Prediction of Biophenol pK_as Using Quantum Chemical Methods

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Following upon earlier quantum chemical studies of the acid dissociation constants of substituted phenols [Gross and Seybold, *Int. J. Quantum Chem. 85*, 569 (2001); Gross, Seybold, and Hadad, *Int. J. Quantum Chem. 90*, 445 (2002)], we have investigated a more diverse set of phenolic compounds to see if similar approaches can be used to estimate the pK_as of these compounds. Correlations are found between several electronic properties of the compounds and their pK_as. In compounds with two or more potential dissociating phenolic sites it is possible to identify the first dissociating site using the methods employed in this analysis.