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Dependence of acidity of organic substances in gaseous and aqueous phases on molecular properties

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Abstract

For a series of aliphatic, unsaturated and aromatic carboxylic acids, as well as alcohols and thiols there have been obtained dependences of anion affinity to proton in gaseous phase on the ionization potential. Linear dependences of pKa in water were obtained on fractional power of the product of molar mass by the value of topological index to the power of 2/3.

Pictures of the location of linear dependences as related to each other ascertain the interdependence of acidic properties of substances and the change of electron energy on transition from acid to anion, as well as the characteristics of the molecular motion in the liquid phase.