Experimental report

22/03/2016

Proposal: **TEST-2362** **Council:** 4/2014

Title: MIL-47 + neopentane

Research area:

This proposal is a new proposal

Main proposer: **Herve JOBIC**

Experimental team: Herve JOBIC

Local contacts: Jacques OLLIVIER

Samples: VO(O2C-C4D4-CO2)
C(CH3)4

Instrument	Requested days	Allocated days	From	To
IN5	3	3	23/07/2014	26/07/2014

Abstract:

Observation of single-file diffusion in a MOF

Hervé Jobic

PCCP (2016) **DOI:** 10.1039/C6CP00410E

From themed collection Neutron Scattering in Catalysis and Energy Materials

Abstract: The translational and rotational dynamics of neopentane adsorbed in the one-dimensional channels of MIL-47(V) has been studied by quasi-elastic neutron scattering. The rotational motion of neopentane is well-described by the rotational diffusion model, with a correlation time of 41 ps at 300 K. The translational motion of the molecule has been fitted by several models: isotropic diffusion, normal 1D and single-file diffusion. It is found that the observed line shapes can only be reproduced by the singlefile diffusion model. The single-file mobility factor, F, is $(8 \pm 1) \times 10^{-14}$ m^2 $s^{-1/2}$ at 300 K. This is the first observation of this unusual diffusion behaviour in a MOF.