Conformations of 2-Substituted Aldehydes

Basic problem: Compute geometries and heats of formation for rotamers about the C-C=O bond for the aldehydes shown below. Determine the *most stable* conformation for each molecule, and the relative energies for higher energy conformations. Use this information to create a conformational energy diagram for each molecule. Look up whatever you can find about the known conformational preferences for aldehydes and ketones. Do your results correspond to known literature preferences (either quantitatively or quantitatively)?

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

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.