Alkene Strain in Endocyclic versus Exocyclic Positions

Basic problem: Compare energies for pairs of alkenes shown below. Compare computed heats of formation to experimental heats of formation where available in the literature. Explain trends for preference in double bond placement as a function of structure.

Method: AM1 and 3-21G(*) are reasonable levels of theory. Strained rings can be a problem for the semiempirical NDO methods like AM1 and PM3. Do you see any evidence in comparing the literature and your computed results that there are problems with AM1 as applied to these systems? Compare results for the semiempirical methods (your choice, but be consistent) to results for the ab initio method. Which one gives results that are closer to experimental data?

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.