Title:	A Theoretical Investigation on the Effect of π − π stacking Interaction on 1 H Isotropic Chemical Shielding in Certain Homo- and Hetero- nuclear Aromatic Systems, Theoretical Chemistry Accounts
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Abstract:	Significant changes in the proton chemical shielding (and hence the chemical shift) are predicted in going from the monomer to the dimer of benzene, naph- thalene, pyridine and quinoline systems and also the trimer of benzene and pyridine. The computed NMR spectra show additional splitting in going from the monomer to the dimer and the trimer of different species. The aromatic protons show a significant upfield shift due to the enhancement of anisotropic shielding by the p electron cloud of the neighboring molecule(s). The nature of the NMR spectra also changes with the orientation of the stacked conform- ers. The results obtained using Møller-Plesset second-order perturbation theory along with the GIAO method show the changes in isotropic shielding, in a reasonable basis set independent fashion.
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