Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

**Structure of deuterated liquid n-butanol by neutron diffraction and molecular dynamics simulations** VIVIANA CRISTIGLIO, Institut Laue Langevin, Grenoble, MIGUEL ANGEL GONZALEZ, GABRIEL JULIO CUELLO, Institut Laue Langevin, Grenoble, FRANCE, CARLOS CABRILLO, CSIS, Instituto de Estructura de la Materia, Madrid, SPAIN, LUIS CARLOS PARDO, ALVARO SILVA-SANTISTEBAN, ETSEIB, Universitat Politcnica de Catalunya, Barcelona, SPAIN — Aliphatic alcohols are the simpler molecular liquids possessing a polar hydroxylic group and a nonpolar alkyl tail. While the structure of the smallest alcohols has been relatively well studied, no much attention has been paid to the temperature dependence of the pre-peak observed before the main diffraction peak. The role of H-bonding in causing this feature and the direct relation between the number of C atoms and their distance were discovered very early, suggesting a liquid picture constituted of straight chains joined by H-bonds with the formation of mesoscopic size clusters. X-rays and neutron diffraction measurements showed that the height of the pre-peak associated with the formation of H-bonds increases with temperature. To explain this counterintuitive effect, a complete diffraction study using two neutron diffractometers D4 and D16 (ILL, Grenoble, France) allowing to cover the range 0.01-23 Åt1 and exploring a temperature range from 100 K (glassy butanol) to 400 K (moderately supercritical conditions) has been conducted. Molecular Dynamics simulations using the OPLS-AA potential were also carried out as a function of temperature and compared to experiment. Experimental and numerical results of liquid n-butanol and its glassy transition will be presented.

Viviana Cristiglio
Institut Laue Langevin, Grenoble

Date submitted: 03 Nov 2015 Electronic form version 1.4