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Ab Initio Conformational Study on Ac-Flp-NHMe: Stereoelectronic Effects on Proline Conformation

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We report here the results on N-acetyl-N′-methylamide of 4-fluoroproline (Ac-Flp-NHMe) 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 stereoelectronic effects on the conformational preference of proline depending on the cis/trans peptide bonds and down/up puckerings along the backbone torsion angle □ in the gas phase, chloroform, and water. In the gas phase, all potential energy surfaces for Ac-Flp-NHMe are quite similar to those of Ac-Pro-NHMe, except that up-puckered conformations are more stabilized than down-puckered ones. In chloroform and water, polyproline structures become dominant, whose populations are larger than those of Ac-Pro-NHMe. In chloroform and water, the populations of polyproline II (i.e., tF conformations) are quite similar to each other, but those of polyproline I (i.e., cF conformations) are larger by 5% in water than in chloroform. In particular, all cis populations for Ac-Flp-NHMe in the gas phase, chloroform, and water are decreased than those of Ac-Pro-NHMe.