

Binding of inorganic cations by *p*-sulfonatocalix[4]arene monitored through competitive fluorophore displacement in aqueous solution

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Experimental Details

DBO was synthesized according to a literature procedure.¹ CX4 (>97%) and metal salts (>99%) were purchased from Fluka and used as received; chloride salts were arbitrarily selected, since anions were shown not to affect the complexation process.^{2,3} All experiments were performed at ambient temperature in D₂O (99.8%, Omnilab). The pD values of the solutions were adjusted by addition of NaOD. pH readings were taken with a WTW 330i pH meter with a combined pH glass electrode (SenTix Mic) and converted to pD (+ 0.40 units).⁴ The corrected steady-state fluorescence spectra ($\lambda_{\text{exc}} = 365 \text{ nm}$) were measured with a Varian Cary Eclipse fluorimeter.

The fitting according to the competitive complexation scheme has been described previously.⁵ The moderate binding constants of DBO (4700 M^{-1} at pD 2.4 and 1200 M^{-1} at pD 7.4)⁵ are ideally suited to quantify also weak binding phenomena. Note that in a competitive binding scheme, to reach 50% displacement of the probe, the product of binding constant and concentration of the competitor must match the value of the same product for the probe; a too large binding constant of the probe, at constant probe concentration, would therefore need to be balanced by exceedingly large metal ion concentrations, *if* the binding of the cation is weak.

References

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