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| Title: | Structure, energetics, and reactivity of boric acid nanotubes: A molecular tailoring approach |
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| Abstract: | Cardinality guided molecular tailoring approach (CG-MTA) [Ganesh et al. J. Chem. Phys. 2006,125, 104019] has been effectively employed to perform ab initio calculations for large molecular clusters of boric acid. It is evident from the results that boric acid forms nanotubes, structurally similar to carbon nanotubes, with the help of an extensive hydrogen-bonding (H-bonding) network. Planar rosette-shaped hexamer of boric acid is the smallest repeating unit in such nanotubes. The stability of these tubes increases due to enhancement in the number of H-bonding interactions as the diameter increases. An analysis of molecular electrostatic potential (MESP) of these systems provides interesting features regarding the reactivity of these tubes. It is predicted that due to alternate negative and positive potentials on O and B atoms, respectively, boric acid nanotubes will interact favorably with polar systems such as water and can also form multiwalled tubes. |
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