using the EMU backscattering spectrometer at ANSTO. This technique is well suited to studying the libration of the butyl chains confined within the host cages, and how the slow dynamics changes with the enclathration of CO<sub>2</sub> molecules. Neutron diffraction was applied on the same samples in order to confirm their crystallographic structure.

QENS measurements are highly sensitive to hydrogen (H) atoms while being very insensitive to the deuterated (D) atoms. As well, the method is also insensitive to the dynamics of CO<sub>2</sub> molecules. We use these characteristics to suppress scattering from the water framework by making it from D<sub>2</sub>O rather than H<sub>2</sub>O. As a result, only the dynamics of the n-butyl chains are observed. Early results suggest the interaction of the CO<sub>2</sub> molecules with the mobile butyl chains is key to the improved selectivity of TBAB semi-clathrates.

## References:

S. Muromachi, K.A. Udachin, K. Shin, S. Alavi, I.L. Moudrakovski, R. Ohmura, J.A. Ripmeester, Guest-induced symmetry lowering of an ionic clathrate material for carbon capture, Chem. Commun. 50 (2014) 11476–11479

## Level of Expertise

Experienced Research

## Speakers Gender

Female

Do you wish to take part in the poster slam

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