Computational Chemistry Research at Queensborough Community College

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We present two undergraduate computational chemistry research projects that are being performed at Queensborough. We have carried out extensive computational study of the intermolecular interactions of protonated amino acid, glycine, with water. At the B3LYP/6-311++G(d,p) and MP2/6-311++G(d,p) level, two unique structures were located for the one-water system in which the protonated glycine interacts with one water molecule. Four structures were located for the two-water system. Seven structures were located for the three-water system. These structures were obtained by full geometry optimizations without restrictions including the structure of water. Frequency calculations have been performed at the same level to confirm that these structures were energy minima. The calculated interaction enthalpies of the protonated glycine with consecutive addition of one, two , and three water molecules were compared to those obtained from the electrospray ionization high pressure mass spectrometry by the researchers from NIH (unpublished). Higher level calculations, including CP corrections are being pursued. In addition, we are also doing computational studies of the conformational equilibria of formic acid, and acetoacetone, in different solutions by using the continuum model in Gaussian 03. Preliminary results will be presented.