Ab Initio Computation of the pKa Values of Neutral Molecules and Anions in Water

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In this paper, we present our progress and results on the computation of the pKa values of some neutral molecules and anions, including the organic carbon acids acetonitrile, methyl acetate, acetamide, N,N-dimethylacetamide, as well as acetate, bicarbonate, and dihydrogenphosphate, in aqueous solution by using a variety of solvation models such as the CPCM in Gaussian 03 and SM6 in Smxgauss along with high level gas phase ab initio MO calculations. In particular, we treated the solute molecule with one, two and three water molecules in the continuum model. This work provides important information on the use of explicit water molecules with the continuum models in the study of pKa values.