

Alkene Strain in Cis versus Trans Geometries

Basic problem: Compare energies for *cis* versus *trans* isomers for sets of alkenes shown below (mostly pairs). Compare computed heats of formation to experimental heats of formation where available in the literature. What happens to the preference for *cis* versus *trans* alkenes as a function of ring size? Does this fit experimental observations?

Method: AM1 and 3-21G(*) are reasonable levels of theory. Compare results for the semiempirical methods to results for the *ab initio* method. Which method works better?

Literature: Use Beilstein Online, Chemical Abstracts, or the NIST Thermodynamic Database (available by request through P. M. Lahti) to get experimental heats of formation and literature references for them.

