Dendrimer-Guest Interactions: Challenging Conventional Wisdom

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Abstract:

Solutions to many future challenges - including water purification, drug delivery, and energy storage - will require innovative new materials. Dendrimers are a class of materials with wide-ranging applications whose behavior is not fully understood. In many potential applications, dendrimers interact with small molecules. Our work focuses on describing the fundamental mechanisms governing the interactions between dendrimers and hydrocarbons using molecular modeling and computer simulations. A common view of dendrimer host-guest interactions is that the guest molecules are encapsulated in protected interior voids within the dendrimer structure. Our results present an alternative picture and show that the association of a model aromatic hydrocarbon, naphthalene (NPH), involves temporary pockets formed by the dendrimer branches and interactions between the NPH molecules themselves.