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The structure, symmetry and dynamics of the benzene dimer

The question 'Do two benzene rings attract each other in the face-to-face or face-to-edge configuration?' has been the subject of much discussion. It is relevant in the determination of the conformation adopted by protein molecules that contain aromatic rings. The study of the benzene dimer, both by analyzing its spectrum and by making theoretical calculations, should answer the question; it is the subject of this talk. It turns out that the attractive force between two benzene molecules is only weakly dependent on their orientations and as a result they both rather freely rotate within the dimer. This greatly complicates the analysis of the spectrum and the theoretical calculations.

