Experimental report

22/03/2016

Proposal: 7-05-435 **Council:** 10/2014

Title: Diffusion of gases and mixtures inthe new MIL-140 materials

Research area: Chemistry

This proposal is a new proposal

Main proposer: Herve JOBIC

Experimental team: Herve JOBIC

Local contacts: Michael Marek KOZA

Samples: MIL-140-A : [ZrO(O2C-C6H4-CO2]
Gases: N2, CO2, CH4 and H2

Instrument	Requested days	Allocated days	From	To
IN6	8	6	24/04/2015	30/04/2015

Abstract:

A series of very stable Metal Organic Frameworks (MOFs), denoted as MIL-140, has been recently prepared. The 1D pore size of MIL-140-A is of 3.2 Å and could thus be used to separate CO2 from other gases in natural gas purification or CO2 capture from flue gas. Functionalised MIL-140-A, obtained after grafting Br and CH3 on the organic linker, have even smaller pore sizes and have therfore the potential to separate H2 and CO2. These separations require full understanding of the diffusion of the different gases and mixtures in the microporous frameworks. This can be obtained by a combination of QENS and molecular simulations.

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Abstract

The diffusivity of H_2 and CO_2 in the small pore Zr-based MOF, MIL-140A(Zr) has been evaluated using a combination of Quasi-Elastic Neutron Scattering measurements and molecular dynamics simulations. These two techniques were used to measure the self-diffusivities of H_2, and the corrected and transport diffusivities of CO_2, as single components and binary mixture. H_2 was shown to be the faster of the two gases to diffuse through the narrow triangular channel of MIL-140A(Zr), its self-diffusvity value being one order of magnitude higher than *that* of CO_2, at the same temperature. In this case, although no specific interaction sites are present, the CO_2 interacts more strongly with the pore wall than H_2, partly a consequence of its greater kinetic radius, which renders it slower than H_2. In the context of a binary mixture, H_2 still diffuses faster between the two, although with a slightly lower self-diffusivity, whilst that of CO_2 increases sligthly. However, the difference in terms of order of magnitude is not altered and makes MIL-140A(Zr) a potential candidate for H_2/CO_2 separation based on kinetics.