E2-06 Chemical speciation - a new approach to titrimetric analysis

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Chemical speciation, i.e. the oxidation state, concentration and composition of each species present in a chemical mixture, is pivotal to any titrimetric procedure. Computer speciation modelling has obvious advantages in understanding chemical titrations.

This work shows how chemical speciation can be used to understand the chemistry behind titrimetric analysis and how speciation modelling* can be used as a quick and easy method of monitoring changes in experimental conditions. (*Equilibrium simulation program, MINTEQA2, was used to perform calculations)

Determination of magnesium by EDTA titration can be done at pH 10 using Eriochrom black T as the indicator. The end point is detected by the colour change of the indicator for red to blue.

Simulation results of the above titration highlight that over the pH range 7 - 11 complexation of magnesium by EDTA and the changes in indicator speciation

are dependent on pH. At pH 7 substantial metal indicator complexation does not take place. A significant amount of blue indicator species is present before the end point and a red indicator species is present throughout. Hence the colour change at the end point is very diffuse. At pH 11 there is no significant amount of blue indicator species formed at the end point. So the colour change is not clear. Thus it shows why the quantitative determination of magnesium by EDTA titration using Eriochrom black T indicator should be done between pH 9 and 10.

The following physical constants are used in this work;
Acid dissociation constants of Eriochrom black T H_3In 1.6, H_2In 6.3, HIn^{2-} 11.6
Formation constant of Mg-EDTA: 8.69

Using computer programs it is relatively easy to calculate the chemical speciation of each step in a titration and so gain a better understanding of why a particular procedure works (or does not work).