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Abstract

Two general topics are covered in this thesis. In the first study the pKₐs of a set of 16 substituted benzoic acids have been modeled using quantum chemical techniques at the density functional theory B3LYP/6-31G* level. A variety of parameters including charges on the dissociating group, energies of dissociation, and the Wiberg bond index were examined in relation to the variations observed in the experimental pKₐs. The best correlation found ($r^2 = 0.978$) was with the Löwdin charges on the dissociating COOH group. In the second study both first-order and second-order cellular automaton models have been employed to simulate the overall chemical kinetics of the classical Lindemann mechanism. It is demonstrated that both models accurately reflect the salient features of this mechanism, including the second-order kinetics at low concentrations of the collision partner M and the apparent first-order behavior at high concentrations of M.