Control of London Dispersion Forces in molecular chemistry

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Project Term
2015 - 2021

Project Areas
Molecular Chemistry

Clusters
Skylla Cluster Gießen

Software
GAUSSIAN, ORCA

Additional Software
Avogadro, Chemcraft

Institute
Institute of Organic Chemistry

University
Justus Liebig University Giessen

Introduction

Introduction: Since attractive forces in molecular chemistry are often neglected in molecular chemistry we want to emphasize on their importance and all abundance in chemistry. We are investigating role model systems and want to determine the explicit influence of these forces on the dimerization and folding behavior of organic compounds in solution as well as in the gas phase, only with joined forces of theory (computational data) and experiment we are able to understand chemistry on a molecular level.

Methods

Methods: We are using Gaussian16 for modeling organic compounds and compare their structure and behavior in silico with experimental values. For our needs to compare experimental data with theory we need to compute our structures on a high level of theory. As basis for geometry optimization serve DFT-Methods such as B3LYP/6-311G(d,p).

But for final energies Coupled Cluster Level of theory is crucial. In each of our investigated molecular systems it is very important how much any of the known forces contributes to the stability of a molecule, for this purpose we use energy decomposition schemes like LED implemented in orca4.1.

Results

In the first period we were able to compute really large structures (up to 200 atoms) (derivatives of hexaphenylethanes)

to understand the influence of their substitution pattern on their stability and dimerization behavior.

Outlook

Ongoing investigations are about the dynamics of cyclooctatetraene hence dispersion forces and the development of new model systems (molecular balances) for quantifying London Dispersion forces in solution.

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