

HSAB analysis of charge transfer in the gas-phase acid-base equilibria of alkyl-substituted alcohols

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A simple model to analyze charge redistribution associated with proton transfer (PT) reaction is derived from a classical ion transport model. The model is applied to the gas-phase acid-base equilibria of alkyl alcohols. Proton transfer is simulated as the motion of a charged particle in an applied external potential defined by the chemical environment of the proton, and represented by the difference in proton affinity (PA) of the conjugated bases RO⁻ and CH₃O⁻; the latter is taken as reference. The electronic chemical potential of transfer accounts for both the amount and direction of charge transfer (CT). The relative acidity for a short series of alkyl alcohols is determined by the difference in proton affinity ($\Delta PA = PA(\text{RO}^-) - PA(\text{CH}_3\text{O}^-)$) of the conjugated bases. The predicted charge transfer is in agreement with the CT pattern obtained from the group hardness and electronegativity analysis. © 1999 American Chemical Society.