Title:	A Computational Investigation of Cyclic Four-Membered Boron Based Systems
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Abstract:	Most of the previous studies on four-membered rings of boron and nitrogen like B2N2H4 have been concerned with their Hückel analysis and to understand their aromaticity or antiaromaticity character. Synthesis of this type of ring is still very difficult and only a few have been isolated with some sterically hindered ligands. In this project, different isomers of diazadiboretine have been examined at first. Calculations have been performed to understand the stability, frequency and ring puckering of different isomers of diazadiboretidine. The most stable conformer has been determined followed by a comparative study between HF, MP2 and CCSD and an extensive basis set study. Comparative studies with other straight chain B-N systems have also been performed and B-N bond length, charge on B and N, deviation of geometry at B from planarity and at N from pyramidalisation etc. have been analyzed thoroughly. H"s bonded to B"s of the most stable form of diazadiboretidine have been substituted by different electron withdrawing and electron donating groups and substitutions have even been performed in the core B2N2 ring to check whether in any of the systems, the geometry around B atom deviates from planarity by a large amount. All the cases have been investigated thoroughly. However, it was not possible to achieve that in any of the boron based cases until we used phosphorus based 4-membered rings. Monoanion of BH3 have also been investigated to see whether the inclusion of an electron can distort the geometry around B and our study suggests that it is not possible. Dianion of 1,3-diazadiboretidine have been examined. Monoanion and dianion of BCl3 have also been investigated and found to be non-planar with a large deviation from planarity, but to confirm the results of this particular case and the dianion of 1,3-diazadiboretidine, more calculations need to be performed.
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