Characterization of Diamondoid Clusters Formed In Helium Nanodroplets

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Abstract: Diamondoids are versatile building blocks in nanomaterial design, but only recently the field expanded to preparation and study of diamondoid covalent assemblies, *i.e.*, molecules composed of diamondoid cage subunits connected by a heteroatom.[1] Spontaneous self-assembly of diamondoid derivatives is known to be strongly influenced by intermolecular London dispersion interactions. We therefore investigated diamondoid agglomeration in helium nanodroplets (HNDs) as that is a medium suitable for characterizing weakly-bound supramolecular clusters.[2,3] We confirmed that organization of diamondoid covalent assemblies in HNDs was indeed predominantly governed by dispersion when derivatives of low polarity (hydrocarbons and ethers)[2] were studied, whereas introduction of more polar functional groups to diamondoid scaffolds[3] resulted in a formation of more complex nanostructured supramolecular networks. By combining experimental results with a computational analysis we gained deeper insights into the forces governing self-organization and agglomeration behavior of diamondoids, which has important implications for their use in nanotechnology.

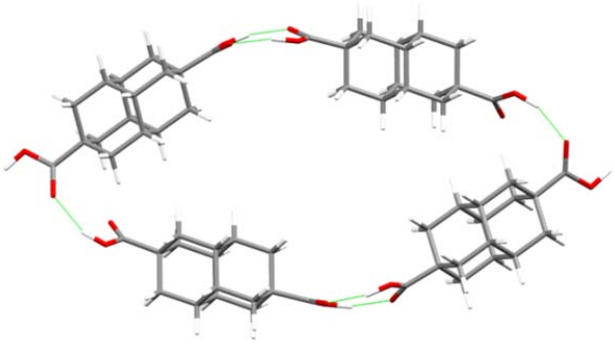

Fig 1. Computed cyclic assembly of 4,9-diamantanedicarboxylic acid molecules formed in HNDs

References:

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