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DMSO Clusters: Non-Covalent Interactions and DFT Benchmarking

Dimethylsulfoxide (DMSO) is one of the most used solvents in industries and in Chemistry. Despite its importance, a very few studies have been reported on DMSO clusters. In this work, we have explored thoroughly the potential energy surfaces (PESs) of the DMSO clusters from dimer to tetramer at the MP2/aug-cc-pVDZ level of theory. In order to understand the non-covalent interactions in DMSO clusters, we have performed a quantum theory of atoms in molecules (QTAIM) analysis. The QTAIM analysis showed that there are eight different types of non-covalent interactions stabilizing the DMSO clusters. The CH$\cdots$O hydrogen bonding and H$\cdots$H bonding are found to be the strongest and the weakest non-covalent interactions in DMSO clusters, respectively. To allow affordable investigations of medium and large sized DMSO clusters in future investigations, we have assessed the performance of ten functionals of the density functional theory (DFT) in calculating the binding energies of the DMSO clusters. The ten DFT functionals have been benchmarked to MP2/CBS and DLPNO-CCSD(T)/CBS. The functionals PW6B95D3 and ωB97XD are recommended for further affordable investigations of the DMSO clusters [1]. It is worth noting that the exploration of the PESs of the DMSO clusters generates several structures of large size. Without HPC resources, these investigations would not be possible. In addition, the calculation of the binding energies at MP2/CBS and DLPNO-CCSD(T)/CBS needs a large amount of memory. It is only with the help of CHPC that we can afford such expensive calculations.

References:
[1] A. Malloum, J Conradie, Non-Covalent Interactions in Dimethylsulfoxide (DMSO) Clusters and DFT Benchmarking, Phys. Chem. Chem. Phys. 2021, Submitted.

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