Hydrogen bonding and dissociation effects on the gas phase proton transfer reactions of ozone

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 Recently, the proton affinity (PA) of ozone was experimentally determined by Cacace and Speranza [Science (1994) 265: 208] using a bracketing technique that involved the proton transfer (PT) reactions: O3H++B? O3. BH+; for different Brönsted bases B. These authors showed that the simple collision model is not adequate to describe PT. We now present a theoretical model reflecting this bracketing procedure by explicitly introducing H-bonding complexing, dissociation and PT contributions, to discuss the kinetic model that assumes that PT occurs through one elementary step. The methods used include semiempirical density functional theory and ab initio Hartree-Fock methods. The procedure is gauged by using estimated PA of ozone obtained from deprotonation reactions including the Brönsted bases B=NH3, H2O, HOCl, SO2, CH3F and Kr. The PA-obtained range was from 145.3 to 160.3 kcal/mol, in fair agreement with the experimental value of 148:0 ± 3 kcal/mol. The model seems