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Hydrogen bonded dimers of small alkyl substituted amides: Structures, energetics, and spectral analyses based on density functional theory calculations

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Abstract

We have performed a density functional theory (DFT) study on the hydrogen bonding patterns for the dimers of small alkyl substituted amides, including formamide, acetamide, and propionamide, as well as their N-methyl substituted counterparts. The dispersion-corrected ωB97X-D exchange-correlation density functional with the aug-cc-pVDZ basis set has been employed in the energy and frequency calculations. To calibrate the DFT calculated binding energies for these dimeric complexes, we perform a benchmark calculation with the coupled cluster with single, double and perturbative triple excitations method at the complete basis set limit [CCSD(T)/CBS]. The binding energies are further analyzed by the energy decomposition method based on the symmetry adapted perturbation theory. The infrared spectra for the alkyl substituted amides and their dimers are simulated with explicit anharmonicities included, and compared with the representative experimental data. Both the dimer formations and the anharmonic corrections have significant effects on the principal spectral features related to hydrogen bonding, while the substitution effects are comparatively marginal.