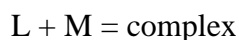


Determination of stability constants from the UV data

Spectrophotometric titration data and nonlinear regression analysis were used to determine the binding constants (K) of the complexes. This procedure was described in details elsewhere⁵³.

In the case of **1b** binding of Mg²⁺ and Ba²⁺ cations the scheme of complexation is



Eqn (1) was used to determine the binding constant (K) and molar absorptivity of the complex (ϵ_{comp}). It was used as the input for a user-defined function in the nonlinear fitting function of Origin, which will then determine the values of K and ϵ_{comp} from the best-fit curve. The procedure was carried out at 2 different wavelengths.

$$A = \frac{C_L}{2 - (1 - KC_M + KC_L) + \sqrt{4KC_M + (1 - KC_M + KC_L)^2}} \times$$

$$\times (2\epsilon_L + \epsilon_{\text{comp}} \times (- (1 - KC_M + KC_L) + \sqrt{4KC_M + (1 - KC_M + KC_L)^2})) \quad (1)$$

where A – optical density (cuvette – 1 cm), C_M and C_L – [M]₀ and [L]₀ correspondingly.
 Model Func_binding_11 (User)

Complexation **1b**-Mg²⁺

