ENERGY ANALYSIS OF THE COMPLEX FORMATION OF AROMATIC MOLECULES IN AN AQUEOUS SOLUTION

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S u m m a r y

The energetics of noncovalent interactions at the self-association of aromatic molecules with various structures and charges has been analyzed. Twelve different molecules have been examined. A method to compute the contributions made by various physical factors to the total Gibbs energy has been developed. The contributions given by hydrogen bonds and entropic factors were found to be always favorable, whereas the contributions made by van der Waals, electrostatic, and/or hydrophobic effects may be stabilizing or destabilizing, depending on the specific system under consideration. The issues concerning the factors that stabilize/destabilize the stacking of aromatic molecules in the solution and their relative importance have been elucidated.