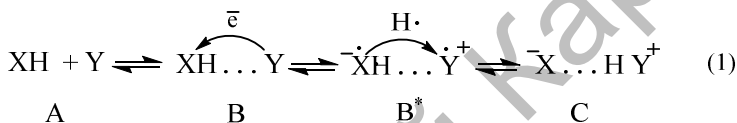


THE IONIZATION POTENTIALS OF ACID-BASE MOLECULES IN FAST PROTOLYTIC REACTIONS

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Investigations of the fast protolytic reactions kinetic by dynamic EPR spectroscopy show that general mechanism of proton transfer process, for example, between H-acid (XH) and organic bases (Y) in toluene medium, may be presented with the next scheme:



If XH is the semiquinone spin probe 3,6-di-tert-butyl-2-oxyphenoxyl (I) then stable radical I gives us molecular complex with hydrogen bond B with molecules of organic solvents, which have the ionization potential values approximately equal or higher than adiabatic IP_a of I: spirits, ethers, water, hexametapol etc.

Bases	$-IP_a$, eV	H-acids	$-IP_a$, eV
Li	5,3917	HOH	10,4474
Na	5,1321	CH ₃ OH	9,3274
K	4,3407	Ĉ ₂ OH	8,0162
NH ₃	8,5200	HCOOH	9,9688
CH ₃ NH ₂	7,7480	CH ₃ COOH	9,3647
(CH) ₂ NH	7,1749	dioxane	6,9966
(CH) ₃ N	6,1851	HCl	11,8596
(C ₂ H ₅) ₃ N	5,7297	HNO ₃	11,1130
tebaine	5,8430	H ₂ SO ₄	10,4240
hexametapol	7,2756	I	7,7132

Alkaline metals, alcaloides and several amines with more small IP_a values than I, form ionic complex with hydrogen bond C in acid-base protolytic reaction (1) between oxyradical (XH) and Y molecules. Table contents IP_a values obtained by ab-initio UHF 3-21G method. This data demonstrate that the elementary electron transfer from bases molecule to acids molecule summary determine proton transfer process in the fast protolytic reaction.