Extraordinary Negative Thermal Expansion in the Smallest Chiral Amino Acid, Alanine

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Amino acid construction consists of a carboxylic acid (-COOH) and an amino (-NH_2) functional group attached to the same tetrahedral carbon atom, the α-carbon. Every amino acid, with the exception of glycine, comes in two forms, a left-handed (L) and a right-handed (D) version, which are identical mirror images of each other. However, protein chains cannot be formed from a mixture of D and L.

We report on high resolution X-ray and neutron scattering diffraction as well as quasi-elastic neutron (QENS) studies on crystalline L- and D-alanine over a wide temperature range. Our aim is to verify the possibility predicted by the Nobel Laureate A. Salam, that a phase transition, related to a break of the as C α-H bond, occurs in alanine. While no change in the space group symmetry was observed, a negative thermal expansion, by discrete steps, along the **c**-axis is observed till the melting point. Additional anomalies are also noticed in the **a** and **b** lattice constants at 170K. Moreover, the evolution of the mean-square displacement, obtained from the QENS, data shows a steadily increase on heating, but near 150K and again near 200K a deviation from the expected behavior is observed. The results suggest the excitation of new degrees of freedom, possibly due to a progressive conformational change of the NH^{3+} group. The ramifications of this study can be extremely interesting for the understanding of homochirality as well as a breakthrough in molecular mapping via non-traditional sources of information.

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