

Are Formal Bonds Realistic Reflections of Electronic Distribution?

Basic problem: Determine charge distributions and bond lengths for the systems shown below. Decide whether the resonance structures shown are the best ones, and if not, suggest a preferred resonance structure and support it based upon bond orders, bond lengths, and/or charge distributions.

Method: AM1 or 6-31G* are reasonable levels of theory. Try twisting the central bond that is shown as a double bond in a plausible resonance structure to find out the bond strength (don't forget to re-optimize the geometries). How strong is the central double bond? Can you explain the dipole moment in this molecule, based on resonance arguments?

Literature: There is limited literature for this, save for computations and qualitative arguments. Use Beilstein Online or Chemical Abstracts to get whatever information you can about these systems.

