

Chem 200/400 Research Project: Prof. John Bartmess, BU 601

### Determining the Gas-phase Basicities of Pharmaceuticals

Modern methods of mass spectrometry allow us to detect and quantify "un-natural" products, such as pharmaceuticals and explosives, by volatilizing them (turning them into gases) and then making ions of them by proton transfer, using their basic properties. However, it has been shown that one analyte in a mixture fed to a mass spectrometer can suppress the signal of another, by competing for the proton in a gas-phase acid-base reaction. It is thus useful to know the relative gas phase basicities of such species, to predict if such "suppression effects" can occur. These gas phase basicities can be measured experimentally, but that is expensive, slow, and in the case of explosives, probably not the safest experiments to carry out. Modern methods of quantum mechanics calculations, however, can compute such energetic quantities both fairly quickly and accurately. To carry these calculations out does **not** require knowledge of quantum mechanics: it's just a computer program, where you input a molecular geometry and method, and then interpret the output. Some knowledge of organic structure and conformations is important in this, as well as computer skills such as using text editors and SSH/telnet file transfers. Most of the work can be done remotely via the Net, with weekly office meetings. This is intended as a one-semester project.