Abstract Submitted
for the TSF17 Meeting of
The American Physical Society

Theoretical Investigations of the Structures and the Ring-Puckering Vibrations for Several Bicyclic Molecules[1] ESTHER J. OCOLA, LAUREN A. WIEDING, JAAN LAANE, Texas A&M University, College Station, TX 77843-3255 — Ab initio calculations using the MP2/cc-pVTZ method have been carried out to calculate the structures and relative energies of the different conformations of five bicyclic molecules including bicyclo[3.1.0]hexane, 3-oxabicyclo[3.1.0]hexane, 6-oxabicyclo[3.1.0]hexane, 3,6-oxabicyclo[3.1.0]hexane, and bicyclo[3.1.0]hexan-3-one. Theoretical ring-puckering potential energy functions in terms of the ring-puckering coordinate have been calculated for each of the molecules and these were compared to those previously determined experimentally from spectroscopic data. Each potential function is asymmetric and has a single energy minimum corresponding to where the five-membered ring is puckered in the same direction as the attached three-membered ring. The calculations show that the ring-puckering motion is somewhat coupled to the ring-twisting and ring-flapping motions. Natural bond orbital analysis has also been performed and studied for these molecules and the wavefunctions for the lowest ring-puckering energy levels have been computed.

[1]The authors wish to thank the Robert A. Welch Foundation (Grant A-0396) for financial support.

Esther Ocola
Texas A&M University, College Station, TX 77843-3255

Date submitted: 28 Sep 2017 Electronic form version 1.4