Alkene Relative Energies as a Function of Structure

Basic problem: Compare computed heats of formation to experimental heats of formation where available in the literature. For the set of C_4 alkenes shown, do the computations reflect experimental energies and relative energetic ordering for the three isomers?

Method: AM1 and 6-31G* are reasonable levels of theory. Compare results for the semiempirical methods to results for the ab initio method. Which one 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.