

## Conformational Preference of Alanine Dipeptide in the Gas Phase and in Solutions

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We report here the results on N-acetyl-N'-methylamide of alanine (Ac-Ala-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 conformational preference of alanine depending on the backbone torsion angles  $\phi$  and  $\psi$  in the gas phase, chloroform, and water. There are seven local minima (LM) in the gas phase and two additional LM are found in chloroform and water. These two additional LM A (an  $\alpha$ -helical structure) and F (a polyproline structure) are stabilized only in solutions. In the gas phase, the lowest LM is the conformation C with a C<sub>7</sub> intramolecular hydrogen bond and the relative conformational energies range from 0.3 to 6.0 kcal/mol. In chloroform, the lowest LM is the conformation E (an extended structure) and the relative conformational energies range from 0.7 to 4.9 kcal/mol. In particular, we identified 14 possible transition states connecting between seven LM in the gas phase. The search for transition states probable in chloroform and water is now in progress.