

Ab Initio Conformational Study on Ac-Pro-NMe₂: a Model of Polyproline

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We report here the results on N-acetyl-N'-dimethylamide of proline (Ac-Pro-NMe₂) calculated using the ab initio molecular orbital method with the self-consistent reaction field (SCRf) theory at the HF level with the 6-31+G(d) basis set to investigate the conformational preference of polyproline depending on the cis/trans peptide bonds and down/up puckerings along the backbone torsion angle ϕ in the gas phase, chloroform, and water. In the gas phase, Ac-Pro-NMe₂ has seven local minima of tFd, tFu, cFd, cFu, cAu, tAu, and cAd conformations. In particular, polyproline conformations tFd, tFu, cFd, and cFu are found to be more stable than α -helical conformations cAu, tAu, and cAd. In contrast, Ac-Pro-NHMe has seven local minima of tCd, tCu, cBd, cAu, tAu, cFd, and cFu conformations. Conformations tCd and tCu are found to be most stable, which is ascribed to the intramolecular hydrogen bond between C=O of acetyl group and $\tilde{N}H$ of N'-methyl amide group. The stability of the cFd conformation (i.e., the polyproline I structure) in chloroform is somewhat increased, relative to that in water, although tFd and tFu conformations (i.e., the polyproline II structure) are dominate both in chloroform and water. The population of backbone conformations feasible in chloroform and water is consistent with the experiments. This work is supported by a Korea Research Foundation Grant (KRF-2002-041-C00129).