Abstract Submitted
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Ab Initio Study of the Barrier to Planarity of Cyclobutane, Silacyclobutane and Germacyclobutane[1] ESTHER J. OCOLA, JAAN LAANE, Department of Chemistry, Texas AM University, College Station, TX-77843-3255, USA — The structures and barriers to planarity of cyclobutane (CB), silacylobutane (SiCB) and germacyclobutane (GeCB) have been computed using MP2, CCSD, MP4(STDQ) and CCSD(T) ab initio methods and the cc-pVTZ basis set in each case. These results were compared to experimental values previously reported. The reported experimental barrier to planarity of CB ranges from 448 to 518 cm^{-1}. The CCSD/cc-pVTZ calculation gives a value of 586 cm^{-1} for CB, which is in closer agreement than the other ab initio results. For SiCB the reported experimental barrier is 440 cm^{-1}. Our calculated CCSD/cc-pVTZ barrier is 472 cm^{-1}, in very good agreement with the experimental value, but the other methods do more poorly. The experimental value of GeCB has not been determined, but we have calculated its CCSD/cc-pVTZ value to be 409 cm^{-1}, which we consider to be a reasonable approximation. The trend to lower barrier heights from CB to SiCB to GeCB is expected since the torsional forces involving SiH_2-CH_2 interactions or GeH_2-CH_2 interactions are less than the CH_2-CH_2 interactions of CB.

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