Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Anharmonicity in Amino Acids[1] HERCULANO MARTINHO, THAMIRES LIMA, MARIANA ISHIKAWA, Universidade Federal do ABC — Two special dynamical transitions of universal character have been recently observed in macromolecules (lysozyme, myoglobin, bacteriorhodopsin, DNA, and RNA) at $T^* \sim 100 - 150$ K and $T_D \sim 180 - 220$ K. The underlying mechanisms governing these transitions have been subject of debate. In the present work it is reported a survey on the temperature dependence of structural, vibrational and thermodynamical properties of a nearly anhydrous amino acid (orthorhombic polymorph of the amino acids L-cysteine and L-proline at a hydration level of 3.5%). The temperature dependence of X-Ray diffraction, Raman spectroscopy, and specific heat were considered. The data were analyzed considering amino acid-amino acid, amino acid-water, and water-water phonon-phonon interactions, and molecular rotors activation. Our results indicated that the two referred temperatures define the triggering of very simple and specific events that govern all the interactions of the biomolecule: activation of CH_2 rigid rotors ($T < T^*$), phonon-phonon interactions between specific amino acid and water dimer vibrational modes ($T^* < T < T_D$), and water rotational barriers surpassing ($T > T_D$).

[1]We would like to thank the Brazilian agencies CNPq (301018/2006-5) and FAPESP (2011/06618-0) for their financial support

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Special instructions:

Date submitted: 11 Nov 2011 Electronic form version 1.4