Computations on N Encapsulations into Smaller Cages

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Endohedral cage compounds have been considered as possible candidate species for molecular memories. In this report, computations are carried out on two hypothetical N-containing endohedral system - N@C_{36} (D_{6h} & D_{2d} cages). Some additional computations on four hypothetical He-containing endohedral system - He@$C_{14}H_{16}$ (isogarudane and garudane cages) and He@C_{36} (D_{6h} & D_{2d} cages) are also included. Geometry optimizations are followed by vibrational analysis in some cases. The geometry optimizations can indeed produce local energy minima for the endohedral systems. While in N@C_{36} D_{6h} the nitrogen atom has a central location, in N@C_{36} D_{2d} exhibits a bonding pattern. Thermodynamic and kinetic stability aspects are discussed, too.