

Supporting Information

Supramolecular Polymer/Surfactant Complexes as Catalysts for Phosphate Transfer Reactions

Adriana P. Gerola,[†] Eduardo H. Wanderlind,[†] Yasmin S. Gomes,[†] Luciano A. Giusti,[†] Luis García Río,[‡] René A. Nome,[#] Anthony J. Kirby,[§] Haidi D. Fiedler,[†] Faruk Nome*,[†]

[†]INCT-Catálise, Departamento de Química, Universidade Federal de Santa Catarina, Florianópolis, SC 88040-900, Brazil

[‡]Departamento de Química Física, Centro de Investigación en Química Biológica y Materiales Moleculares, Universidad de Santiago de Compostela 15782 Santiago de Compostela, Spain

[#]Instituto de Química, Universidade Estadual de Campinas, Campinas, SP 13083-970, Brazil

[§]Department of Chemistry, University of Cambridge, Cambridge CB2 1EW, UK

*e-mail: faruk.nome@ufsc.br

Supporting Information - Summary	
Figure S1. ^1H NMR spectrum of PAIM in D_2O at 25°C	2
Figure S2. Potentiometric pH–titration curve of PAIM with KOH.	3
Figure S3. Specific conductance for CTAB in water, in the presence of PAIM.	3
Figure S4. Specific conductance <i>versus</i> $\log_{10}[\text{CTAB}]$	4
Figure S5. Diameter of PAIM/CTAB complex at pH	5
Figure S6. Pyrene $I_{\text{I}}/I_{\text{III}}$ intensity ratio in ethanol/water mixtures.	6
Figure S7. Pyrene $I_{\text{Ex}}/I_{\text{M}}$ intensity ratio <i>versus</i> [CTAB] in the presence of PAIM.	6
Figure S8. Rate constants for the dephosphorylation of DEDNPP (in the presence of PAIM and as a function of CTAB and pH).	7
Figure S9. Rate constants for the dephosphorylation of DEDNPP in aqueous solutions as a function of [Imidazole]	8
Figure S10. Rate constants for the dephosphorylation of DEDNPP in aqueous solutions as a function of $[\text{CH}_3\text{COONa}]$	8
Treatment of the Binding isotherms of CTAB to PAIM	9

Figures

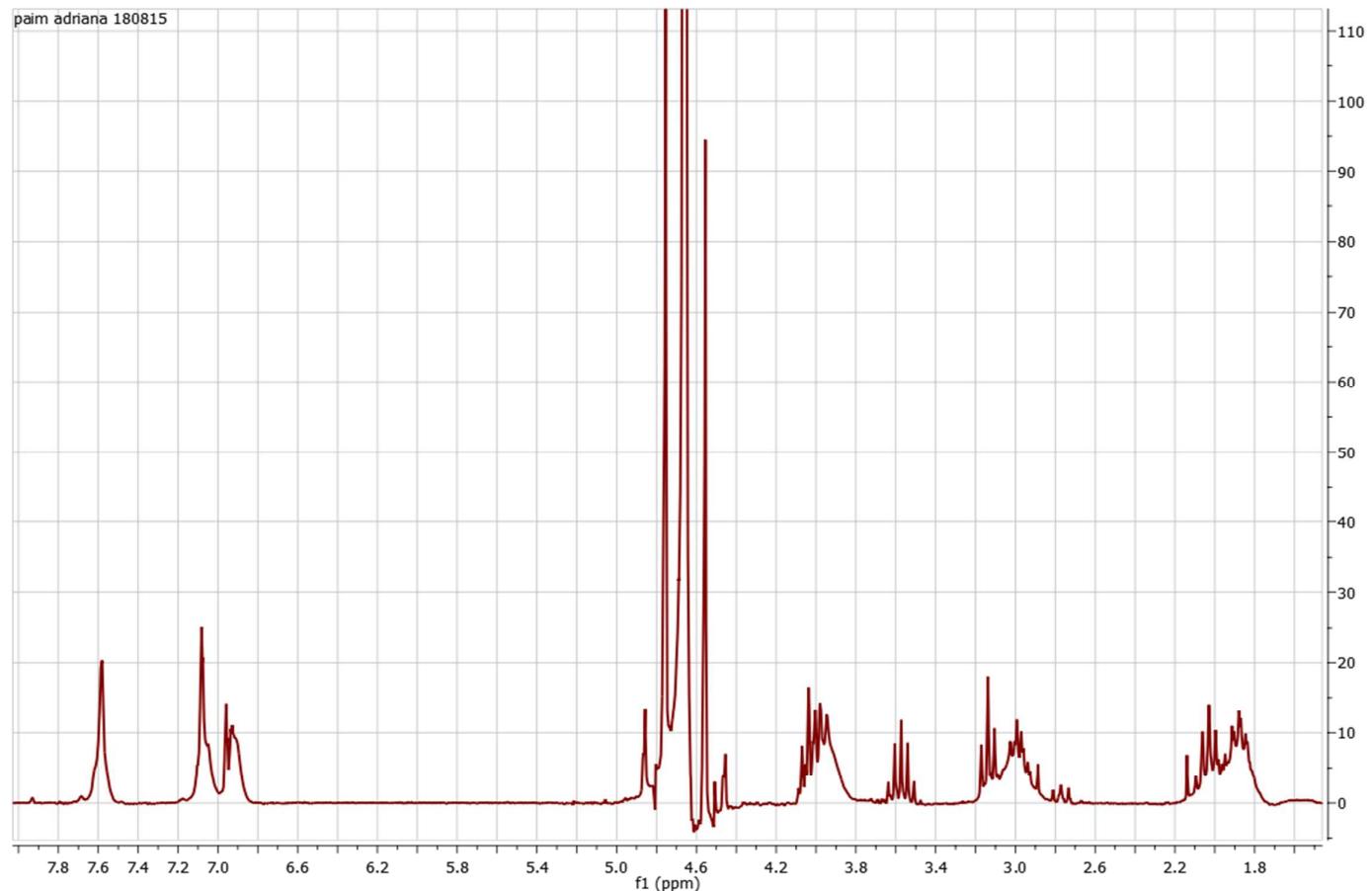
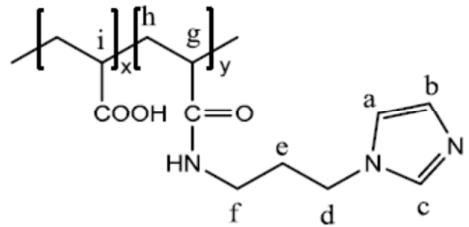


Figure S1. ¹H NMR spectrum of PAIM in ²D_O at 25°C.

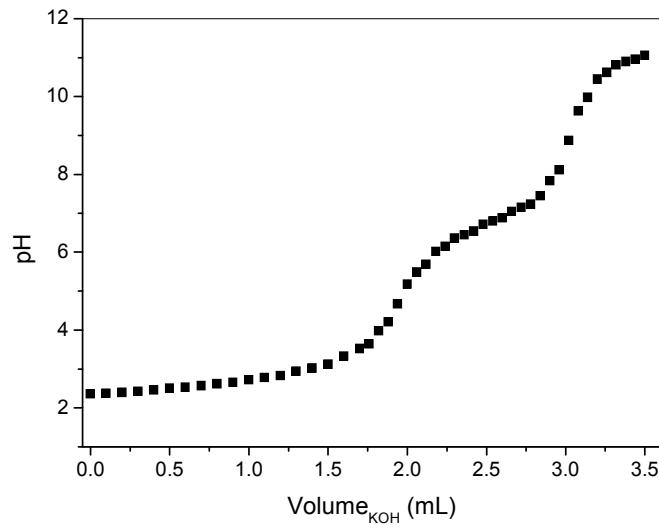


Figure S2. Potentiometric pH–titration curve of PAIM with KOH. The extent of PAA functionalization was evaluated by Potentiometric titration. The experimental data were fitted using the FITEQL program. Results obtained indicated a functionalization of nearly 50%, with functional groups carboxylate and imidazole in approximately 1:1 ratio.

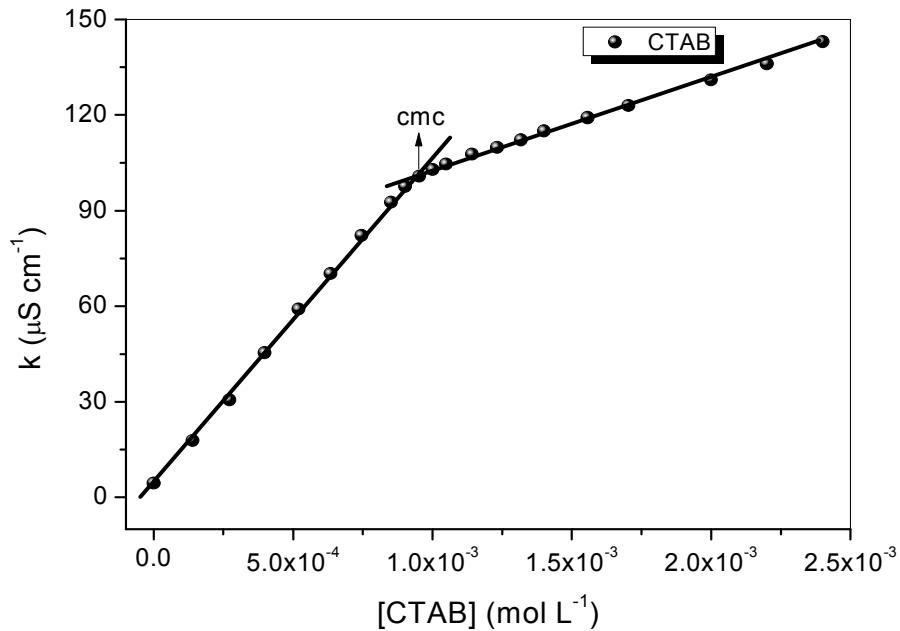


Figure S3. Specific conductance for CTAB in Milli-Q water at 25.0 °C and $[PAIM] = 2 \times 10^{-4} \text{ mol L}^{-1}$.

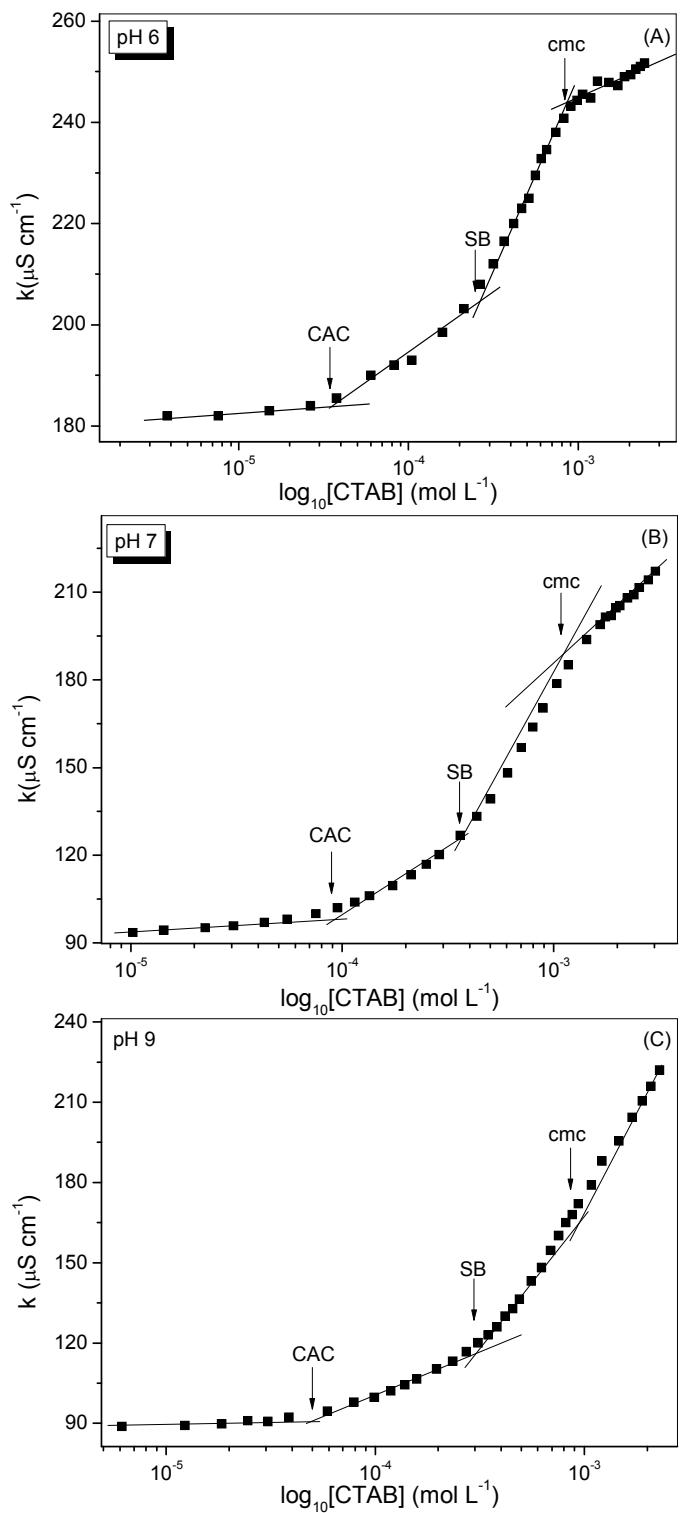


Figure S4. Specific conductance *versus* $\log_{10}[CTAB]$ in PAIM solutions (2×10^{-4} mol L $^{-1}$) at pH 6 (A), pH 7 (B) and pH 9 (C), at 25.0 °C.

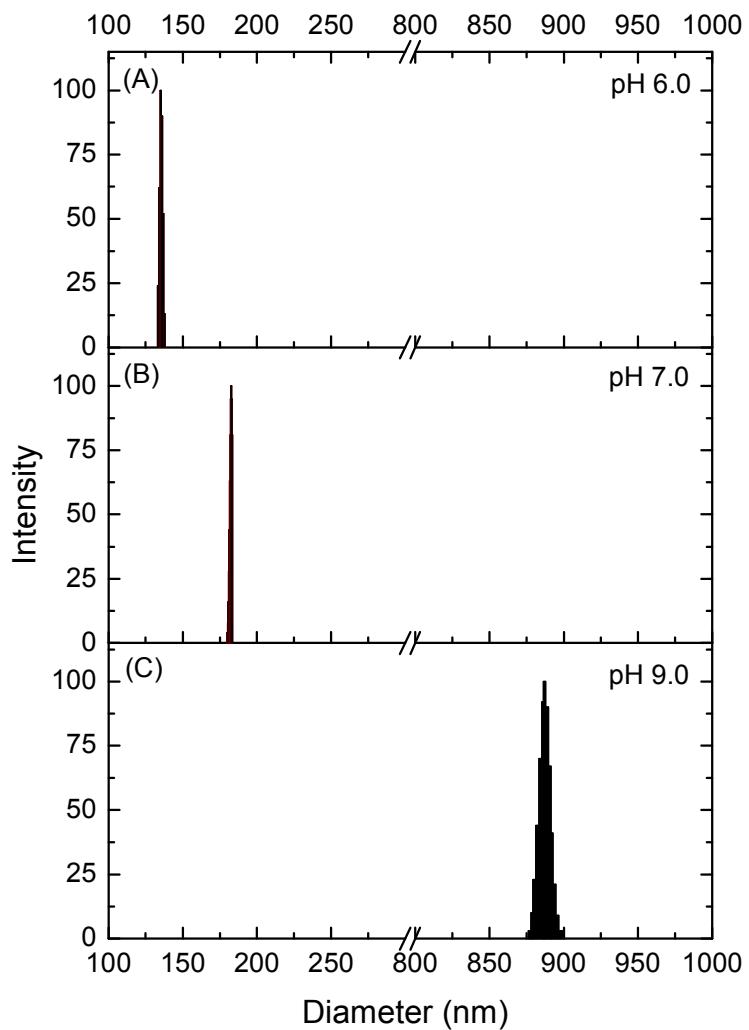


Figure S5. Diameter of PAIM/CTAB complex at pH 6 (A), pH 7 (B) and pH 9 (C). $[PAIM] = 2.0 \times 10^{-4} \text{ mol L}^{-1}$ and $[CTAB] = 2.4 \times 10^{-4} \text{ mol L}^{-1}$ at 25.0°C .

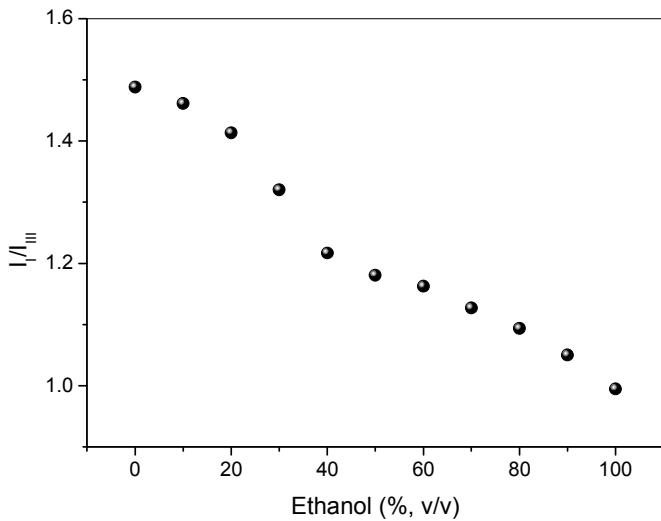


Figure S6. Pyrene I_I/I_{III} intensity ratio *versus* percentage of ethanol in mixtures ethanol/water ($\lambda_{\text{exc}} = 334 \text{ nm}$). [Pyrene] = $5 \times 10^{-7} \text{ mol L}^{-1}$.

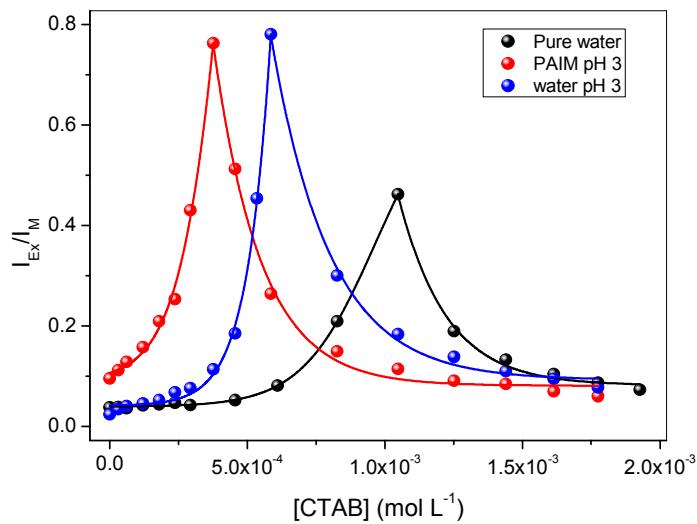


Figure S7. Pyrene I_{Ex}/I_M intensity ratio *versus* [CTAB] in absence and presence of PAIM ($2 \times 10^{-4} \text{ mol L}^{-1}$) at water and pH 3 ($\lambda_{\text{exc}} = 334 \text{ nm}$). [Pyrene] = $5 \times 10^{-7} \text{ mol L}^{-1}$.

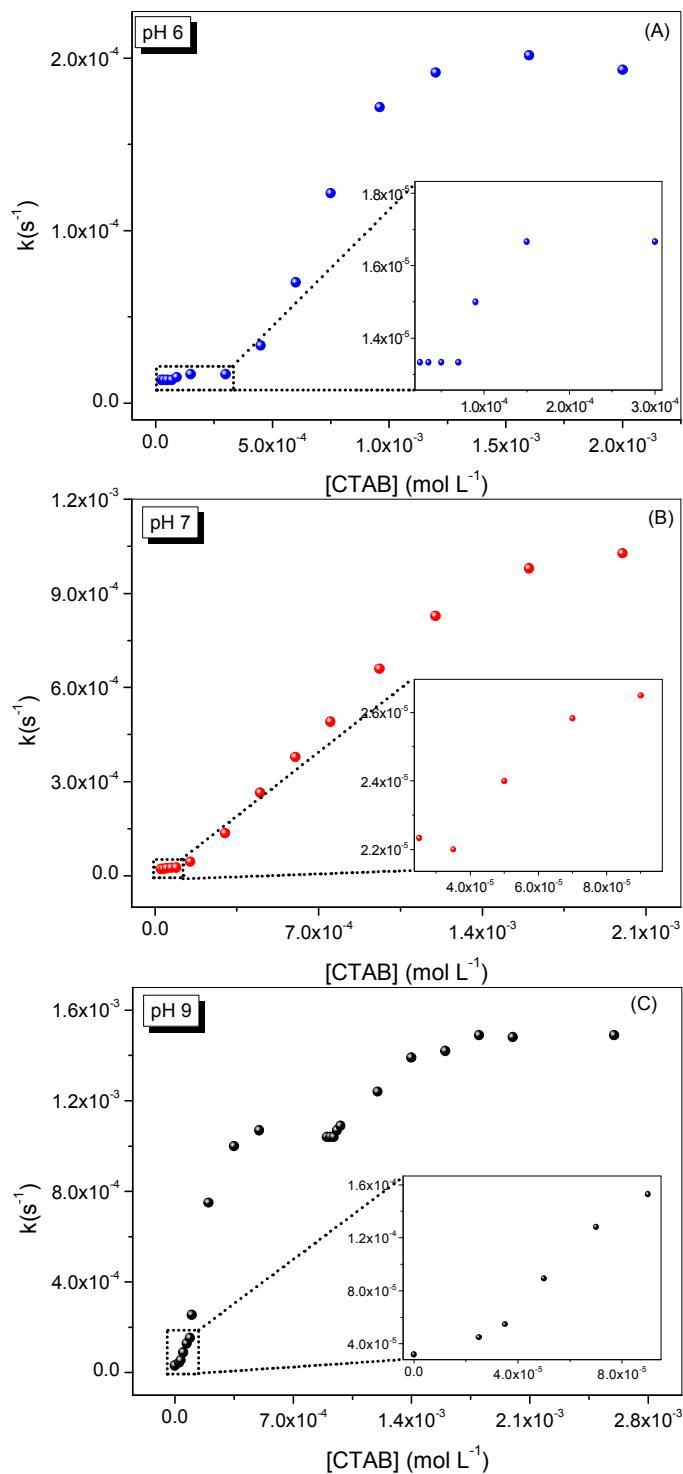


Figure S8. Rate constants for the dephosphorylation of DEDNPP (5.0×10^{-5} mol L $^{-1}$) in aqueous solutions in the presence of PAIM (2.0×10^{-4} mol L $^{-1}$) as a function of [CTAB] at (A) pH 6, (B) pH 7 and (C) pH 9, at 25.0 °C.

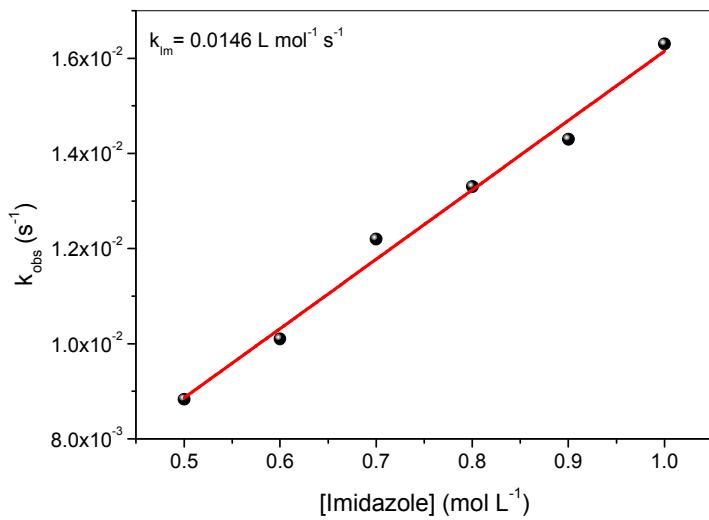


Figure S9. Rate constants for the dephosphorylation of DEDNPP (5.0×10^{-5} mol L⁻¹) in aqueous solutions as a function of [Imidazole] at 25.0 °C.

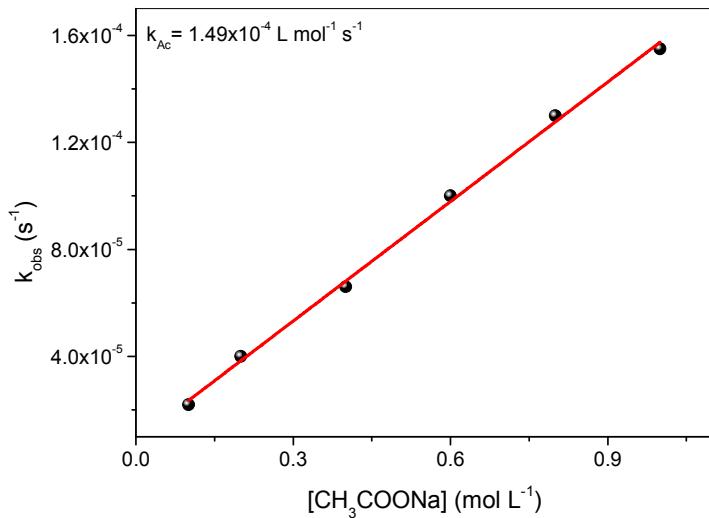


Figure S10. Rate constants for the dephosphorylation of DEDNPP (5.0×10^{-5} mol L⁻¹) in aqueous solutions as a function of [CH₃COONa] at 25.0 °C.

Treatment of the Binding isotherms of CTAB to PAIM

The binding constants (K) of CTAB with PAIM were evaluated by Pyrene I_1/I_{III} intensity ratio at pH 3, 6 and 9 ($\lambda_{exc} = 334$ nm, [Pyrene] = 5×10^{-7} mol L $^{-1}$. [PAIM] = 2×10^{-4} mol L $^{-1}$). The experimental data were theoretically fitted using equation S1:

$$IR = \frac{IR_0 + IR_m K[CTAB]}{1 + K[CTAB]}$$

where IR is the Pyrene I_1/I_{III} intensity ratio, IR_m is the intensity ratio of PAIM bound to the surfactant, IR_0 is the intensity ratio of unbound PAIM, K is the binding constant and [CTAB] is the surfactant concentration.