

COMPARISON OF INTRAMOLECULAR FORCES IN DIPEPTIDES WITH TWO AROMATIC RINGS: DOES DISPERSION DOMINATE?

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IR/UV double resonance spectroscopy has shown that the structure of the capped dipeptide Ac-Trp-Tyr-NH₂ is dominated by a hydrophobic interaction between the aromatic rings on the side chains. Using the same method, a similar molecule, Ac-Phe-Phe-NH₂, had three experimentally observed conformers including one similar to that of Ac-Trp-Tyr-NH₂. In this work, calculations were performed on additional dipeptides containing two aromatic rings to determine if the dispersion-dominated structure was among the lowest energy structures in all such cases.

The B3LYP-DCP method developed by DiLabio and Torres was used to calculate the conformations of each dipeptide. Appending dispersion correction potentials (DCP) to B3LYP input files improves results for systems containing dispersion interactions without significantly increasing the calculation time. This method was used first on Ac-Trp-Tyr-NH₂ and Ac-Phe-Phe-NH₂ to confirm that it successfully identified the experimentally observed structures among the lowest energy results and was then applied to other capped dipeptides containing two aromatic rings including Ac-Phe-Tyr-NH₂ and Ac-Tyr-Phe-NH₂.