

Are Formal Charges Realistic Reflections of Electronic Distribution?

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

Method: PM3 or 6-31G* are reasonable levels of theory. PM3 is good for hypervalent systems, and 6-31G* (while slow) is good for systems with polar bonds.

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 cationic systems (for example, as oxonium ions versus carbocations).

