Experimental Report

Proposal: **TEST-2275** **Council:** 10/2012

Title: Molecular diffusion in metal-organic frameworks

This proposal is a new proposal

Researh Area:

Main proposer: **JOBIC HERVE**

Experimental Team: JOBIC HERVE
RIVES Sebastien
KOLOKOLOV Daniil

Local Contact: OLLIVIER Jacques

Samples: MIL-53: Cr(OD)(O2C-C4D4-CO2) +C6D6
UiO-66: Zr6O4(CO2)12(C6D3)CO2D + C6H14

Instrument	Req. Days	All. Days	From	To
IN5	2	2	15/07/2013	17/07/2013

Abstract:

The diffusion of benzene in MIL-53(Cr) was studied at different temperatures on IN5. Some typical spectra are shown in Figure 1. The QENS results are now compared with ^{2}H NMR and molecular simulations.

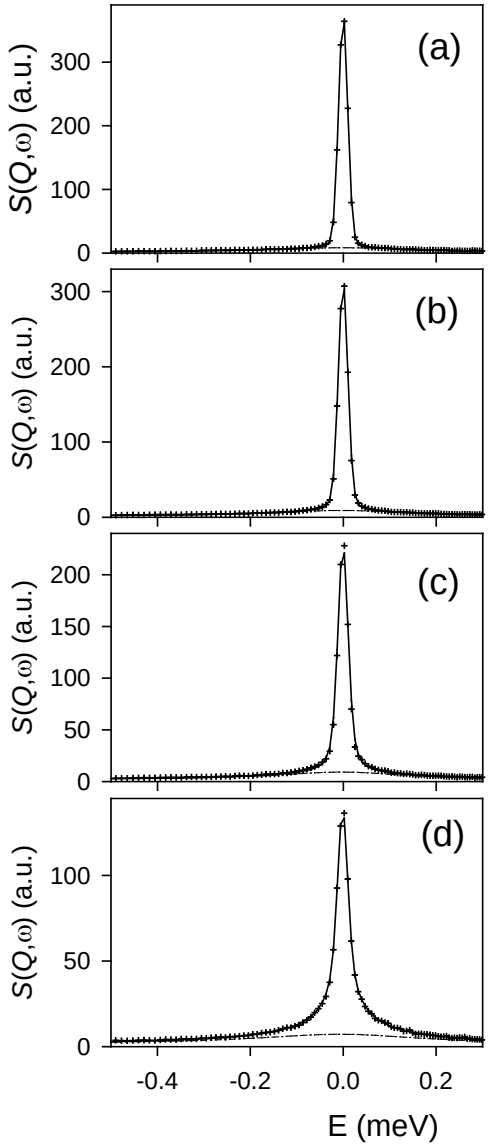

Figure 1. Comparison between experimental (crosses) and fitted (solid lines) QENS spectra obtained for benzene in MIL-53(Cr) at different temperatures: (a) 300, (b) 350, (c) 400, (d) 450 K. The dashed lines indicate the contribution from rotation (Q = 0.36 Å^{-1}).