Combining X-Rays and Neutrons to Shed Light in the Conformational Changes in L-Methionine

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In recent years crystalline amino acids have attracted a lot of attention due to their rich vibrational and structural properties [J. A. Lima Jr., et al, J. Raman Spect. 2008, 39, 1356; J. M. de Souza, et al., J. Phys. Chem. B 2007, 111, 5034; H. N. Bordallo, et al., J. Phys. Chem. B 2008, 112, 8748]. In addition, as a building block of proteins and peptides, amino acids are extremely important biological substances. Finally, understanding their ability to form polymorphs is a great challenge as it can later be extended to the design of smart materials. L-Methionine is an essential amino acid, important in the methylation process playing a key role in the immune system affected by HIV and other diseases [R. van Brummelen and D. Toit, Amino Acids 2007, 33,157; R. Pal, et al, J. Exp. Brain Res. 2007, 180, 765; E. Martignoni, et al, J. Neurol. Sci. 2007, 257, 31]. However very few studies of crystalline L-methione have been reported in the literature, thus very little is known about its physical properties. According to recent experiments, including Raman spectroscopy, thermal analysis, neutron diffraction and inelastic neutron scattering, changes in the conformational states of L-methionine induce a variety of structural arrangements between 220 and 340 K [J. Fischer, private communication; P.T.C Freire, private communication]. In order to analyse the structural arrangements of the intermediate conformational states high resolution X-ray measurements as a function of temperature are essential. Here we present the first results from X-ray synchrotron (LNLS-XPD) and neutron diffraction (IPEN) which combined to the previous results confirm that subtle structural changes in L-Methionine lead to a rich phase diagram in this important amino acid.

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