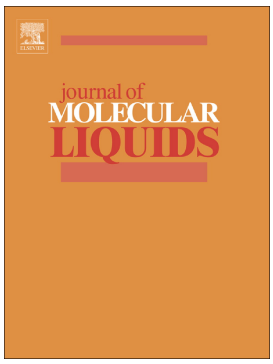

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Understanding the Quantum Mechanical Properties of Hydrogen Bonds in Solvated Biomolecules from Cluster Calculations

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Abstract

Here we use a combination of molecular mechanics force fields and high level ab initio calculations to study hydrogen bonding interactions in small hybrid peptide-water clusters relevant for larger biological aggregates. Potential energy surfaces interrogating pairwise interactions, constructed from popular biological force fields and water models, are in relatively good agreement with those from first principles. We also examine the importance of 3-body interactions in peptide-peptide and peptide-water hydrogen bonds and show that they can contribute between 4-19% of the total interaction energy. Using an energy decomposition analysis we show that this mostly originates from many-body polarization. The variations are caused by changes in the topology of the network and vibrational distortions of protons

Keywords: hydrogen bond, many body interaction, polarization, peptide aggregates

1. Introduction

Hydrogen bonds (HBs) form one of the most important and studied interactions in the physical chemistry and chemical physics of biological

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