

SYNTHESIS AND PROPERTIES OF HIGHLY LIPOPHILIC PHOSPHAZENE BASES

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This work reports synthesis and characterisation of twelve novel phosphazene-based indicator molecules (with the structure $X-C_6H_4-N=N-C_6H_4-N=PR_3$) for the basic pH range with unusual combination of properties: 0/+1 charge states, high lipophilicity of both neutral and charged forms, lack of localized charges in the cations. They have been synthesized by the Staudinger reaction and characterized by UV-Vis spectral properties, pK_a values in acetonitrile (MeCN) and water, as well as by lipophilicities ($\log P$ values). The UV-Vis spectrophotometric titration method was used to establish the pK_a values in MeCN medium. Estimates of aqueous pK_a values were obtained from pK_a values in MeCN via correlation analysis. $\log P$ values between aromatic (toluene) and aliphatic (1-octanol) solvent and aqueous medium were determined using the shake-flask method. The possible extraction of ion pairs into the organic phase was considered and the results corrected accordingly. The new bases have wide pK_a range (14.9–20.8 pK_a units in MeCN, 7.7–10.6 in water), high lipophilicities ($\log P$ values in the range of 5.4–9.2 in toluene-water system) and significant spectral changes in the visible region on protonation/deprotonation. Indicators with this set of properties are expected to find application in production of lipophilic membranes, design of sensors, etc.

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