عنوان مقاله:

DFT Study of dimers of dimethyl sulfoxide in gas phase

محل انتشار:

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خلاصه مقاله:

Density functional (DFT) calculations at M05-2x/aug-cc-pVDZ level were used to analyze the interactions between dimethyl sulfoxide (DMSO) dimers. The structures obtained have been analyzed with the Atoms in Molecules (AIMs) and Natural Bond Orbital (NBO) methodologies. Four minima were located on the potential energy surface of the dimers. Three types of interactions are observed, CH···O, CH···S hydrogen bonds and orthogonal interaction between the lone pair of the oxygen with the electron-deficient region of the sulfur atom. Stabilization energies of dimers including BSSE and ZPE are in the range 27–40 kJmol-1. The most stable conformers of dimers at DFT level is cyclic structure with antiparallel orientation of S=O groups pairing with three C–H···O and a S···O interactions.

کلمات کلیدی:

Hydrogen bonding, DMSO, DFT, dimers