Supporting Information

Anomalous Acid-Base Equilibria in Biologically Relevant Water Nanopools

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Received July 17, 2012, Accepted July 23, 2012

Experimental

6HQ (98%), purchased from Sigma-Aldrich, was used after being purified via column chromatography and vacuum sublimation. AOT (> 99%) was used as purchased from Sigma-Aldrich, while *n*-heptane (anhydrous, ≥ 99%), purchased from Sigma-Aldrich, was stored over molecular sieves of 4 Å prior to use. Aqueous solutions of 6HQ were prepared by dissolving 6HQ in water (≥ 18 MΩ cm) which was distilled triply with a Milli-Q system (Millipore). 0.2 mM of 6HQ in AOT reverse micelles was prepared by dissolving 2.9 mg of 6HQ in a 100 mL heptane solution of 0.09 M AOT. In our samples, practically no more than one 6HQ molecule can be present in an AOT micelle consisting of 20 AOT molecules because [6HQ]/[micelle] is 0.04. pH was adjusted by adding a dilute HCl or NaOH aqueous solution to triply distilled water, and then a requisite amount of pH-adjusted water was added to the AOT solution to control w_0. Absorption spectra were obtained using a UV/vis spectrometer (Scinco, S-3100) while pH was measured using a pH meter (Fisher Scientific, AR15) calibrated with three buffers of pH 4, 7, and 10. All the measurements were carried out at room temperature.

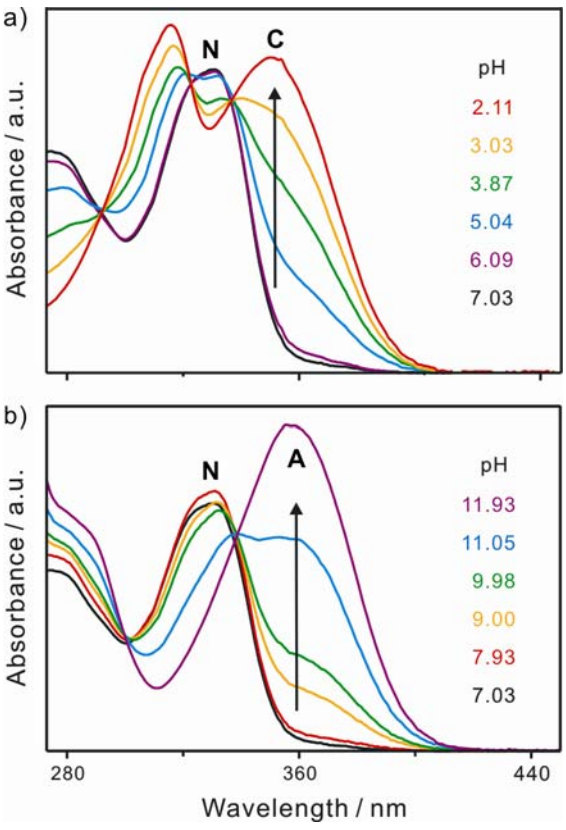

Figure S1. pH-dependent absorption spectra of 6HQ in acidic (a) and basic (b) water nanopools of AOT reverse micelles having w_0 = 36. pH values are indicated inside, and absorption bands of neutral, cationic, and anionic species of 6HQ are marked as **N**, **C**, and **A**, respectively.

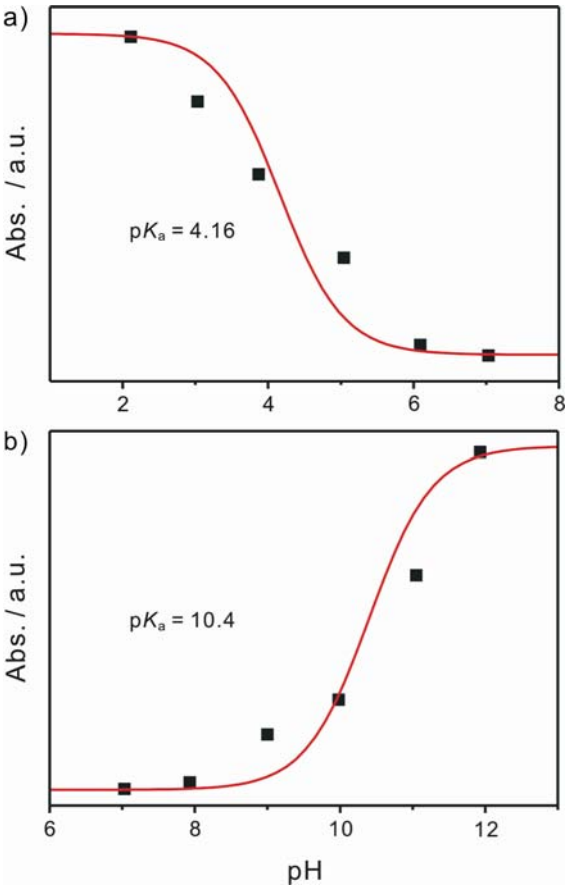

Figure S2. pH-dependent absorbance, in AOT reverse micelles having w_0 = 36, of **C** at 350 nm (a) and **A** at 358 nm (b). Solid lines are the best-fitted curves of Eq. (1) to extract pK_a values indicated inside