Stabilizing power of dispersion forces in aromatic compounds

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Dispersion forces are a subclass of attractive forces that arise between molecules and molecular fragments even in the absence of charges or permanent electric moments. While the dispersion forces are moderate in small molecules, the strength of the forces accumulates as the number of atoms increases. This fact makes the study of dispersion forces challenging and promising for such areas as molecular design, protein and enzyme structure research, chemical selectivity studies, and many others.

The idea of this research is to find out more about the stabilizing power of the dispersion forces between the rings of aromatic compounds through quantification. To understand the phenomenon, we focused on different classes of aromatic substances, such as substituted benzophenones, di-benzyl ketone, poly-phenyls, bi-fluorenes, and substituted ferrocenes. We have developed two independent approaches to quantify dispersion interactions. The first approach is based on experimental thermochemistry, including combustion calorimetry, differential scanning calorimetry, thermogravimetry, vapour pressure determination with combined Quartz Crystal Microbalance Langmuir method, Knudsen method, and transpiration technique. The second approach is pure theoretical and based on Density Functional Theory method with Becke-Johnson dispersion correction (D3BJ). The comparison of experimental and theoretical results enables the development of quantitative scales of dispersion forces, dependant on the structures of molecules under study.

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