Resonance Effects in Nonalternant Aromatic Hydrocarbons

Basic problem: You will optimize the structures of a set of nonalternant hydrocarbons (systems that contain odd-member rings) to isoatomic alternant analogs. You will then examine bond lengths, bond orders, charge distributions, and dipole moments, in order to look for effects of charge-separated resonance contributions.

Method: AM1 and 3-21G* are reasonable levels of theory for these comparisons. Build and geometry optimize the following systems using AM1 and RHF/3-21G*. Compare heats of formation or energies to decide which member of each pair is more stable, and compare to experimental data where available. Do the results confirm the expectation that benzene-type rings are particularly favorable? Compare bond lengths to experimental bond lengths to decide whether aromatic bond delocalization (near-equal) bond lengths occur in either, neither, or both of the molecules. Use resonance arguments to try to explain the trends in bond lengths and dipole moments/charge density populations. Explain the difference between the dipole moments of the two molecules computed at the ab initio level of theory.

Literature: Use Beilstein Online, Chemical Abstracts, and the NIST Thermodynamic Database (see P. M. Lahti to get access to the NIST database) to get experimental information and literature references for them.