

Abstract Submitted
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Structural Isotopic Effects in the smallest chiral amino acid: Observation of a structural phase transition in fully deuterated alanine. HELOISA BORDALLO¹, HMI, JOELMA DE SOUZA, PAULO DE TARSO, Universidade Federal do Ceara, DIMITRI ARGYRIOU, HMI — A first study of possible changes instigated by deuteration in amino acids was carried out using neutron diffraction, inelastic neutron scattering and Raman scattering in L-alanine, $C_2H_4(NH_2)COOH$. Careful analysis of the structural parameters shows that deuteration of L-alanine engenders significant geometric changes as a function of temperature, which can be directly related to the observation of new lattice vibration modes in the Raman spectra. The combination of the experimental data suggests that $C_2D_4(ND_2)COOD$ undergoes a structural phase transition (or a structural rearrangement) at about 170 K. Considering that this particular amino acid is a hydrogen-bonded system with short hydrogen bonds ($O \dots H \sim 1.8 \text{ \AA}$), we evoke the Ubbelohde effect to conclude that substitution of hydrogen for deuterium gives rise to changes in the hydrogen-bonding interactions. The structural differences suggest distinct relative stabilities for the hydrogenous and deuterated L-alanine. De Souza et al. - Journal of Physical Chemistry B (Letters) **111**, 5034-39 (2007)

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