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Please use this identifier to cite or link to this item: http://hdl.handle.net/123456789/1601 Title: Restricted backbone preference in the conformational landscape of amino acids: Do they have a role to play in the peptide structure? Authors: Dubey, Pankaj (/jspui/browse?type=author&value=Dubey%2C+Pankaj) Keywords: Conformational Landscape Amino Acids Ab initio Computations Issue Date: May-2019 Publisher: IISER Mohali Abstract: Conformational preferences of  $\alpha\text{-amino}$  acids were studied using matrix isolation infrared and ab initio computations. As a result of this study, the factors that determine the conformational stability of amino acids were recognized. It turns out that the low energy conformers of  $\alpha$ -amino acids prefer predominantly two types of backbone structures (i.e. the relative orientation of COOH and NH 2 moiety) and these two preferred orientations were labelled as "type I or II". An analysis of the conformer population indicates that ~80 % of the amino acid populations take up backbone type I and II structures. For these backbone structures, the various orientations of the side chain in the amino acids gave rise to a variety of conformers for each amino acid. The question was then addressed to see if these preferred backbone structures had a role to play in the intrinsic propensity and the structural preferences in peptides.

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