

Acidity of aromatic sulfoacids in gas and water phase

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Abstract

The acidity of aromatic sulfoacids is described within the framework of quantitative Pearson's HSAB theory on base of conceptual DFT. It is discovered that values their pKa are in linear correlation on local electrophilicity of reaction centre (the atom of the oxygen) and its electrostatic potential, both in gas phase, and water ambience. That dependence is considered in accordance with physical sense of electrophilicity as electron capacity of reaction centre.