Toward spectroscopic studies of biologically relevant systems: Vibrational spectrum of adenine as a test case for performances of long-range/dispersion corrected density functionals

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Several recently introduced models rooted into the density functional theory and designed for the study of weakly bound molecular systems, with particular reference to the role of dispersion interactions, have been tested for their performances in prediction of vibrational properties for adenine molecule. Results obtained by semi-empirical correction for dispersion (DFT-D), semi-local density-functionals (M05-2X, M06-2X), and long-range correction scheme (LC-ωPBE, CAM-B3LYP) have been compared to the PT2 anharmonic frequencies computed by B3LYP functional and to the experimental results. From the tested computational models only the B3LYP-D/DM scheme provided quantitative agreement with the reference data and at the same time correctly described binding of adenine dimer.

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