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BENCHMARK STUDY FOR SYSTEMS WITH DOUBLE AND SINGLE BONDS

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The interactions of model system with π-bonds are important and have been studied with interest. Presence of π-bonds can affect the properties and behavior of various systems and processes. For example, fatty acids, which contain molecules with π-bonds, and have a significant role in living organisms and influence human health.

Previous study performed calculations for different interactions of *cis*- and *trans*-unsaturated molecules. We used three groups of non-covalent interactions: (1) interactions of *cis*- and *trans*-2-butene dimers, (2) interactions between 2-butene and butane, and (3) interactions of butane dimers. SAPT decomposition analysis of interaction energies showed some different nature between the three groups of the studied model systems. Hence, one can assume that different methods should be used to study these three groups of systems. This study is based on detailed benchmark study using MP2 and large number of DFT-D methods, with various basis sets.

In benchmark study eleven methods: MP2, BLYP-D3, BP86-D3, M05-D3, M052X-D3, M06-D3, M06HF-D3, TPSS-D3, PBE1PBE-D3, B3LYP-D3 and B2PLYP-D3 and four basis sets: cc-pVDZ, cc-pVTZ, aug-cc-pVDZ and 6-311++G** for each of the method have been analyzed. The results obtained with these methods were compared with high level accurate CCSD(T) method at complete basis set (CBS) approximation.

The geometries used for calculations have been studied in all possible parallel and displaced parallel interactions. All calculations on interaction energies have been performed in Gaussian 09 (version D.01). RMTD values represent the results that have the best agreement with CCSD(T)/CBS values. As it was expected, different set of method with basis set for each of the model systems groups showed the best agreement with CCSD(T)/CBS values. For (1) interactions of 2-butene the best agreement showed method B3LYP-D3/cc-pVTZ with RMTD value of 0.0318, for (2) interactions between 2-butene and butane the best method was B2PLYP-D3/cc-pVTZ with value or RMTD 0.0293, and (3) interactions of butane dimers the best agreement has B2PLYP-D3/6-311++G** method with RMTD value of 0.0734. These results show which methods should be used to study systems with double and single bonds.

Key words: CCSD(T)/CBS, Pi-interactions, alkenes, DFT

THERMODYNAMIC
METAL CATIONS BY

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e-

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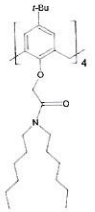
2- Department of Organic Chemist

Calixarenes are macro
residues linked by methylene
are known to be very efficient,
molecules.

Complexation of alkal
derivatives (**1**, **2**) in acetonitril
was studied at 25°C by mea
spectroscopies. Computationa
studied systems were carried o
previously obtained by studyi
amide derivative (**3**).[1,2]



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The stability constan
by different methods being
complexation enthalpies and
found to be favourable for th
of the complexes were quite
MeCN > PhCN > MeOH), w
in the solvation of the ligand
solvents used. The strong i
compound **3** (not present i
molecules into the calixarene
determining the calixarene-c
results were fully supported b

Key words: calixarenes, con

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1. G. Horvat *et al.*, *Inorg. Chem*
2. G. Horvat *et al.*, *Inorg. Chem*