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Estimation of the pK_as of Aliphatic Amines Using Quantum Chemical Descriptors

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Abstract. Earlier theoretical studies [Gross & Seybold, *Int. J. Quantum Chem*. 80, 1107 (2000); Gross et al., *J. Org. Chem*. 66, 6919 (2001); Gross, Seybold, and Hadad, *Int. J. Quantum Chem*. 90, 445 (2002)] showed that the variations in several quantum chemical charge and energy parameters were strongly correlated with the pK_a variations in substituted anilines. In this work we extend this examination to the pK_as of a variety of aliphatic amines, including halogenated compounds and some biochemically active species. Good correlations are found between the pK_as of these compounds and the energy differences (ΔE) between the parent amines and their cations as well as the natural charges on the $-NH_2$ and $-NH_3^+$ groups calculated at the B3LYP/6-311++G(d,p) level.