Abstract Submitted
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Theoretical Investigations, Structure, and the Ring-Puckering Vibration of 3-Oxabicyclo[3.1.0]hexane[1] LAUREN A. WIEDING, ESTHER J. OCOLA, JAAN LAANE, Department of Chemistry, Texas AM University, College Station, TX 77843-3255 — Ab initio computations using the MP2/cc-pVTZ method have been carried out to calculate the structures and energies of the conformations of 3-oxabicyclo[3.1.0]hexane (OBCH). A theoretical potential energy function for the ring-puckering vibration was also determined. The minimum energy conformation of OBCH has the ring puckering angle of the five-membered ring at a calculated value of 34.0 degrees and a three-membered ring bending angle of 69.2 degrees. The theoretical potential energy function and the experimental potential energy function, previously determined from spectroscopic data, are in good agreement. Both of these functions are asymmetric and have the conformation with the lowest energy puckered in the same direction as the attached three-membered ring. The calculations also show that the ring-puckering vibration is somewhat coupled to the ring-flapping and ring-twisting motions. The observed far-infrared ring-puckering transitions for OBCH agree with the calculated values to within 1%. The wavefunctions for the lowest ring-puckering energy levels have also been computed.

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