Entropy versus aromaticity in the conformational dynamics of aromatic rings.

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Comparison of the results of Car-Parrinello molecular dynamics simulations of isolated benzene, pyrimidine and 1,2,4-triazine molecules reveals that the unusually low population of planar geometry of the benzene ring is caused by entropy effects despite its high aromaticity. The decrease in symmetry of the molecule results in smaller changes in entropy and Gibbs free energy due to out-of-plane deformations of the ring, leading to an increase in the population of planar geometry of the ring. This leads to differences in the topology of potential energy and Gibbs free energy surfaces.

Słowa kluczowe

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