

Electronic Supplementary Material

Metal complexation chemistry used for phosphate and nucleotide determination: an investigation of the Yb^{3+} -pyrocatechol violet sensor

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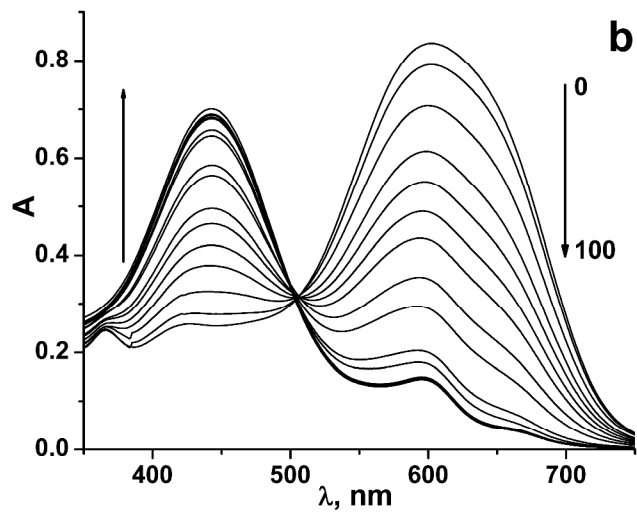
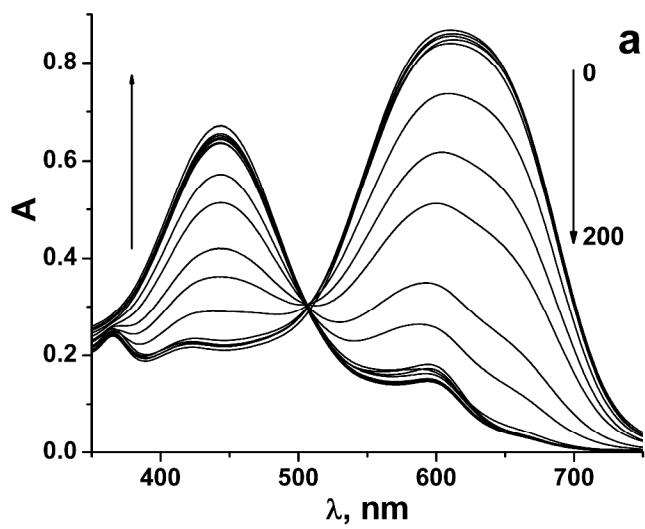


Figure S1. The absorbance spectra upon addition of ATP to the 100 μM Yb^{3+} and 50 μM PV solution (a) and to the 50 μM Yb^{3+} and 50 μM PV solution (b) in 10 mM HEPES buffer (pH 7.0). ATP concentration range (in μM) is shown next to the spectra.

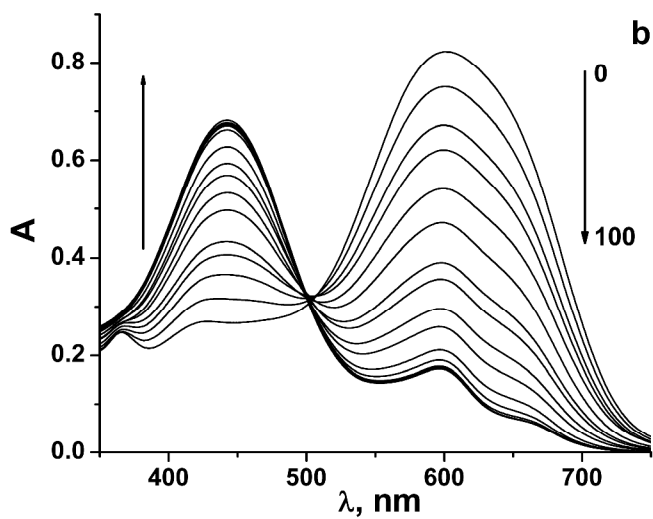
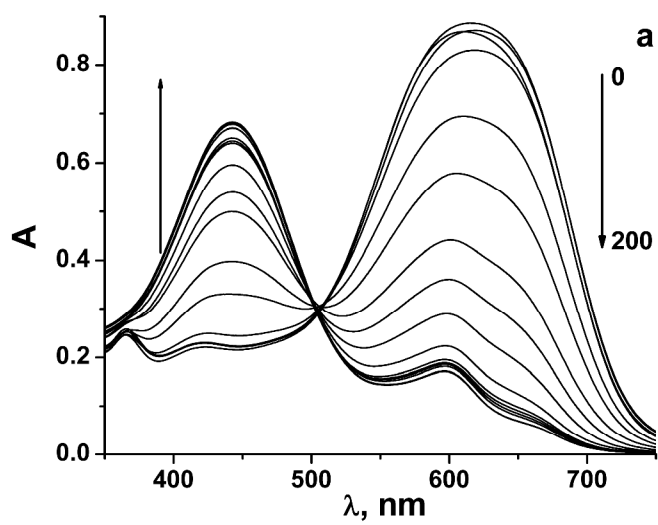


Figure S2. The absorbance spectra upon addition of P_i to the 100 μM Yb^{3+} and 50 μM PV solution (a) and to the 50 μM Yb^{3+} and 50 μM PV solution (b) in 10 mM HEPES buffer (pH 7.0). P_i concentration range (in μM) is shown next to the spectra.

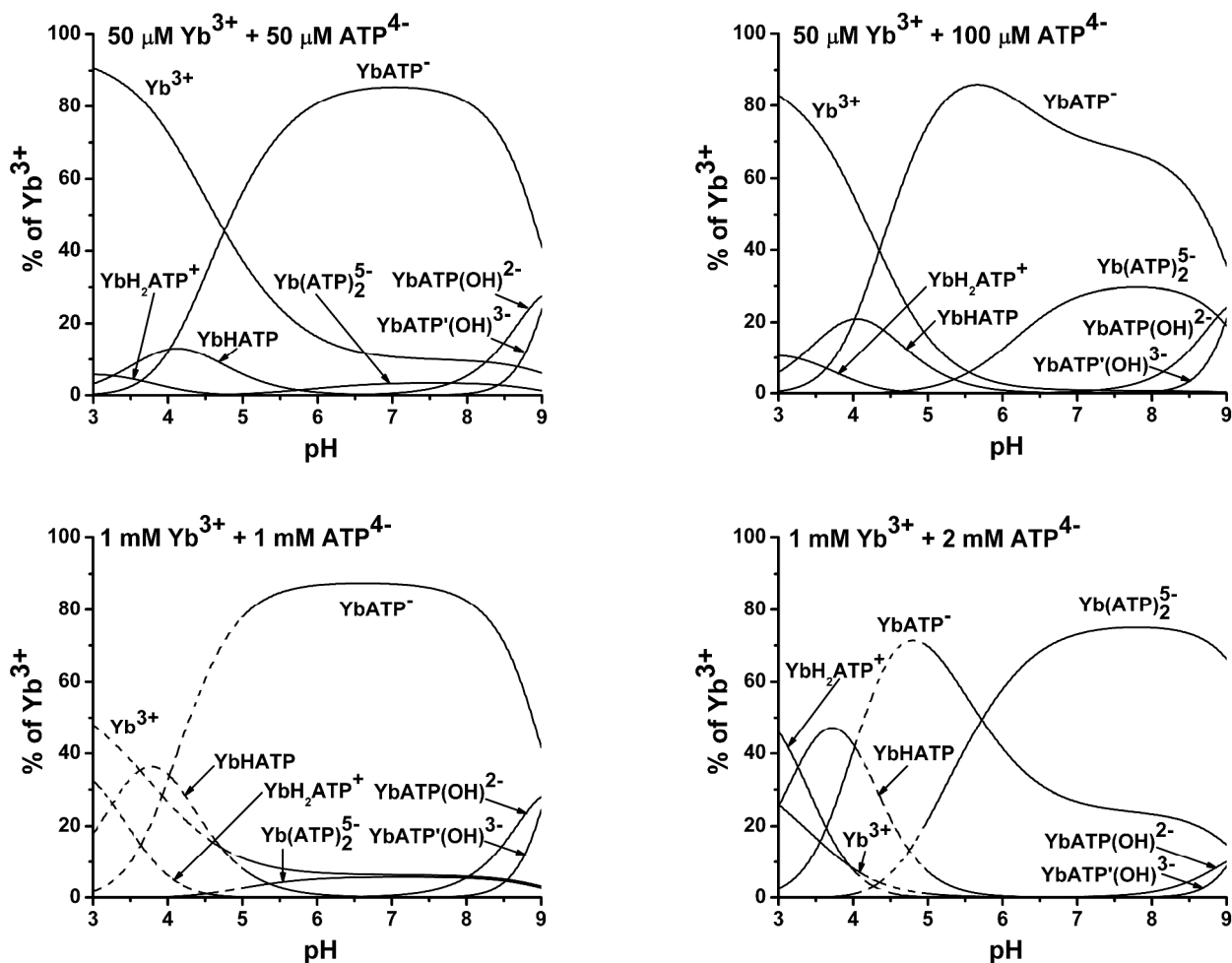


Figure. S3. Speciation diagrams for solutions of Yb³⁺ and ATP in 0.1 M KCl. The data used were derived from Ref. [28]: ATPH³⁻ (log β₀₁₁ = 6.47), ATPH₂²⁻ (log β₀₁₂ = 10.47), ATPH₃⁻ (log β₀₁₃ = 12.64), ATPH₄ (log β₀₁₄ = 14.69) ATP'H₁ (log β₀₁₋₁ = -11.78), YbATP⁻ (log β₁₁₀ = 6.44), YbATPH (log β₁₁₁ = 10.46), YbATPH₂⁺ (log β₁₁₂ = 13.72), YbATP(OH)₂²⁻ (log β₁₁₋₁ = -2.73), YbATP'(OH)₃³⁻ (log β₁₁₋₂ = -11.79), YbATP₂⁵⁻ (log β₁₂₀ = 10.56). Dashed lines indicate conditions where precipitates may form.

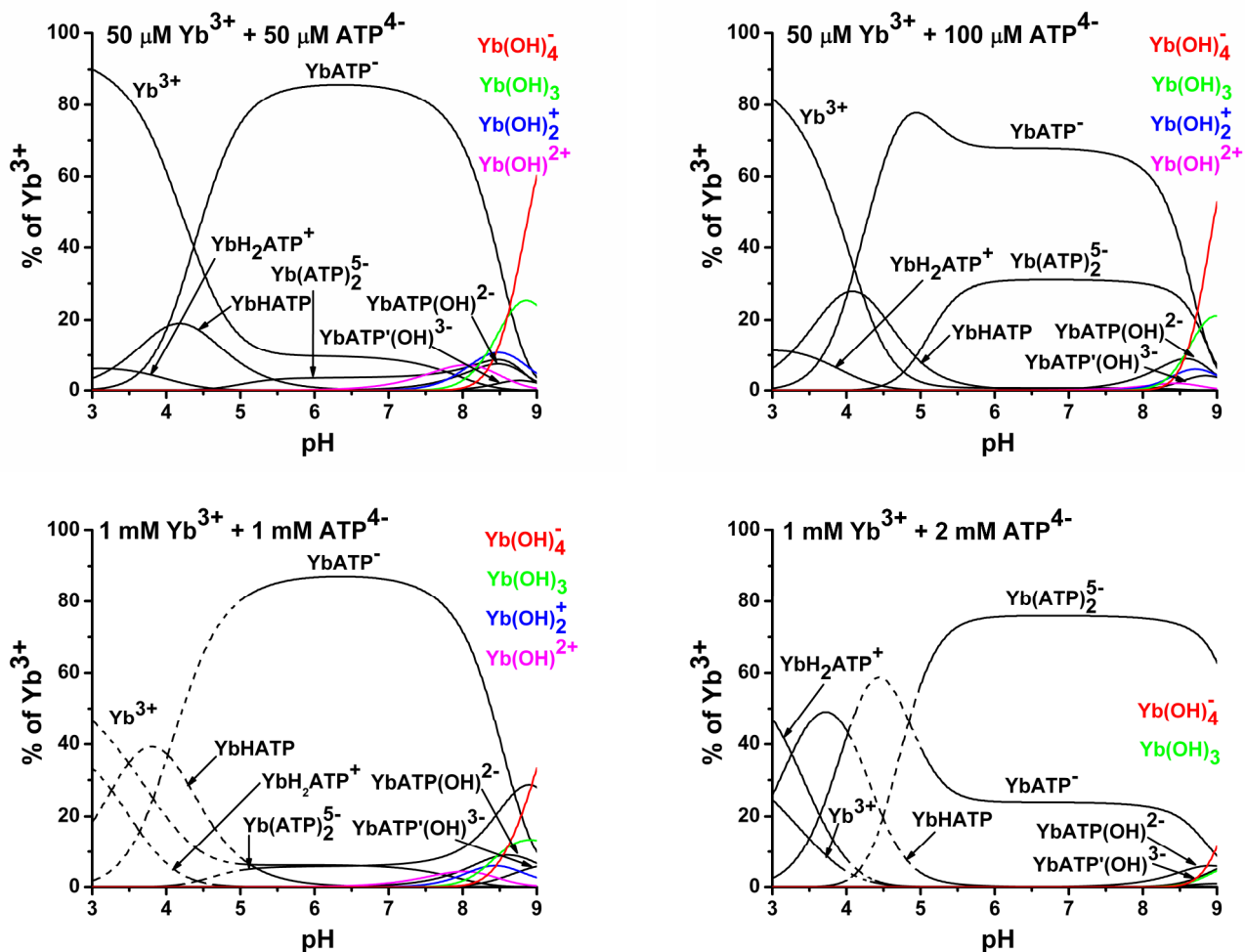


Figure. S4. Speciation diagrams for solutions of Yb^{3+} and ATP^{4-} . The data used were derived from Ref. [28]: ATPH^{3-} ($\log \beta_{011} = 6.47$), ATPH_2^{2-} ($\log \beta_{012} = 10.47$), ATPH_3^{-} ($\log \beta_{013} = 12.64$), ATPH_4 ($\log \beta_{014} = 14.69$) $\text{ATP}'\text{H}_1$ ($\log \beta_{01-1} = -11.78$), YbATP^{-} ($\log \beta_{110} = 6.44$), YbATPH ($\log \beta_{111} = 10.46$), YbATPH_2^{+} ($\log \beta_{112} = 13.72$), YbATP(OH)^{2-} ($\log \beta_{11-1} = -2.73$), YbATP'(OH)^{3-} ($\log \beta_{11-2} = -11.79$), YbATP_2^{5-} ($\log \beta_{120} = 10.56$). Yb^{3+} hydrolysis species formation constants were taken from Ref. [50]: Yb(OH)^{2+} ($\log \beta_{10-1} = -7.7$), Yb(OH)_2^{+} ($\log \beta_{10-2} = -15.8$), Yb(OH)_3 ($\log \beta_{10-3} = -24.1$), and Yb(OH)_4^{-} ($\log \beta_{10-4} = -32.7$). Dashed lines indicate conditions where precipitates may form.