

COMPARISON OF NMR AND ISOTHERMAL TITRATION CALORIMETRY ON ENTHALPY DETERMINATION OF CATION-RECEPTOR BINDING

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Studying the thermodynamic parameters- enthalpy, entropy and Gibbs free energy – of receptor-guest binding reactions gives important information about the binding process. The determination of these parameters is commonly carried out using the isothermal titration calorimetric method (ITC) [1]. An alternative method to this determination is using NMR analysis with van't Hoff equation [2]. However, this alternative method has previously been characterized in literature as “less reliable” [3], at the same time, no clear reasons have been stated.

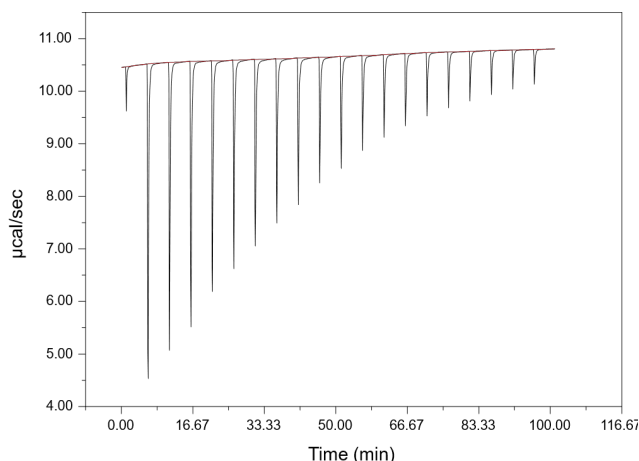


Fig.1 Example of an ITC experiment- 0.01M 18-crown-6 titration with 0.1M BaCl₂

In this work, comparison experiments with 18-crown-6-ether binding a number of alkali and alkaline-earth metal cations (K^+ , Na^+ , Ca^{2+} , Ba^{2+} , Sr^{2+}) in water were carried out with ITC and NMR. Results obtained with both methods are compared with literature data and a detailed analysis is made to determine the possible shortcomings of the NMR method with van't Hoff data treatment.

References

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