Abstract

Conformational preferences of α-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 α-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.