Experimental report

12/10/2015

Proposal: 7-05-423 **Council:** 4/2014

Title: Diffusion of methane and carbon dioxide in ZIF-8

Research area: Chemistry

This proposal is a new proposal

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Samples: carbon dioxide: CO2
ZIF-8: Zn(2-methylimidazole)2
methane: CH4

Instrument	Requested days	Allocated days	From	To
IN6	6	6	24/09/2014	30/09/2014

Abstract:

Some hybrid porous solids are non rigid. This is the case for ZIF-8 (ZIF stands for zeolitic imidazolate framework). While the crystallographic pore size was calculated to be of 3.4 Å, larger molecules have been found to enter the pore structure, indicating that the linkers are flexible. Computed diffusivities of molecules with a size close to the window size are very sensitive to the force field. Studying the diffusion of methane and carbon dioxide in ZIF-8 will allow us to test the various force fields available in the literature.

Diffusion of CH_4 in ZIF-8 Studied by Quasi-Elastic Neutron Scattering

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J. Phys. Chem. 119 (2015) 16115-16120.

Abstract

Quasi-elastic neutron scattering (QENS) measurements have been performed to characterize at the molecular level the diffusion of CH_4 adsorbed at various concentrations in ZIF-8. This allows to compare for the first time diffusivities obtained in a MOF by microscopic and mesoscopic techniques. The good agreement which is observed between the different methods shows that there are no defects obstructing diffusion, which is often the case in zeolites. Even if the effective size of ZIF-8 windows is larger than the diameter derived from crystallography, the characteristic time for intercage diffusion (~ ns) is much longer than the time between jumps within a cage (~ 10 ps) indicating that the organic linkers severely hinder molecule passage.