Title:	Influence of stacking on the ground and excited states of 2-aminopyridine
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
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Abstract:	In the present work, the ground and excited electronic state properties of seven isomers of 2-aminopyridine (2AMP) stacked dimer have been investigated at the estimated CCSD(T)/CBS limit and RI-CC2/def2-TZVP levels of theory, respectively. The interaction energy values for the seven isomers fall in the range of −7.7 to −4.9 kcal/mol. The most stable dimer is stabilized by two weak hydrogen bonds as well as by stacking interaction between the two moieties. The performance of several density functional theoretical methods has been tested for the ground state as well as the excited states. For the ground state, the functionals B3LYP-D3 and B97D were found to perform the best, giving a mean absolute deviation of 0.3 kcal/mol. For the excited states, the use of the functionals M06-2X and CAM-B3LYP led to results in good agreement with those of the RI-CC2 method, giving a mean absolute deviation of 2.3 kcal/mol. In addition, the vertical excitation energy values for a single proton transfer in the hydrogen bonded (planar) 2-aminopyridine dimer and double proton transfer in the stacked dimer of (2AMP)2 are also reported.
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