Symmetry-adapted perturbation theory analysis of the N···HX hydrogen bonds.

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The main aim of the study was the detailed investigation of the interaction energy decomposition in dimers and trimers containing N···HX bonds of different types. The study of angular dependence of interaction energy terms partitioned according to the symmetry-adapted perturbation theory (SAPT) was performed for the dimers containing N···HX bonds as mentioned above: ammonia-HX (X = F, Cl, Br) and pyridine-HF complexes. It was found that the electrostatic and induction terms exhibit strong angular dependence, while the exchange contributions are less affected. The dispersion terms are virtually nondirectional. In addition, the three-body SAPT interaction energy analysis for the mixed acid-base $NH_3\cdots(HF)_2$ and $(NH_3)_2\cdots HF$ trimers revealed strong differences between interactions of similar strength but different types (i.e., hydrogen bond and general electrostatic interaction). The importance of the induction terms for the nonadditivity of the interaction energy in strongly polar systems was confirmed.

Adres publiczny

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https://www.acs.org/content/acs/en.html