Determination of Acivity Coefficient from Conductometry data

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Prologue

Extension of one of our practical laboratory experiments.

Some stuffs related to conductivity

- $\mathsf{C} = \frac{1}{R} = (\frac{1}{\rho})(\frac{a}{l})$
- $\Lambda = 1000\frac{\kappa}{c}$
- $\Lambda = \alpha\Lambda_o$

Some stuffs related to conductivity

- $C = \frac{1}{R} = (\frac{1}{\rho})(\frac{a}{l})$
- $\Lambda = 1000\frac{\kappa}{c}$
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- Debye Huckel Limiting Law

$$log(f_{\pm}) = -|z_+ z_-| A I^{\frac{1}{2}}$$
$$I = \frac{1}{2}\Sigma {z_i}^2 c_i$$
$$I = \frac{1}{2}(c_+ {z_+}^2 + c_- {z_-}^2)$$

- $A = \frac{F^3}{4\pi N_A ln(10)}(\frac{\rho}{2\epsilon^3 R^3 T^3})^{\frac{1}{2}}$

In the practical class:

$$CH_3COOH \rightleftharpoons CH_3COO^- + H^+$$

$$K_a = \frac{c\alpha^2}{1-\alpha}$$

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$$K_a = \frac{(\Lambda^2 c)^2}{[(\Lambda_o - \Lambda)\Lambda_o]}$$

$$\frac{1}{\Lambda} = \frac{1}{\Lambda_o} + \frac{1}{K_a {\Lambda_o}^2}\Lambda c$$

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Data of c vs κ available.

Calculate $\frac{1}{\Lambda}$ and Λc and do linear fitting.

Need for using activity coefficient

Interactions between ions are so strong that the approximation of replacing activities by concentrations is valid only in very dilute solutions, and in precise works activities themselves must be used.

Our Work:

- To calculate the value of $f_{\pm}$ instead of taking it to be 1.
- The corresponding equation is: $\frac{1}{\Lambda} = \frac{1}{\Lambda_o} + \frac{1}{K_a {\Lambda_o}^2} \Lambda c {f_{\pm}}^2$

Our Work:

- To calculate the value of $f_{\pm}$ instead of taking it to be 1.
- The corresponding equation is: $\frac{1}{\Lambda} = \frac{1}{\Lambda_o} + \frac{1}{K_a {\Lambda_o}^2} \Lambda c {f_{\pm}}^2$
- Instead of simply doing a linear fit, we implemented the following algorithm, which enabled us to get not only Λ_o and K_a but also the values of $f_{\pm}$ for different concentrations.

Our Program:

- The Algorithm
  1. Take all the values of $f_{\pm}$ to be 1 initially.
  2. Arbitrarily fix the initial values of Λ_o and K_a to 0.
  3. Calculate an array of values of $\frac{1}{\Lambda}$ and $\Lambda c {f_{\pm}}^2$ using experimental data and current values of $f_{\pm}$.

Our Program:

- The Algorithm
  1. Take all the values of $f_\pm$ to be 1 initially.
  2. Arbitrarily fix the initial values of Λ_o and K_a to 0.
  3. Calculate an array of values of $\frac{1}{\Lambda}$ and $\Lambda c {f_\pm}^2$ using experimental data and current values of $f_\pm$.
  4. Fit the calculated values to $\frac{1}{\Lambda} = \frac{1}{\Lambda_o} + \frac{1}{K_a {\Lambda_o}^2} \Lambda c {f_\pm}^2$.
  5. Determine the values of Λ_o and K_a.
  6. Calculate values of $f_\pm$ using the formula $f_\pm = -A\sqrt{\frac{\Lambda c}{\Lambda_o}}$.
  7. If(Old and new constants differ by more than 0.0001 %) then (goback to 3) else (continue).
  8. Plot the final values of $log(f_\pm) vs \sqrt{\mu}$.

Results:

- Values obtained by considering $f_{\pm} = 1$:

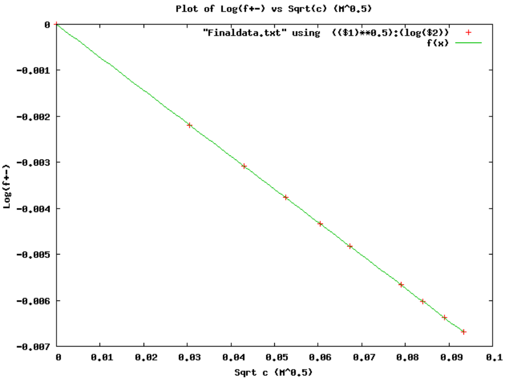
$$K_a = 8.67 * 10^{-5}$$
$$\Lambda_o = 196.46 \ SM^{-1}$$

- Values obtained by using our program:

$$K_a = 7.8 * 10^{-5}$$
$$\Lambda_o = 204.46 \ SM^{-1}$$

Some more results:

Graph obtained by taking $f_{\pm} = 1$



Conclusion

- Obtained $f_{\pm}$ values for different concentrations of acetic acid.
- Obtained the values of Λ_o and K_a.

Acknowledgment

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THANK YOU