Solutions to Problems

Chapter 1

 a. A dipolar resonance structure has aromatic character in both rings and would be expected to make a major contribution to the overall structure.

b. The "extra" polarity associated with the second resonance structure would contribute to the molecular structure but would not be accounted for by standard group dipoles.

c. There are three major factors contributing to the overall dipole moments: (1) the σ-bond dipole associated with the C-O and C-N bonds; (2) the π-bond dipole associated with delocalization of π electrons from the heteroatom to the ring; and (3) the dipole moment associated with the unshared electron pair (for O) or N-H bond (for N). All these factors have a greater moment toward rather than away from the heteroatom for furan than for pyrrole. For pyrrole, the C-N π dipole should be larger and the N-H moment in the opposite direction from furan. These two factors account for the reversal in the direction of the overall dipole moment. The AIM charges have been calculated.



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Lucio Gelmini, Robert Hilts

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