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FitAll

nonlinear regression analysis

Chemistry Functions Guide

MTR

SOFTWARE

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Contents

Introduction

This ***FitAll***™ **Chemistry Functions Guide** describes the functions contained in the **Chemistry Functions Library** and has an appendix that explains how to get help from ***MTR* Software**.

Function Reference 2

Appendix 150

Function Reference Overview

This section describes each of the functions in ***FitAll***'s Chemistry Functions Library.

In most cases, a graph of the function is shown. These graphs were created using "typical" parameter and constant values.

The actual appearance of a function depends on the parameter and constant values and may look quite different from the illustrations shown.

Equation

Gives the equation and its variations. The variations are listed in order of increasing complexity.

Constants

Lists the constants, K, that are used in the function. The default values for the constants also are given.

Parameters

Lists the parameters, P, that are used in the function.

Multi-Fits

Describes the Multi-Fit functionality of "Multi-Fit enabled" functions.

Sample Applications

Gives examples of some situations in which the function is known to be used.

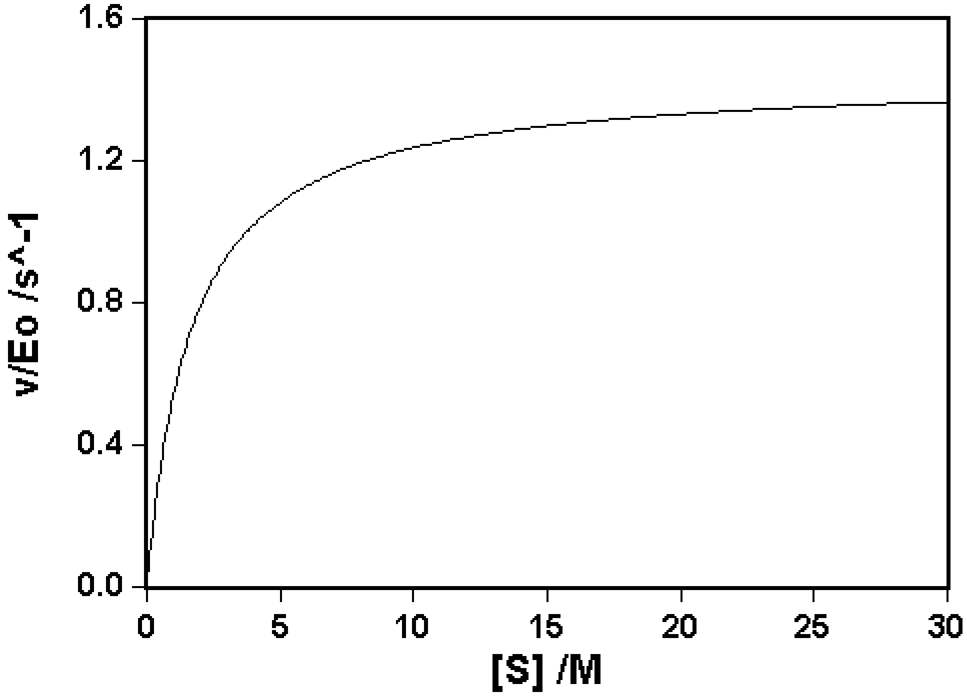
Remarks

Provides general comments and hints, and lists any known limitations or restrictions that should be observed when using the function.

Also see

Provides links or references to other related functions.

Ftn 0401: Michaelis-Menton Kinetics



Equation

Three variations of the function are available. For example:

- $$Y = \frac{P1 * X}{(P2 + X)}$$
- $$Y = \frac{P1 * X}{(P2 + X)} + \frac{P3 * X}{(P4 + X)}$$
- $$Y = \frac{P1 * X}{(P2 + X)} + \frac{P3 * X}{(P4 + X)} + \frac{P5 * X}{(P6 + X)}$$

in which

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Parameters

Parameter	**Name**	**Comments**
P1	k2	First order rate constant for the conversion of the enzyme-substrate complex, ES, of the first enzyme or isozyme to products.
P2	Km	Michaelis constant for the first enzyme (or isozyme).
P3	k2b	First order rate constant for the conversion of the enzyme-substrate complex, ES, of the second enzyme or isozyme to products.
P4	Kmb	Michaelis constant for the second enzyme (or isozyme).
P5	k2c	First order rate constant for the conversion of the enzyme-substrate complex, ES, of the third enzyme or isozyme to products.
P6	Kmc	Michaelis constant for the third enzyme (or isozyme).

Sample Applications

- Fitting initial rate data for the enzyme catalyzed conversion of a substrate, S, to a product, P

  For one enzyme, the reaction scheme (mechanism) is:

  $$E + S \underset{k_{1r}}{\overset{k_{1f}}{=}} ES \xrightarrow{k_{2f}} E + P$$

  , and

  $K_M = \frac{(k_{1r} + k_{2f})}{k_{1f}}$, $k_2 = k_{2f}$, Y = v/Eo, X = [S], Eo is the initial (total) enzyme concentration (in moles/L) and v is the initial rate of product formation (in moles/L/s).

- When more then one enzyme (or isozyme) is present, the second and / or third variations of this function can be used.

- Binding of a ligand or substrate to a metal or receptor.

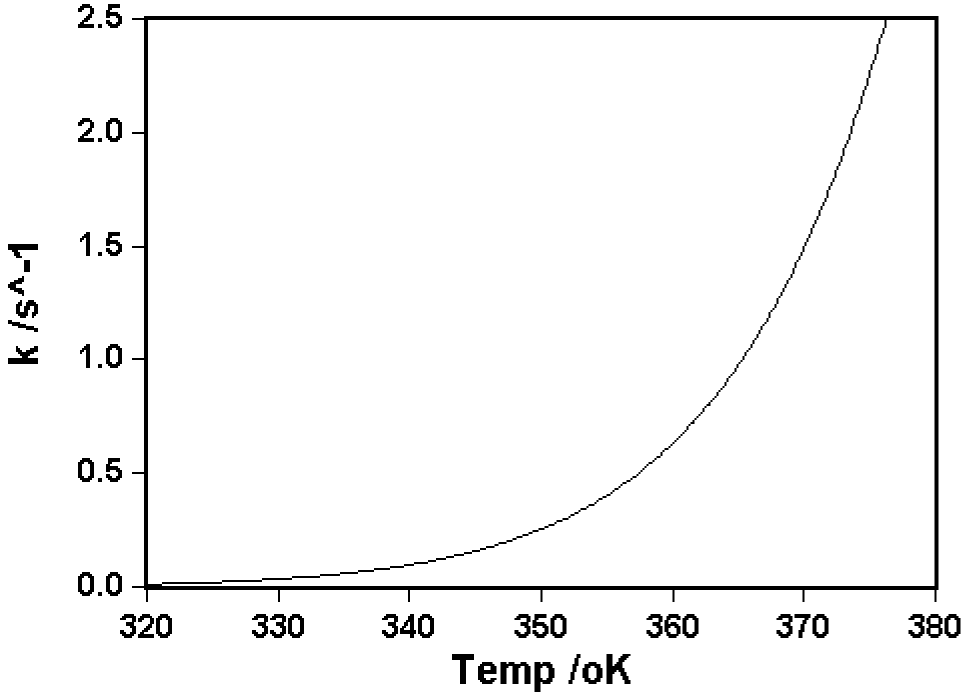
Remarks

This function is very similar to the saturation curve described by function 0205 in the **Binding Curves *FitAll* Function Library**. The only difference is that the parameters are defined in a slightly different way.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Frequently, the best fitting strategy is to fit your data, or a segment of it, to one Michaelis-Menton curve before attempting fits with the more complicated forms of this function.

Ftn 0402: Arrhenius Activation Energy



Equation

$$Y = P1 * e^{\left[\frac{-P2}{(K1*X)}\right]}$$

in which

- Y is the measured response, usually the rate constant
- X is the independent variable, the temperature in ºK.

Constants

Constant	**Name**	**Comments**
K1	R	Universal Gas Constant, R = 8.3143 J/ºK/mole or R = 1.986 cal/ºK/mole The default value is 8.3143.

Parameters

Parameter	**Name**	**Comments**
P1	A	Arrhenius pre-exponential factor.
P2	Ea	Arrhenius activation energy.

Sample Applications

- Determining the Arrhenius activation energy, Ea, from the temperature dependence, X = temperature in ^oK, of the rate constant, Y in s^{-1}.

- Determining the activation energy from the temperature dependence of the rate of a crystallization process.

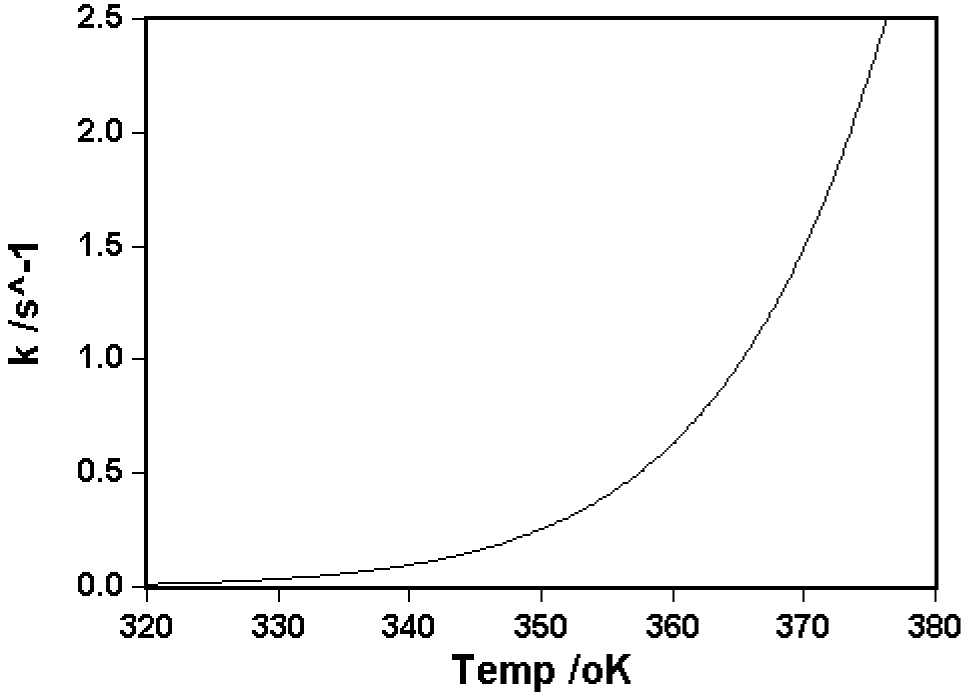
- Determining the band-gap energy of a semi-conductor from the temperature dependence of the electrical resistivity.

Remarks

Arrhenius activation energy is applicable only over very limited temperature ranges as Ea is also temperature dependent. A better fit of the temperature dependence of a chemical reaction's rate constant usually can be obtained using the equation derived from Absolute Rate Theory, function 0403 8, to obtain the activation enthalpy, $dH^{\#}$, and activation entropy, $dS^{\#}$.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0403: Activation Enthalpy and Entropy



Equation

$$Y = K1 * X * e^{\left[\frac{-P1}{(K2 * X)} + \frac{P2}{K2}\right]}$$

in which

- Y is the measured response, usually the rate constant.
- X is the independent variable, the temperature in degrees K.

Constants

Constant	**Name**	**Comments**
K1	k/h	Ratio: Boltzmann's Constant / Plank's Constant = 2.0842 x 10^{42}/ºK/s.
K2	R	Universal Gas Constant, R = 8.3143 J/ºK/mole or R = 1.986 cal/ºK/mole. The default value is 8.3143.

Parameters

Parameter	Name	Comments
P1		Activation Enthalpy
P2		Activation Entropy

Sample Applications

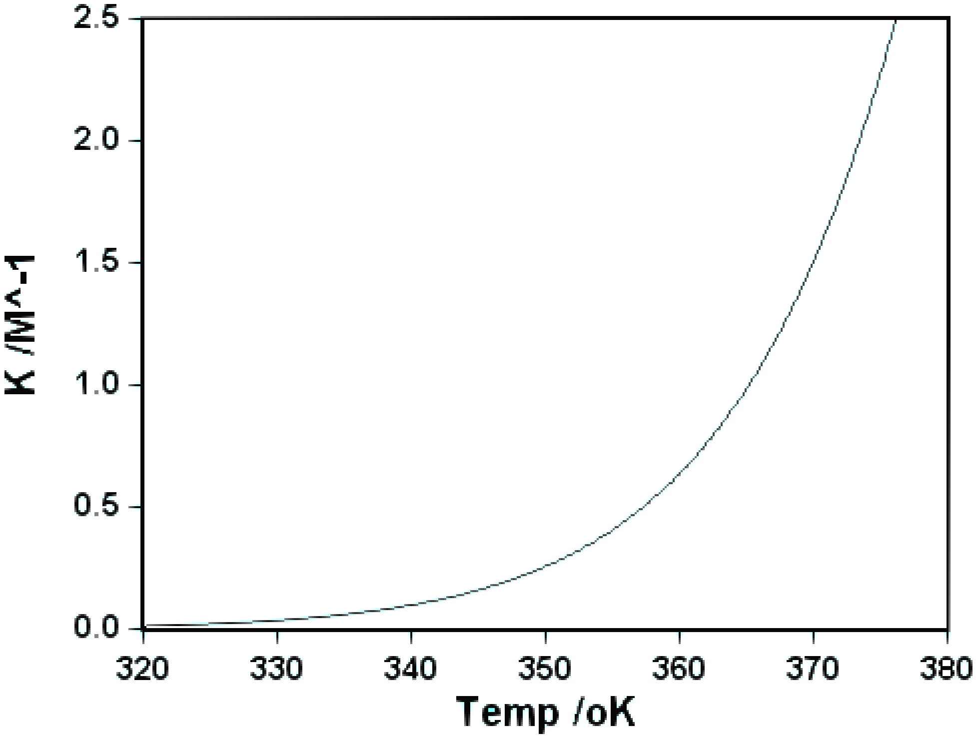
- Determining the activation parameters from the temperature dependence of a first order rate constant; that is, Y is the observed rate constant in s^{-1} and X is the temperature in ºK.

Remarks

The choice of value for K2, = R, determines whether the activation enthalpy, dHº, will have units of cal/mole or Joules/mole.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0404: Equilibrium Enthalpy and Entropy



Equation

$$Y = e^{\left[\frac{-P1}{(K1 * X)} + \frac{P2}{K1}\right]}$$

in which

- Y is the measured response.
- X is the independent variable, the temperature in degrees K.

Constants

Constant	**Name**	**Comments**
K1	R	Universal Gas Constant, R = 8.3143 J/ºK/mole or R = 1.986 cal/ºK/mole. The default value is 8.3143.

Parameters

Parameter	Name	Comments
P1	dH	Equilibrium Enthalpy
P2	dS	Equilibrium Entropy

Sample Applications

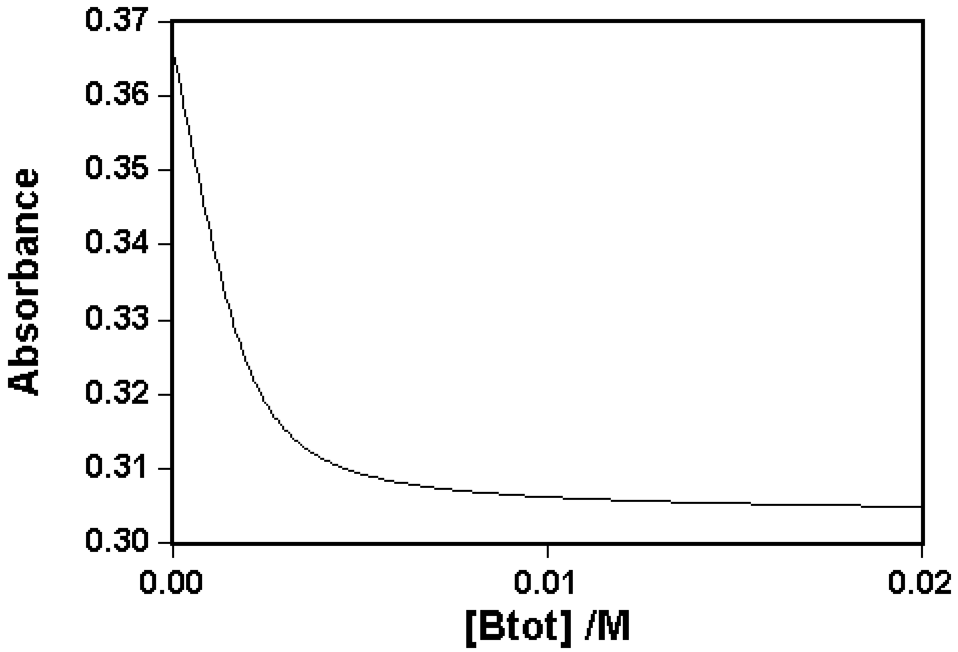
- Determining the Enthalpy, dH, and Entropy, dS, from the temperature dependence of an equilibrium or stability constant.

Remarks

The choice of value for K1, = R, determines whether the enthalpy, dH, will have units of cal/mole or Joules/mole.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0405: Reversible Chemical Equilibrium_1: A + B = C, X1 = Btot, K1 = Atot



Equation

Three variations of the function are available:

- $$Y = P3 * K1 + P4 * X1 + (P2 - P3 - P4) * \left\{ \frac{P1 * (K1 + X1) + 1 - \sqrt{\left(\left[P1 * (K1 + X1) + 1 \right]^2 - 4 * P1^2 * K1 * X1 \right)}}{2 * P1} \right\}$$
- $$Y = P3 * K1 + (P2 - P3) * \left\{ \frac{P1 * (K1 + X1) + 1 - \sqrt{\left(\left[P1 * (K1 + X1) + 1 \right]^2 - 4 * P1^2 * K1 * X1 \right)}}{2 * P1} \right\}$$
- $$Y = P2 * \left\{ \frac{P1 * (K1 + X1) + 1 - \sqrt{\left(\left[P1 * (K1 + X1) + 1 \right]^2 - 4 * P1^2 * K1 * X1 \right)}}{2 * P1} \right\}$$

in which

- Y is the measured response.

- X1 is the total concentration of B, [Btot].

Constants

Constant	Name	Comments
K1	[Atot]	Total (constant) concentration of component A.

Parameters

Parameter	Name	Comments
P1	Q	Equilibrium (association or formation) quotient (constant) defined as: Q = [C]/([A]*[B]).
P2	Rc	Specific response factor for C; for example, the extinction coefficient, absorbtivity, or specific conductivity of C. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to C, Yc, is given by: Yc = Rc * [C].
P3	Ra	Specific response factor for substance A. In the third variation of this function it is assumed that Ra = 0.
P4	Rb	Specific response factor for substance B. In the second and third variations of this function it is assumed that Rb = 0.

Sample Applications

- Determining the equilibrium (stability or formation) constant for binding of a ligand or substrate to a metal ion or an enzyme.

Remarks

Alternate ways of expressing the same type of chemical reaction are:

- A + B = AB

- M + L = ML

- E + S = ES

This function was derived assuming that:

- The total concentration of A, [Atot], is the same (constant) for all data points. If this is not the case, see function 0406 15.

- Initially no C is present. That is, all of the reaction product, C, is derived from the substances A and B that are admixed.

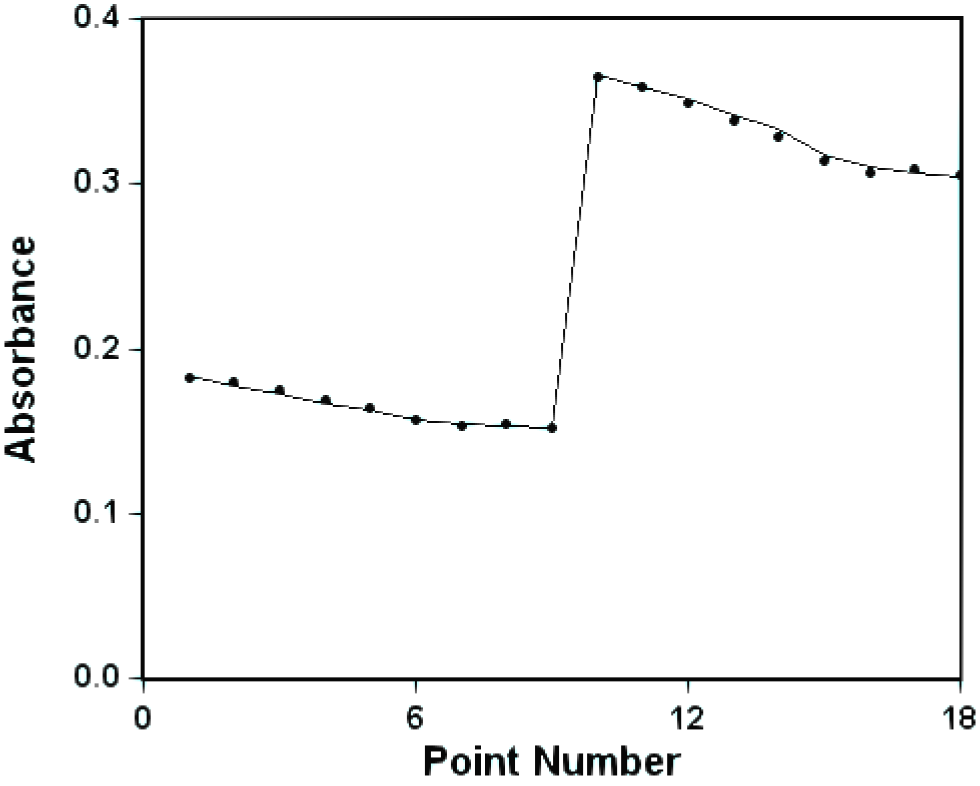
- The total concentrations of A and B may be of similar magnitude. That is, under some conditions the reaction of A with B may consume a significant amount of B.

- If the concentration of B is always much larger than that of A, [Btot] >> [Atot], the function can be simplified and closely approximated by a simpler saturation curve, see functions 0203 and 0206 in the **Binding Curves *FitAll* Function Library**.

- The reaction is reversible and its stoichiometry is 1:1:1.

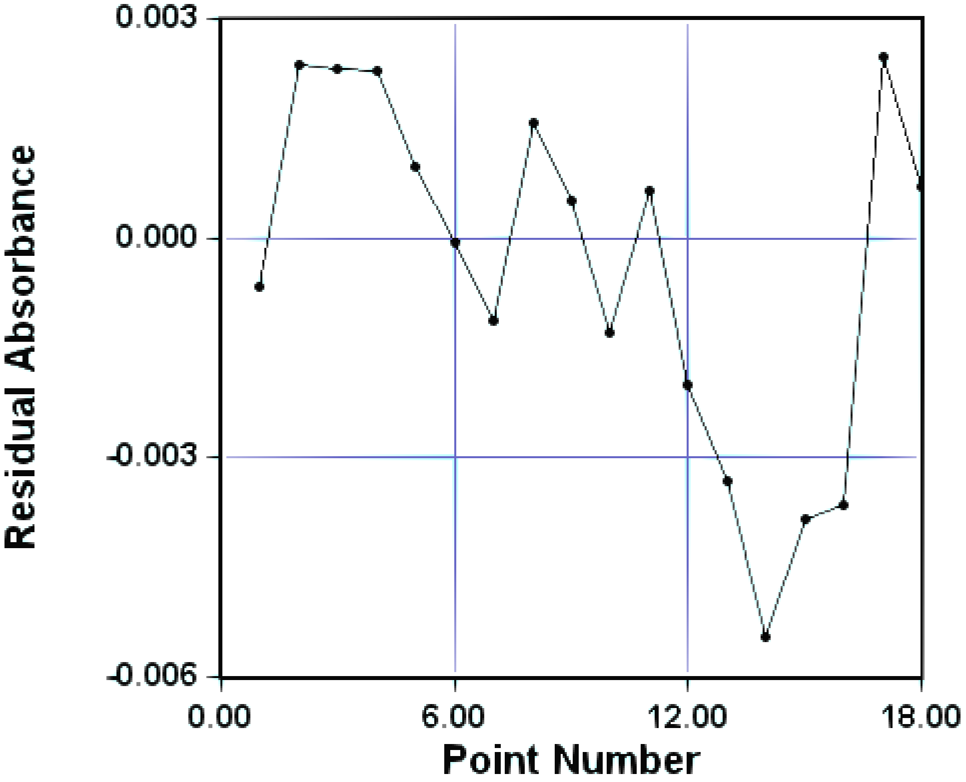
When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0406: Reversible Chemical Equilibrium_2: A + B = C, X1 = Btot, X2 = Atot



NOTE:
This function has two independent variables, Atot (X2) and Btot (X1). The only way to plot a meaningful fit graph in this situation is to plot Y versus the "Point Number" rather than the value of the independent variable, X.

The best way to get a visual indication of the quality of the fit is to view the residuals graph, such as the one shown below.



Equation

Three variations of the function are available:

- $$Y = P3 * X2 + P4 * X1 + (P2 - P3 - P4) * \left\{ \frac{P1 * (X2 + X1) + 1 - \sqrt{\left(\left[P1 * (X2 + X1) + 1\right]^2 - 4 * P1^2 * X2 * X1\right)}}{2 * P1} \right\}$$
- $$Y = P3 * X2 + (P2 - P3) * \left\{ \frac{P1 * (X2 + X1) + 1 - \sqrt{\left(\left[P1 * (X2 + X1) + 1\right]^2 - 4 * P1^2 * X2 * X1\right)}}{2 * P1} \right\}$$
- $$Y = P2 * \left\{ \frac{P1 * (X2 + X1) + 1 - \sqrt{\left(\left[P1 * (X2 + X1) + 1\right]^2 - 4 * P1^2 * X2 * X1\right)}}{2 * P1} \right\}$$

in which

- Y is the measured response.
- X1 is the total concentration of B, [Btot].
- X2 is the total concentration of A, [Atot].

Parameters

Parameter	**Name**	**Comments**
P1	Q	Equilibrium (association or formation) quotient (constant) defined as: Q = [C]/([A]*[B]).
P2	Rc	Specific response factor for C; for example, the extinction coefficient, absorbtivity, or specific conductivity of C. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to C, Yc, is given by: Yc = Rc * [C].
P3	Ra	Specific response factor for substance A. In the third variation of this function it is assumed that Ra = 0.
P4	Rb	Specific response factor for substance B. In the second and third variations of this function it is assumed that Rb = 0.

Sample Applications

- Determining the equilibrium (stability or formation) constant for binding of a ligand or substrate to a metal ion or an enzyme.

Remarks

Alternate ways of expressing the same type of chemical reaction are:

- A + B = AB
- M + L = ML
- E + S = ES

This function was derived assuming that:

- Initially no C is present. That is, all of the reaction product, C, is derived from the substances A and B that are admixed.

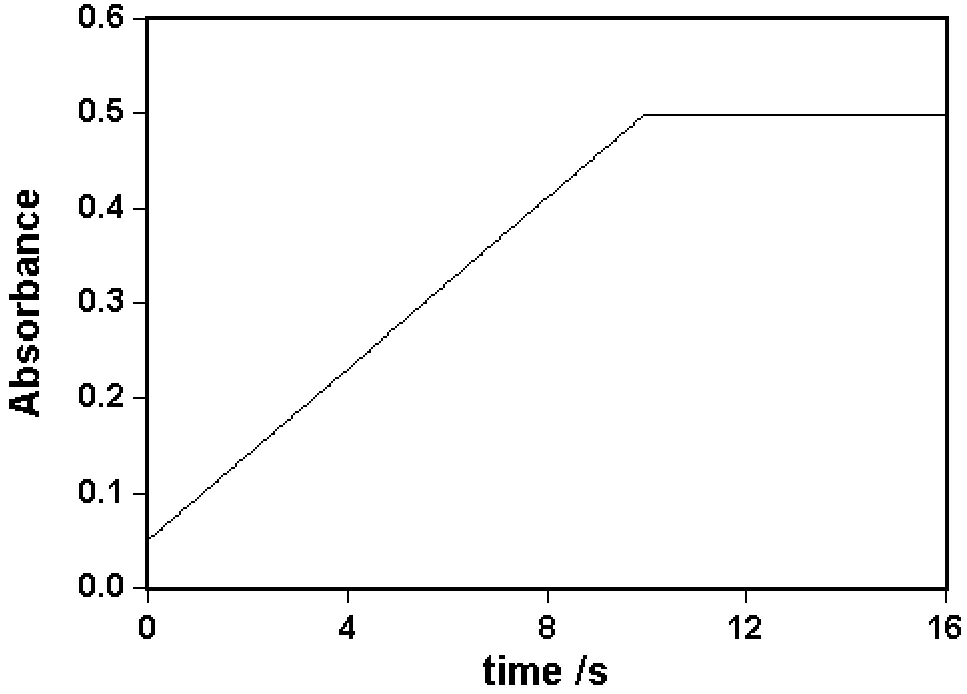
- The total concentrations of A and B may be of similar magnitude. That is, under some conditions the reaction of A with B may consume a significant amount of B.

- The reaction is reversible and its stoichiometry is 1:1:1.

Because this function has two independent variables, X1 and X2, there is no convenient way for ***FitAll*** to automatically calculate the initial parameter estimates.

In some cases, you can obtain these estimates by fitting part of the data to function 0405 12. When you do this, choose an analysis range over which the X2-values are (reasonably) constant and assign K1 a value equal to the average of these X2-values.

Ftn 0407: Chemical Kinetics: Zero-Order Rxn: A -> B, -dA/dt = k



Equation

Two variations of the function are available:

- $$Y = \begin{cases} P2 * K1, & \text{for } X < 0 \\ P2 * K1 + (P3 - P2) * P1 * X, & \text{for } 0 \le X \le \dfrac{K1}{P1} \\ P3 * K1, & \text{for } X > \dfrac{K1}{P1} \end{cases}$$
- $$Y = \begin{cases} P2 * K1, & \text{for } X < 0 \\ P2 * (K1 - P1 * X), & \text{for } 0 \le X \le \dfrac{K1}{P1} \\ 0, & \text{for } X > \dfrac{K1}{P1} \end{cases}$$

in which

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Constants

Constant	Name	Comments
K1	Ao	Total (initial) concentration of component A. Default value is 1.0.

Parameters

Parameter	Name	Comments
P1	k	Rate constant.
P2	Ra	Specific response factor for A; for example, the extinction coefficient, absorbtivity, or specific conductivity of A. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to A, Ya, is given by: Ya = Ra * [A]. If the analysis is done using the default value of K1 (= 1.0), the resolved value of P2 corresponds to Ra*Ao.
P3	Rb	Specific response factor for substance B. If the analysis is done using the default value of K1 (= 1.0), the resolved value of P3 corresponds to Rb*Ao. In the second variation of this function it is assumed that Rb = 0.

Sample Applications

- Determining the rate constant for a zero-order decomposition of a chemical substance or enzyme.

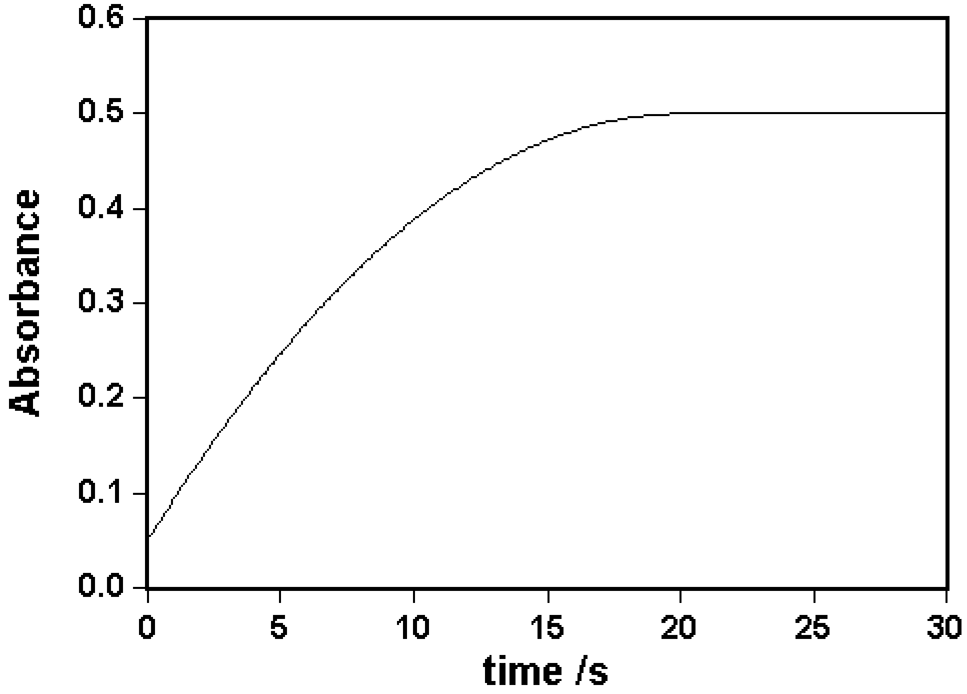
Remarks

This function was derived assuming that:

- The reaction stoichiometry is 1:1.
- Initially, no B is present. That is, all of the reaction product, B, is derived from A.
- The reaction is irreversible; that is, it goes to completion.
- The reaction rate is given by: d[A]/dt = k.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0408: Chemical Kinetics: Half-Order Rxn: A -> B, dA/dt = k*A^(1/2)



Equation

Two variations of the function are available:

- $$Y = \begin{cases} P2 * K1, & \text{for } X < 0 \\ P2 * K1 + (P3 - P2) * P1 * X * \dfrac{4 * \sqrt{K1} - P1 * X}{4}, & \text{for } 0 \le X \le \dfrac{2 * \sqrt{K1}}{P1} \\ P3 * K1, & \text{for } X > \dfrac{2 * \sqrt{K1}}{P1} \end{cases}$$
- $$Y = \begin{cases} P2 * K1, & \text{for } X < 0 \\ P2 * \left[K1 - P1 * X * \dfrac{4 * \sqrt{K1} - P1 * X}{4} \right], & \text{for } 0 \le X \le \dfrac{2 * \sqrt{K1}}{P1} \\ 0, & \text{for } X > \dfrac{2 * \sqrt{K1}}{P1} \end{cases}$$

in which

- Y is the measured response.

- X is the independent variable, often the time in seconds.

Constants

Constant	Name	Comments
K1	Ao	Total (initial) concentration of component A. Default value is 1.0. An appropriate value must be assigned to K1 if meaningful results are to be obtained.

Parameters

Parameter	Name	Comments
P1	k	Rate constant.
P2	Ra	Specific response factor for A; for example, the extinction coefficient, absorbtivity, or specific conductivity of A. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to A, Ya, is given by: Ya = Ra * [A]. If the analysis is done using the default value of K1 (= 1.0), the resolved value of P2 corresponds to Ra*Ao.
P3	Rb	Specific response factor for substance B. If the analysis is done using the default value of K1 (= 1.0), the resolved value of P3 corresponds to Rb*Ao. In the second form of this function it is assumed that Rb = 0.

Sample Applications

- Determining the rate constant for a half-order decomposition of a chemical substance or enzyme.

Remarks

This function was derived assuming that:

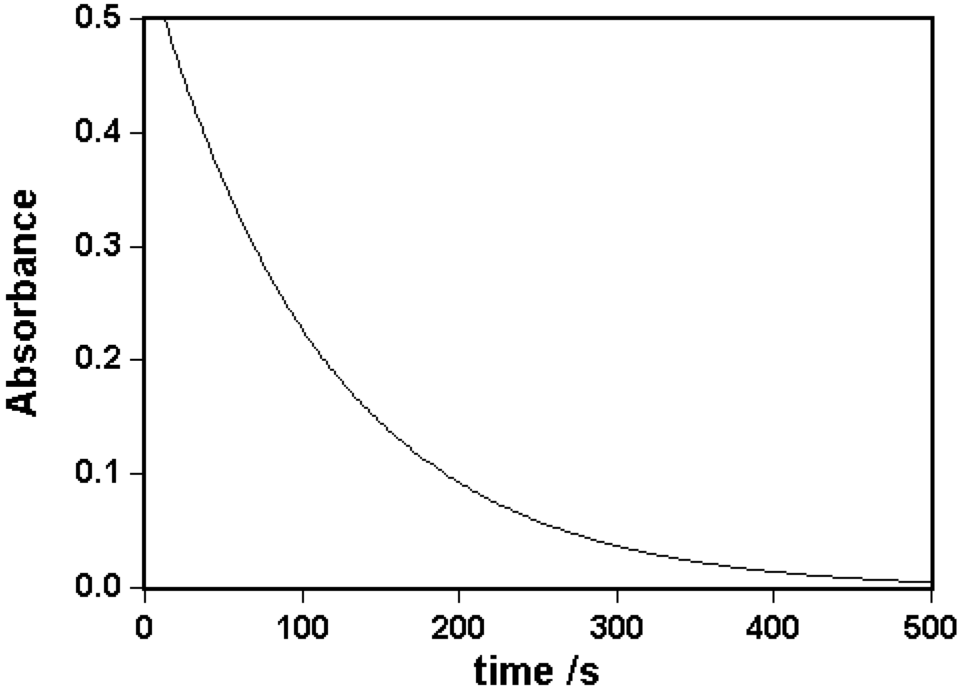
- The reaction stoichiometry is 1:1.

- Initially, no B is present. That is, all of the reaction product, B, is derived from A.

- The reaction is irreversiblereversible; that is, it goes to completion.
- The reaction rate is given by: $d[A]/dt = k^*[A]^{1/2}$.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0409: Chemical Kinetics: First-Order Rxn: A -> B, dA/dt = k*A



Equation

Two variations of the function are available:

- $Y = K1 * [P2 + (P3 - P2) * (1 - e^{-P1*X})]$
- $Y = K1 * P2 * e^{-P1*X}$

in which

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Constants

Constant	Name	Comments
K1	Ao	Total (initial) concentration of component A. Default value is 1.0.

Parameters

Parameter	Name	Comments
P1	k	Rate constant.
P2	Ra	Specific response factor for A; for example, the extinction coefficient, absorbtivity, or specific conductivity of A. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to A, Ya, is given by: Ya = Ra * [A]. If the analysis is done using the default value of K1 (= 1.0), the resolved value of P2 corresponds to Ra*Ao.
P3	Rb	Specific response factor for substance B. If the analysis is done using the default value of K1 (= 1.0), the resolved value of P3 corresponds to Rb*Ao. In the second form of this function it is assumed that Rb = 0.

Sample Applications

- Determining the rate constant for a first-order decomposition of a chemical substance or enzyme.

Remarks

This function was derived assuming that:

- The reaction stoichiometry is 1:1.

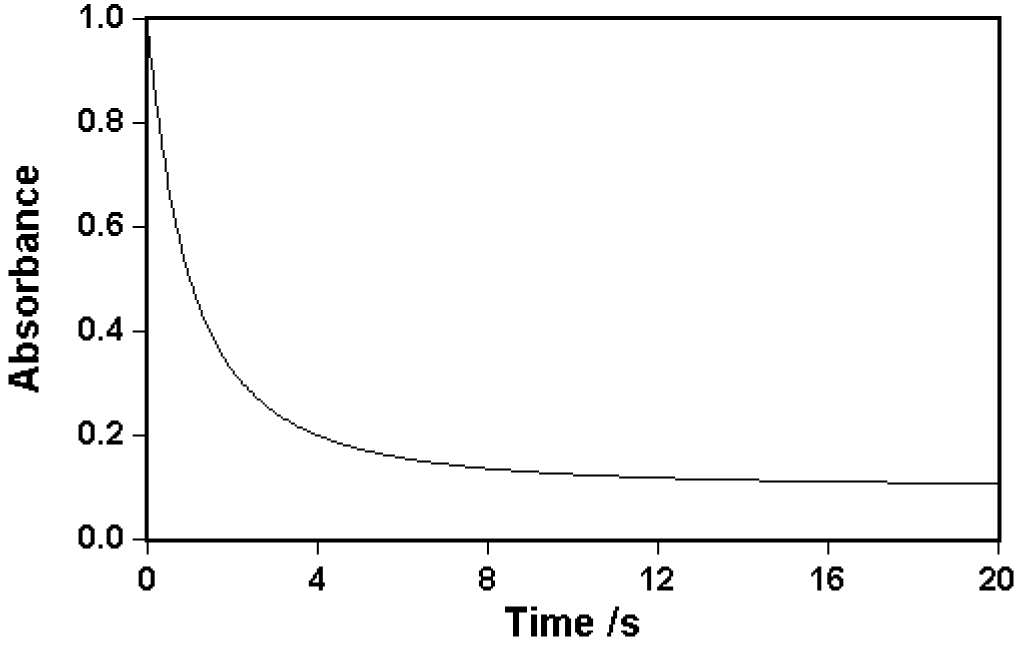
- Initially, no B is present. That is, all of the reaction product, B, is derived from A.

- The reaction is irreversiblereversible; that is, it goes to completion.

- The reaction rate is given by: d[A]/dt = k*[A].

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0410: Chemical Kinetics: (3/2)-Order Rxn: A -> B, dA/dt = k*A^(3/2)



Equation

Two variations of the function are available:

- $$Y = K1 * P2 + (P3 - P2) * K1 * \left(1 - \frac{4}{(2 + P1 * \sqrt{K1} * X)^2}\right)$$
- $$Y = K1 * P2 - P2 * K1 * \left(1 - \frac{4}{(2 + P1 * \sqrt{K1} * X)^2}\right)$$

in which

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Constants

Constant	**Name**	**Comments**
K1	Ao	Total (initial) concentration of component A. Default value is 1.0.

Parameters

Parameter	Name	Comments
P1	k	Rate constant.
P2	Ra	Specific response factor for A; for example, the extinction coefficient, absorbtivity, or specific conductivity of A. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to A, Ya, is given by: Ya = Ra * [A]. If the analysis is done using the default value of K1 (= 1.0), the resolved value of P2 corresponds to Ra*Ao.
P3	Rb	Specific response factor for substance B. In the second form of this function it is assumed that Rb = 0.

Sample Applications

- Determining the rate constant for a (3/2)-order decomposition of a chemical substance or enzyme.

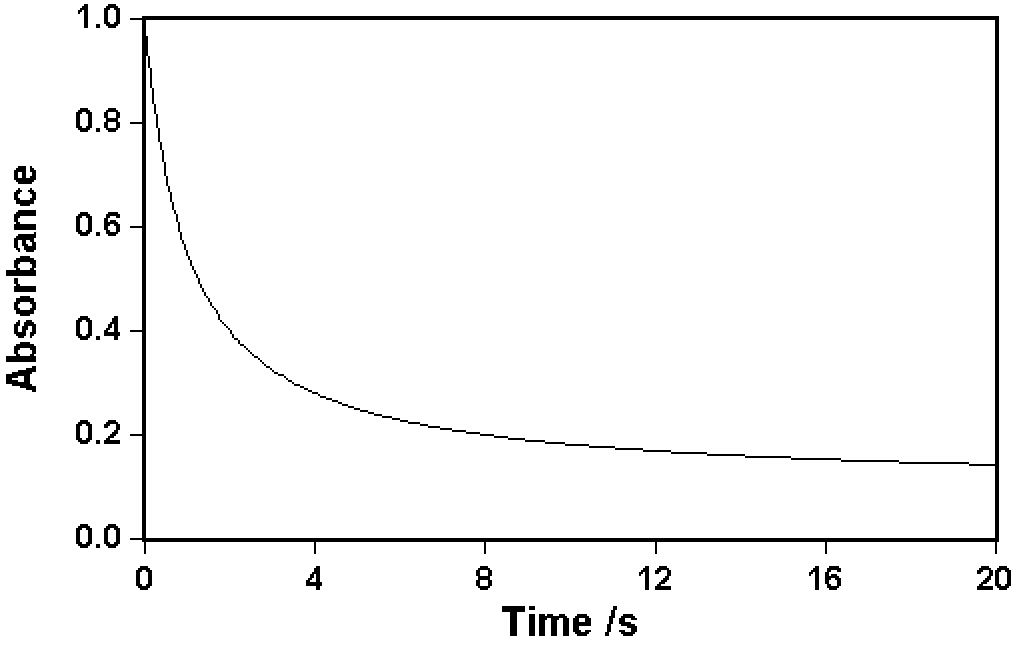
Remarks

This function was derived assuming that:

- The reaction stoichiometry is 1:1.
- Initially, no B is present. That is, all of the reaction product, B, is derived from A.
- The reaction is irreversiblereversible; that is, it goes to completion.
- The reaction rate is given by: $d[A]/dt = k*[A]^{3/2}$.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0411: Chemical Kinetics: Second-Order (equal) Rxn_1: A -> B, dA/dt = k*A^2



Equation

Two variations of the function are available:

- $$Y = K1 * P2 + \frac{(P3 - P2) * P1 * K1^2 * X}{(1 + P1 * K1 * X)}$$
- $$Y = K1 * P2 - \frac{P2 * P1 * K1^2 * X}{(1 + P1 * K1 * X)}$$

in which

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Constants

Constant	Name	Comments
K1	Ao	Total (initial) concentration of component A. Default value is 1.0. An appropriate value must be assigned to K1 if meaningful results are to be obtained.

Parameters

Parameter	Name	Comments
P1	k	Rate constant.
P2	Ra	Specific response factor for A; for example, the extinction coefficient, absorbtivity, or specific conductivity of A. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to A, Ya, is given by: Ya = Ra * [A].
P3	Rb	Specific response factor for substance B. In the second form of this function it is assumed that Rb = 0.

Sample Applications

- Determining the rate constant for a second-order chemical reaction.

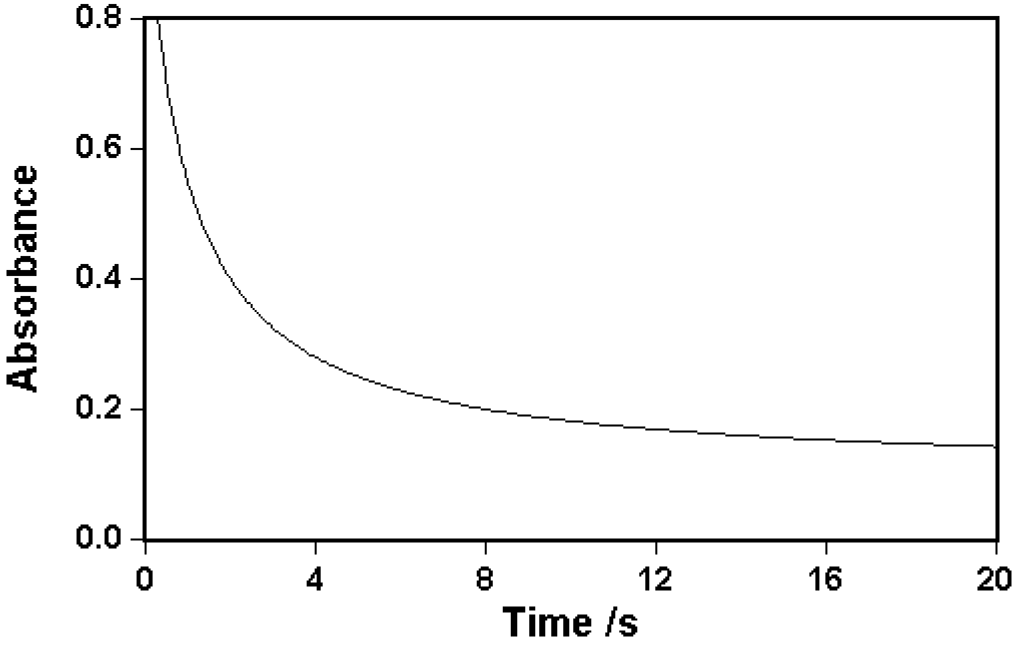
Remarks

This function was derived assuming that:

- The reaction stoichiometry is 1:1.
- Initially, no B is present. That is, all of the reaction product, B, is derived from A.
- The reaction is irreversiblereversible; that is, it goes to completion.
- The reaction rate is given by: $d[A]/dt = k*[A]^2$.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0412: Chemical Kinetics: Second-Order (equal) Rxn_2: 2A -> B, dA/dt = k*A^2



Equation

Two variations of the function are available:

- $$Y = K1 * P2 + \frac{\left(\frac{P3}{2} - P2\right) * P1 * K1^2 * X}{(1 + P1 * K1 * X)}$$
- $$Y = K1 * P2 - \frac{P2 * P1 * K1^2 * X}{(1 + P1 * K1 * X)}$$

in which

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Constants

Constant	Name	Comments
K1	Ao	Total (initial) concentration of component A. Default value is 1.0. An appropriate value must be assigned to K1 if meaningful results are to be obtained.

Parameters

Parameter	Name	Comments
P1	k	Rate constant.
P2	Ra	Specific response factor for A; for example, the extinction coefficient, absorbtivity, or specific conductivity of A. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to A, Ya, is given by: Ya = Ra * [A].
P3	Rb	Specific response factor for substance B. In second form of this function it is assumed that Rb = 0.

Sample Applications

- Determining the rate constant for a second-order chemical reaction.

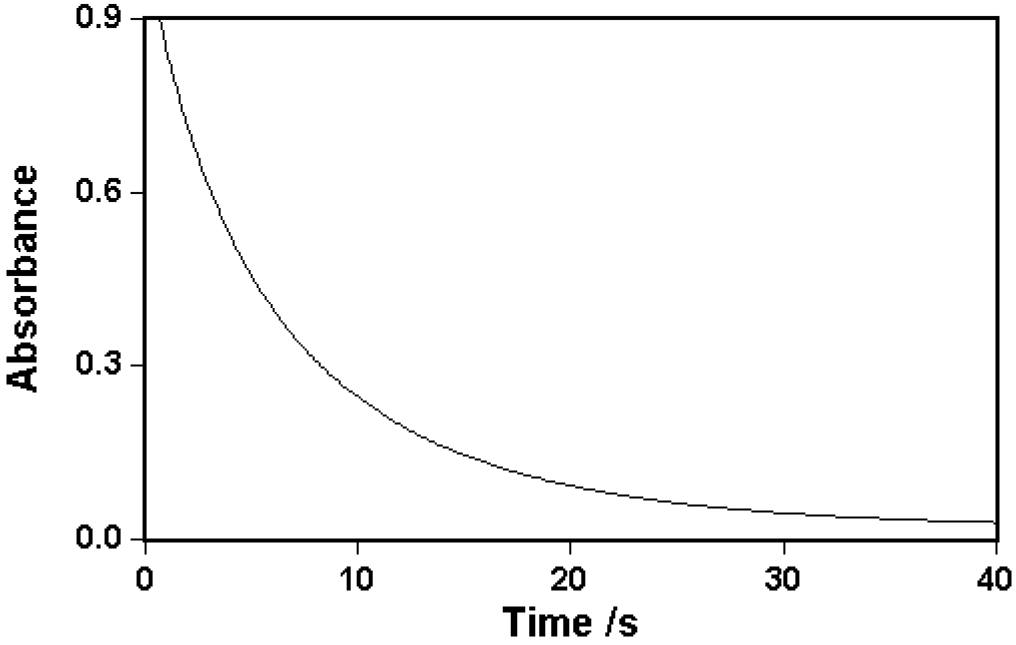
Remarks

This function was derived assuming that:

- The reaction stoichiometry is 2:1.
- Initially, no B is present. That is, all of the reaction product, B, is derived from A.
- The reaction is irreversible; that is, it goes to completion.
- The reaction rate is given by: $d[A]/dt = k*[A]^2$.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0413: Chemical Kinetics: Second-Order (unequal) Rxn: A + B -> C, dA/dt = k*A*B



Equation

Two variations of the function are available:

- $$Y = K1 * P2 + K2 * P3 + \frac{(P4 - P3 - P2) * K1 * K2 * [1 - e^{(K2 - K1) * P1 * X}]}{K1 - K2 * e^{(K2 - K1) * P1 * X}}$$
- $$Y = K1 * P2 + K2 * P3 - \frac{(P3 + P2) * K1 * K2 * [1 - e^{(K2 - K1) * P1 * X}]}{K1 - K2 * e^{(K2 - K1) * P1 * X}}$$

in which

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Constants

Constant	Name	Comments
K1	Ao	Total (initial) concentration of component A. Default value is 1.0.

Constant	Name	Comments
		An appropriate value must be assigned to K1 if meaningful results are to be obtained.
K2	Bo	Total (initial) concentration of component B. Default value is 2.0. An appropriate value must be assigned to K2 if meaningful results are to be obtained.

Parameters

Parameter	Name	Comments
P1	k	Rate constant.
P2	Ra	Specific response factor for A; for example, the extinction coefficient, absorbtivity, or specific conductivity of A. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to A, Ya, is given by: Ya = Ra * [A].
P3	Rb	Specific response factor for substance B. In the second form of this function it is assumed that Rb = 0.

Sample Applications

- Determining the rate constant for a second-order chemical reaction.

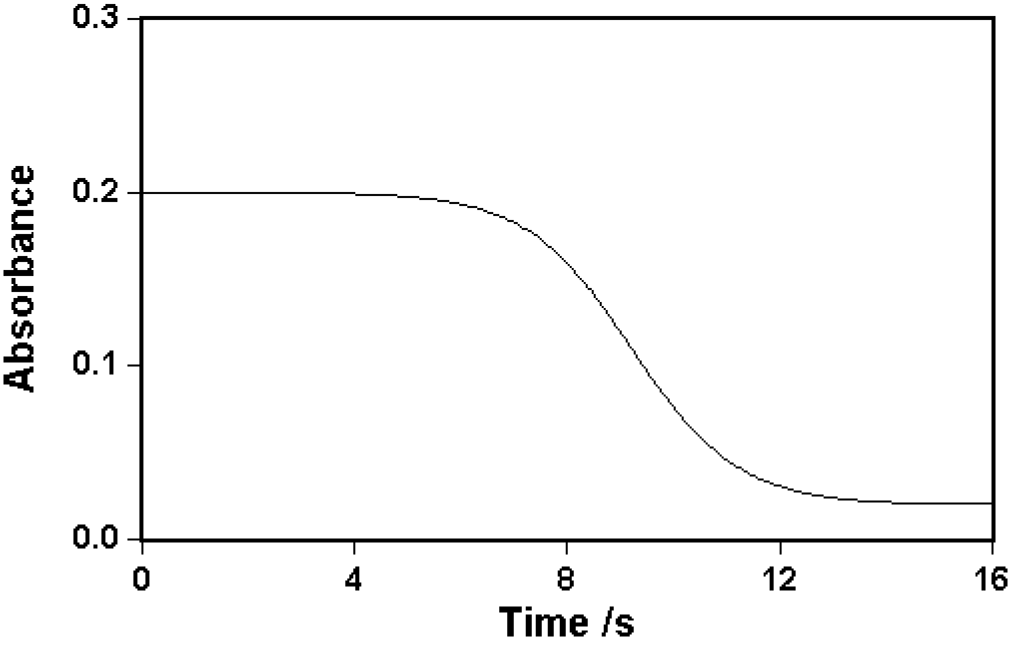
Remarks

This function was derived assuming that:

- The reaction stoichiometry is 1:1:1.
- Initially, no C is present. That is, all of the reaction product, C, is derived from A and B.
- The reaction is irreversible; that is, it goes to completion.
- The reaction rate is given by: d[A]/dt = k*[A]*[B].

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0414: Chemical Kinetics: Autocatalysis_1: A -> B, dA/dt = k*A*B, Bo Known



Equation

Two variations of the function are available:

- $$Y = K1 * P2 + K2 * P3 + \frac{(P3 - P2) * K1 * K2 * \left(1 - e^{[(K2 - K1) * P1 * X]}\right)}{K2 + K1 * e^{[(K2 - K1) * P1 * X]}}$$
- $$Y = K1 * P2 - \frac{P2 * K1 * K2 * \left(1 - e^{[(K2 - K1) * P1 * X]}\right)}{K2 + K1 * e^{[(K2 - K1) * P1 * X]}}$$

in which

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Constants

Constant	Name	Comments
K1	Ao	Total (initial) concentration of component A. Default value is 1.0. An appropriate value must be assigned to K1 if meaningful results are to be obtained.
K2	Bo	Total (initial) concentration of component B. Default value is 1.0 * 10^-4. An appropriate value must be assigned to K2 if meaningful results are to be obtained.

Parameters

Parameter	Name	Comments
P1	k	Rate constant.
P2	Ra	Specific response factor for A; for example, the extinction coefficient, absorbtivity, or specific conductivity of A. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to A, Ya, is given by: Ya = Ra * [A].
P3	Rb	Specific response factor for substance B. In the second form of this function it is assumed that Rb = 0.

Sample Applications

- Determining the rate constant for an auto-catalytic chemical or biochemical reaction which has been "spiked" with a (small) known amount of the product, B, to initiate the reaction.

Remarks

This function was derived assuming that:

- The reaction stoichiometry is 1:1.

- Initially, there is a (small) known amount of B is present.

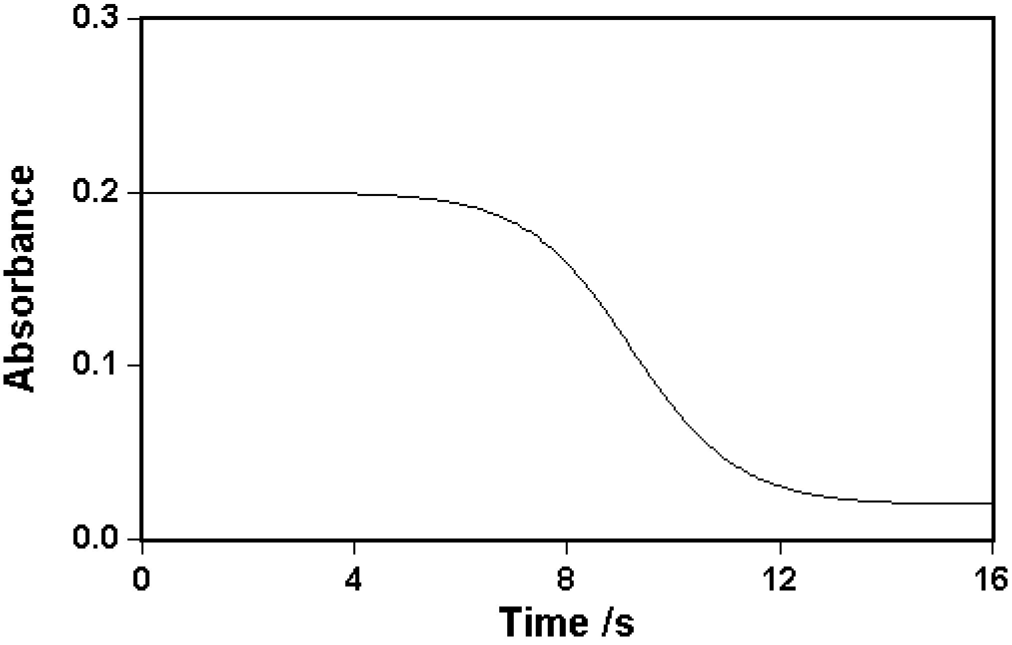
- The reaction is irreversiblereversible; that is, it goes to completion.

- The reaction rate is given by: d[A]/dt = k*[A]*[B].

If the reaction is initiated by the spontaneous decomposition of a very small (unknown) amount of A, function 0415 38 should be used to analyze the data.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0415: Chemical Kinetics: Autocatalysis_2: A -> B, dA/dt = k*A*B, Bo UnKnown



Equation

Two variations of the function are available:

- $$Y = K1 * P3 + P2 * P4 + \frac{(P4 - P3) * K1 * P2 * \left(1 - e^{\left[(P2 - K1) * P1 * X\right]}\right)}{P2 + K1 * e^{\left[(P2 - K1) * P1 * X\right]}}$$
- $$Y = K1 * P3 - \frac{P3 * K1 * P2 * \left(1 - e^{\left[(P2 - K1) * P1 * X\right]}\right)}{P2 + K1 * e^{\left[(P2 - K1) * P1 * X\right]}}$$

in which

- Y is the measured response.
- X is the independent variable, often the time in seconds.

Constants

Constant	Name	Comments
K1	Ao	Total (initial) concentration of component A. Default value is 1.0. An appropriate value must be assigned to K1 if meaningful results are to be obtained.

Parameters

Parameter	Name	Comments
P1	k	Rate constant.
P2	[B]o	Total (initial) concentration of component B.
P3	Ra	Specific response factor for A; for example, the extinction coefficient, absorbtivity, or specific conductivity of A. Specific response factors, R, are assumed to be directly proportional to the concentration of the substance being monitored. For example, the response due to A, Ya, is given by: Ya = Ra * [A].
P4	Rb	Specific response factor for substance B. In the second form of this function it is assumed that Rb = 0.

Sample Applications

- Determining the rate constant for an auto-catalytic chemical or biochemical reaction which has been "spiked" with a (small) unknownknown amount of the product, B, to initiate the reaction. The B initially present may have resulted from the spontaneous decomposition of A or it may have been present as an impurity in the reagents.

Remarks

This function was derived assuming that:

- The reaction stoichiometry is 1:1.

- Initially, there a (small) unknownknown amount of B is present.

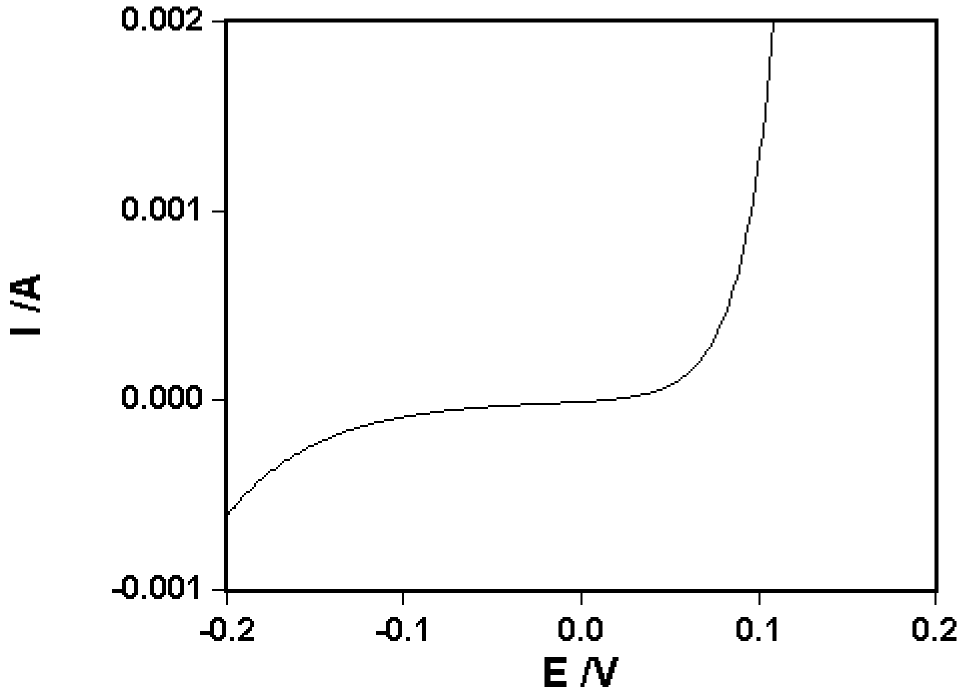
- The reaction is irreversiblereversible; that is, it goes to completion.

- The reaction rate is given by: d[A]/dt = k*[A]*[B].

If the reaction is initiated by the spontaneous decomposition of a very small known amount of A, function 0414 35 should be used to analyze the data.

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

Ftn 0416: Current - Over Potential



Equation

Two variations of the function are available:

- $$Y = P1 * \left\{ e^{\left[\frac{K1*(X-P4)}{P2}\right]} - e^{\left[\frac{-K1*(X-P4)}{P3}\right]} \right\}$$
- $$Y = P1 * \left\{ e^{\left[\frac{K1*(X-P4-Y*P5)}{P2}\right]} - e^{\left[\frac{-K1*(X-P4-Y*P5)}{P3}\right]} \right\}$$

in which

- Y is the measured response, the current in amperes.
- X is the independent variable, the applied voltage in volts.

Constants

Constant	**Name**	**Comments**
K1	Ln(10)	Default value is 2.30258509.
K2	Max I /amps	The maximum value of the current, I, that ***FitAll*** will use during the regression analysis. By default this is set to two times the maximum value of I in the current data set when the function is selected. Manually adjusting this value to a lower value may help to reduce the occurrence of "numeric overflow" or "invalid floating point operation" errors during the analysis.

Parameters

Parameter	**Name**	**Comments**
P1	Io	Exchange current or current density (in A or A/cm^2). In corrosion studies, the corrosion current or current density. **Note**: The sign convention used is: Anodic currents and voltages are positive. That is, positive voltages result in positive currents. Cathodic currents and voltages are negative. That is, the sign of the current, Y, is opposite to that often used in polarography.
P2	ba	Anodic Tafel constant (in V). In electrochemistry, this is equal to: $\frac{2.3RT}{\alpha nFT}$
P3	bc	Cathodic Tafel constant (in V). In electrochemistry, this is equal to: $\frac{2.3RT}{(1-\alpha nFT)}$
P4	Eo	Equilibrium potential (in V).
P5	Ru	Uncompensated solution resistance (in ohms or ohm.cm^2).

Parameter	Name	Comments
		When doing a fit, it is often advantageous to limit the value of Ru to values greater than or equal to zero. These are the only physically meaningful values of Ru.

Sample Applications

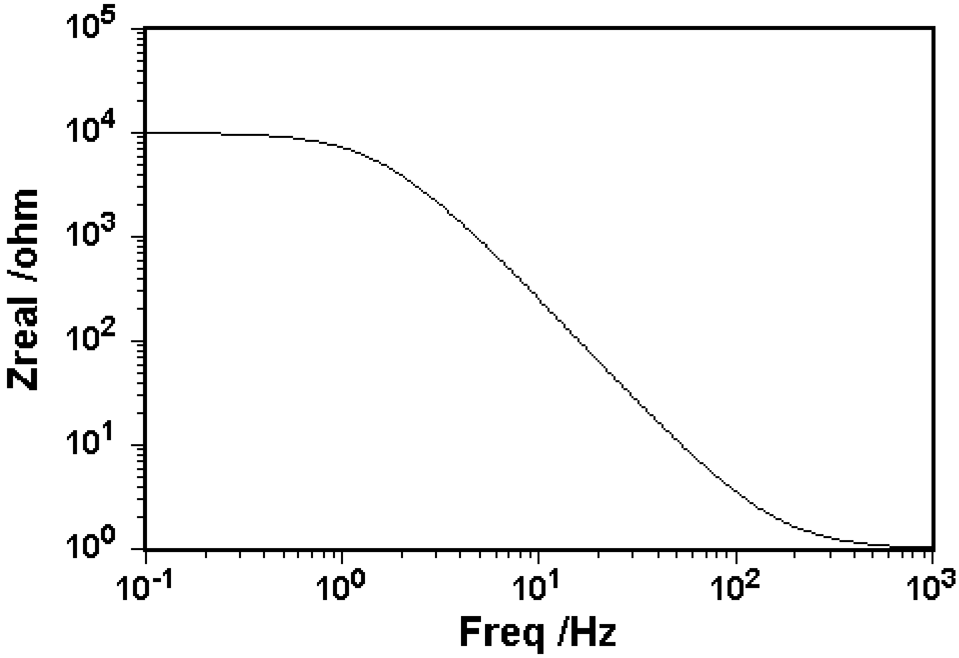
- Characterizing the current - over potential behaviour of a reversible electrochemical reaction.
- Characterizing the current - over potential behaviour of a corrosion reaction.

Remarks

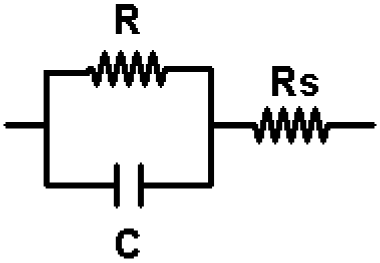
In most cases the current, Y, data will span a wide range of values, for example, three or four orders of magnitude. Because of this, it is strongly advised that you weight the data using a weighting factor of $1/(\text{SigmaY})^2$ or $1/(0.1Y)^2$.

When you plot the fit, plot Log[Y] vs. X so that you will be able to see the deviations at low Y-values as well as at high Y-values.

Ftn 0417: Real Impedance of a Parallel RC+Rs Circuit



Equivalent Circuit



Equation

Two variations of the function are available:

- $$Y = \frac{P1}{\left[1 + (2 * \pi * P1 * P2 * X)^2\right]}$$
- $$Y = \frac{P1}{\left[1 + (2 * \pi * P1 * P2 * X)^2\right]} + P3$$

in which

- Y is the measured response, the "in-phase" or "real" component of the impedance, Zre (in ohm or ohm.cm).

- X is the independent variable, the frequency, f, in Hertz (cycles per sec).

Parameters

Parameter	**Name**	**Comments**
P1	R	Resistance or resistivity of the resistor, R.
P2	C	Capacitance of the capacitor, C.
P3	Rs	Resistance or resistivity of the series resistor, Rs. This is the limiting value of the impedance at high frequencies.

Sample Applications

- Determining the resistance and capacitance of a parallel RC circuit that is in series with a resistor, Rs, from the frequency dependence of the "real" or "in-phase" component of the impedance. The impedance measurements are frequently made using a Frequency Response Analyzer or similar instrument.
- Determining the polarization resistance of an electrochemical (or corrosion) reaction from the frequency dependence of the impedance.

Remarks

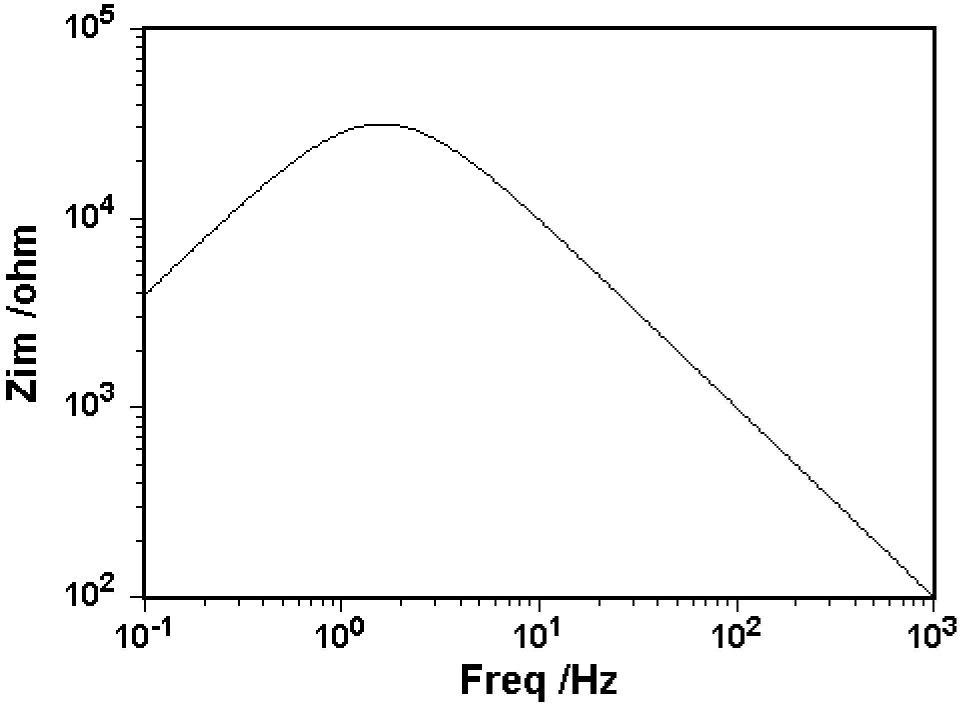
Because impedance measurements are made over a wide range of frequencies, X, it is normally advisable to use a weighting factor of $1/(\text{SigmaY})^2$ or $1/(0.01Y)^2$ when doing the fit.

If the series resistor, Rs = P3, is not present, the "real" impedance is described by the first equation.

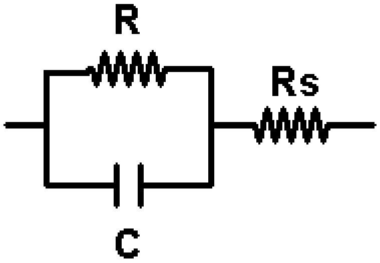
At low values of the frequency, X, the in-phase impedance, Y, approaches a limiting value of (R + Rs).

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1, that is, the X-values.

Ftn 0418: Imaginary Impedance of a Parallel RC or RC+Rs Circuit



Equivalent Circuit



Equation

$$Y = \frac{-(2*\pi*P1)^2*P2*X}{\left[1+(2*\pi*P1*P2*X)^2\right]}$$

in which

- Y is the measured response, the "out-of-phase" or "imaginary" component of the impedance, Zim (in ohm or ohm.cm).
- X is the independent variable, the frequency, f, in Hertz (cycles per sec).

Parameters

Parameter	Name	Comments
P1	R	Resistance or resistivity of the resistor, R.
P2	C	Capacitance of the capacitor, C.

Sample Applications

- Determining the resistance and capacitance of a parallel RC circuit that is in series with a resistor, Rs, from the frequency dependence of the "imaginary" or "out-of-phase" component of the impedance. The impedance measurements are frequently made using a Frequency Response Analyzer or similar instrument.

- Determining the polarization resistance of an electrochemical (or corrosion) reaction from the frequency dependence of the impedance.

Remarks

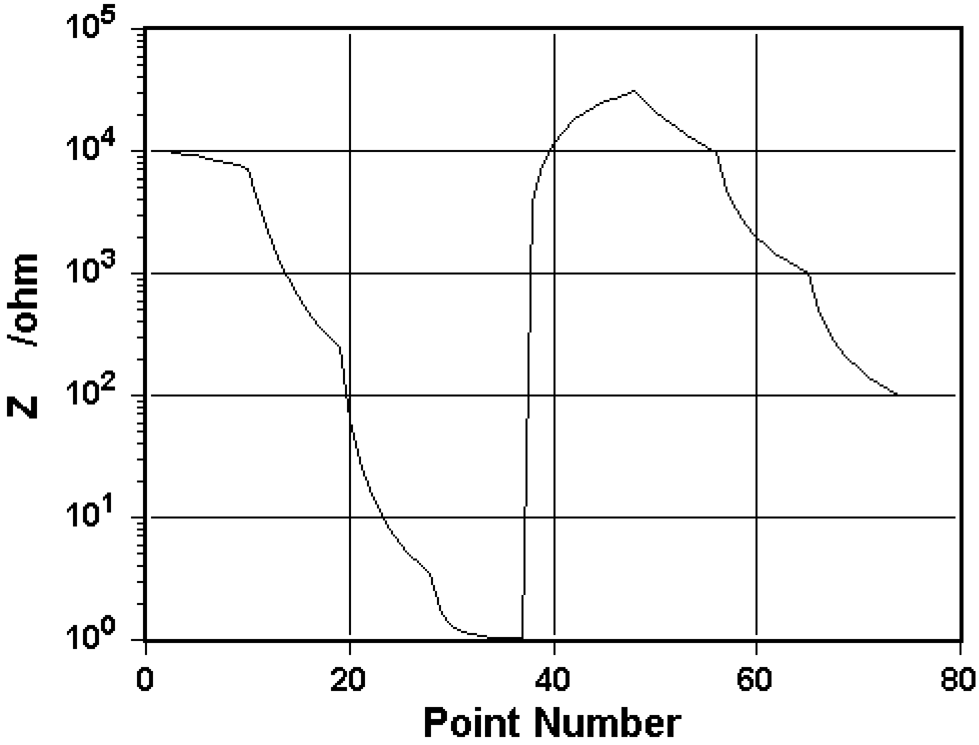
Because impedance measurements are made over a wide range of frequencies, X, it is normally advisable to use a weighting factor of $1/(\mathrm{SigmaY})^2$ or $1/(0.01Y)^2$ when doing the fit.

The out-of-phase, imaginary, impedance is independent of the value of the series resistance, Rs.

At low values of the frequency, X, the in-phase impedance, Y, approaches a limiting value of (R + Rs).

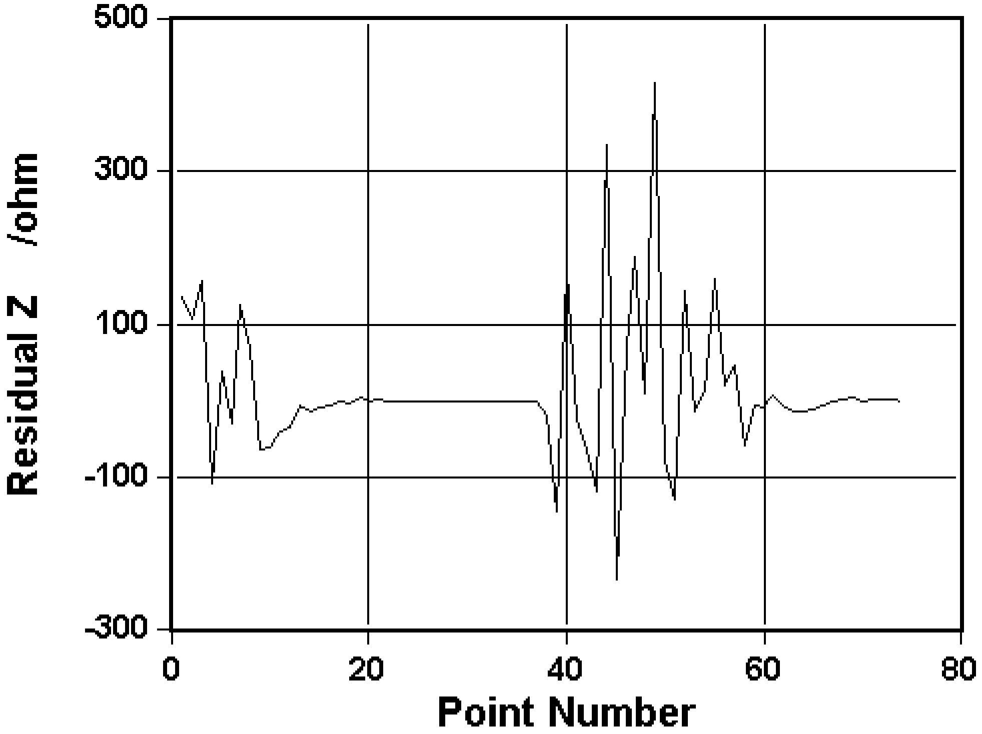
When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1, that is, the X-values.

Ftn 0419: Real and Imaginary Impedance of a Parallel RC+Rs Circuit

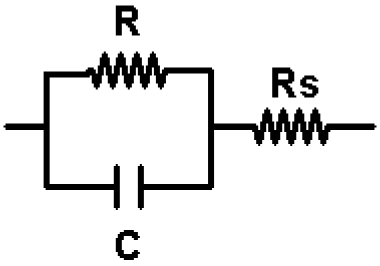


NOTE:
This function has two independent variables, X1 (the frequency) and X2 (a selector that indicates whether the Y-value is Zre or Zim). The only way to plot a meaningful fit graph in this situation is to plot Y against the "Point Number" rather than the value of the independent variable, X1.

The best way to get a visual indication of the quality of the fit is to view the residuals graph, such as the one shown below.



Equivalent Circuit



Equation

$$Y = \begin{cases} \dfrac{P1}{\left[1 + (2 * \pi * P1 * P2 * X1)^2\right]} + P3\,, & \text{for } X2 = 0 \\[2ex] \dfrac{-(2 * \pi * P1)^2 * P2 * X1}{\left[1 + (2 * \pi * P1 * P2 * X1)^2\right]}\,, & \text{for } X2 \neq 0 \end{cases}$$

in which

- The dependent variable, Y, is the "real" or "imaginary" component of the impedance, Zre or Zim , (in ohm or ohm.cm) depending on the value of X2.

- The independent variable, X1, is the frequency, f, (in Hz).

- The independent variable, X2, is a "selector" that, when zero indicates that Y is the "real" component of the impedance and, when non-zero that Y is the "imaginary" component of the impedance.

Parameters

Parameter	**Name**	**Comments**
P1	R	Resistance or resistivity of the resistor, R.
P2	C	Capacitance of the capacitor, C.
P3	Rs	Resistance or resistivity of the series resistor, Rs. This is the limiting value of the impedance at high frequencies.

Sample Applications

- Determining the resistance and capacitance of a parallel RC circuit that is in series with a resistor, Rs, from the frequency dependence of the "real" or "in-phase" and the "imaginary" or "out-of-phase" components of the impedance. The impedance measurements are frequently made using a Frequency Response Analyzer or similar instrument.

- Determining the polarization resistance of an electrochemical (or corrosion) reaction from the frequency dependence of the impedance.

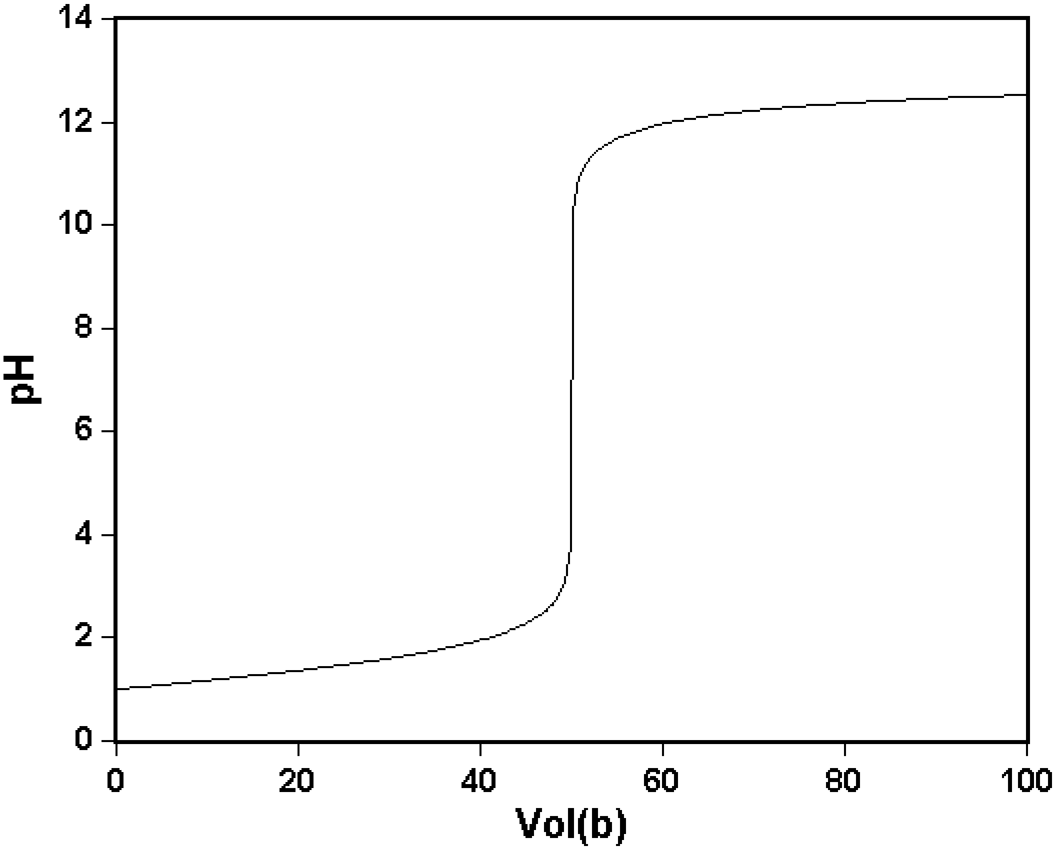
Remarks

Because impedance measurements are made over a wide range of frequencies, X, it is normally advisable to use a weighting factor of $1/(\text{SigmaY})^2$ or $1/(0.01Y)^2$ when doing the fit.

At low values of the frequency, X, the in-phase impedance, Y, approaches a limiting value of (R + Rs).

When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1, that is, the X-values.

Ftn 0421: Titration: Strong Acid w/ Strong Base: Cso



Equation

$A*[H^+]^2 + B*[H^+] + C = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$VT = K[2] + X$,

$A = 1.0$,

$B = (K[1]*X - P[1]*K[2])/VT$,

$C = -Kw$,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quadratic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	Name	Comments
P1	Cso	Initial concentration of the acid in moles/L.

Sample Applications

- Determining the concentration, Cso, of a strong monoprotic acid solution.

- Determining the total concentration, Cso, of a mixture of strong monoprotic acids.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

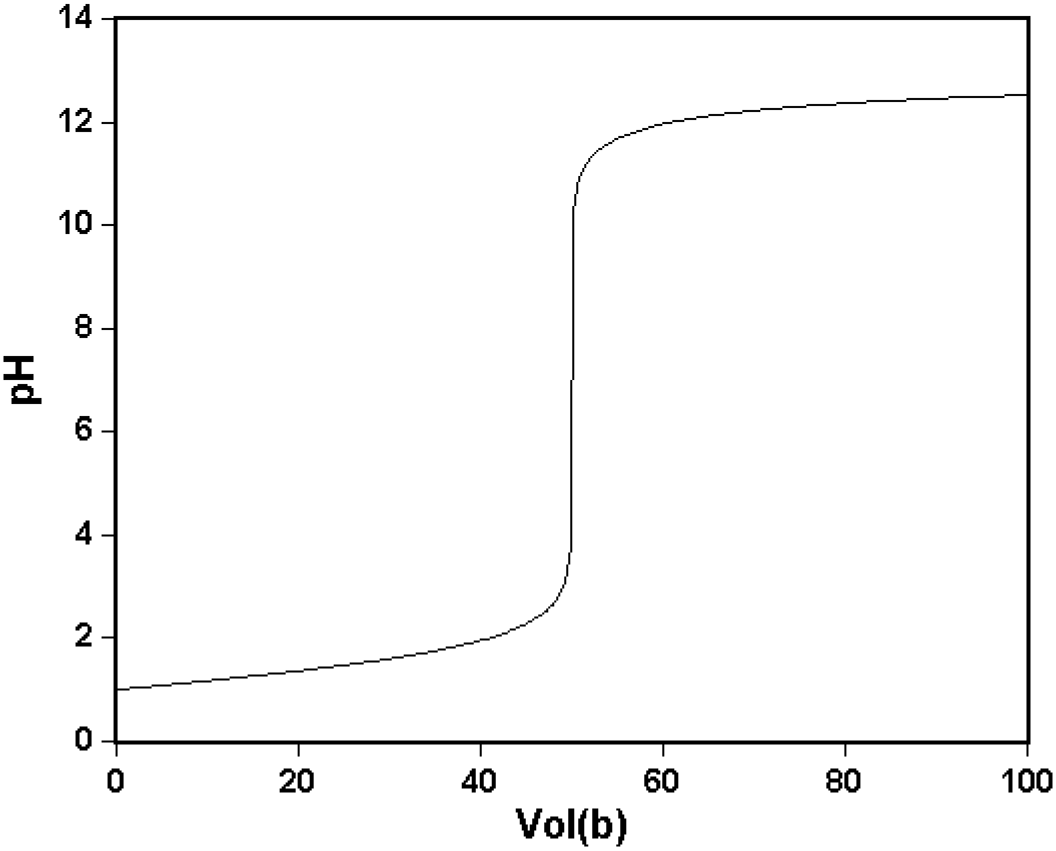
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0422 53

Ftn 0423 55

Ftn 0422: Titration: Strong Acid w/ Strong Base: Cso & pKw



Equation

$A*[H^+]^2 + B*[H^+] + C = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[2]}$,

VT := K[2] + X,

A := 1.0,

B := (K[1]*X - P[1]*K[2])/VT,

C := -Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quadratic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	Name	Comments
P1	Cso	Initial concentration of the acid in moles/L.
P2	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the concentration of a strong acid solution, Cso, and the water autoprotolysis constant, pKw.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

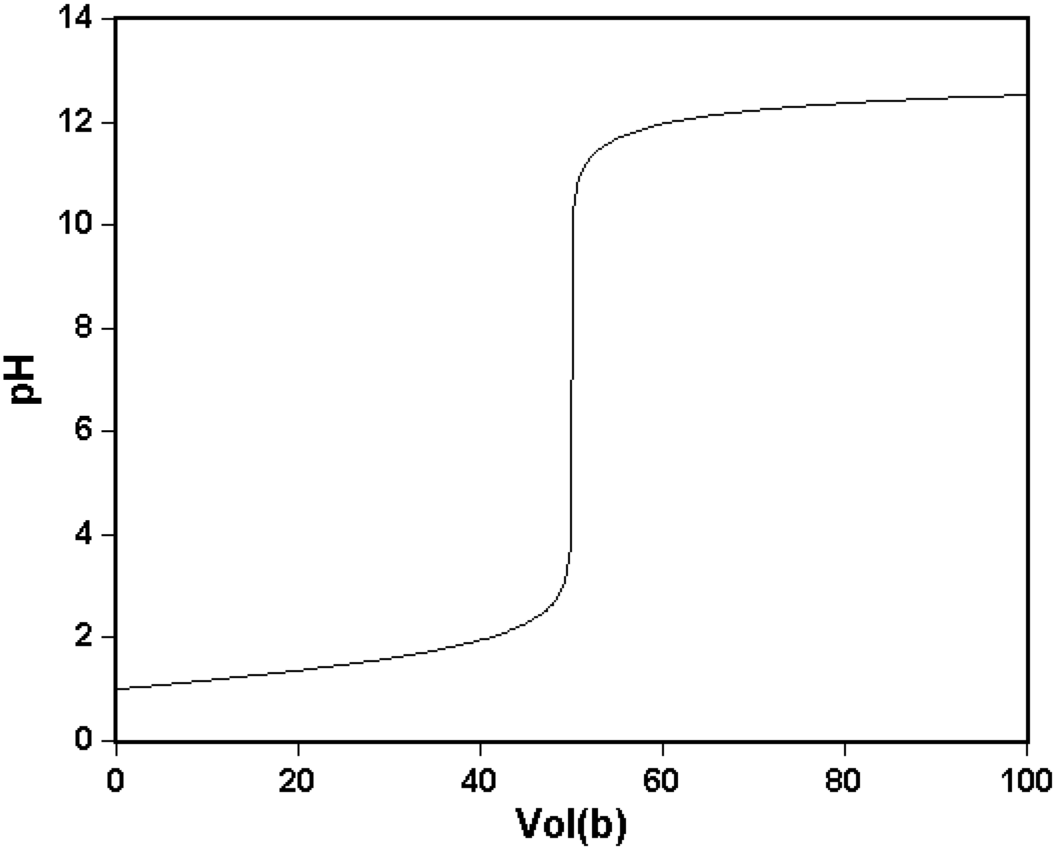
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0421 51

Ftn 0423 55

Ftn 0423: Titration: Strong Acid w/ Strong Base: pKw



Equation

$A*[H^+]^2 + B*[H^+] + C = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[1]}$,

VT = K[2] + X,

A = 1.0,

B = (K[1]*X - K[3]*K[2])/VT,

C = -Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quadratic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	Cso	Initial concentration of the acid in moles/L.

Parameters

Parameter	Name	Comments
P1	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the water autoprotolysis constant, pKw.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

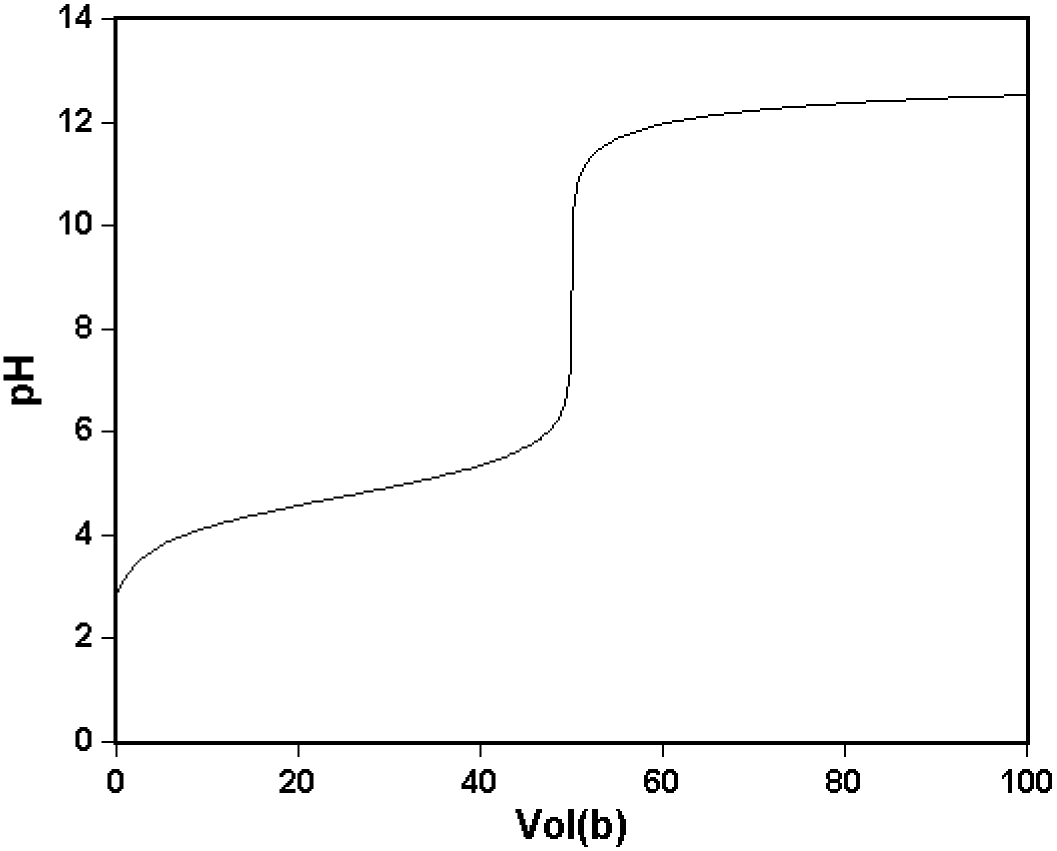
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0421 51

Ftn 0422 53

Ftn 0425: Titration: Weak Monoprotic Acid w/ Strong Base: pKa



Equation

HA ⇌ $H^+ + A^-$ with acid dissociation constant Ka = $[H^+] * [A^-] / [HA]$

H_2O ⇌ $H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$A*[H^+]^3 + B*[H^+]^2 + C*[H^+] + D = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka = 10^{-P[1]}$,

VT = K[2] + X,

A = 1.0,

B = Ka + K[1]*X/VT,

C = [Ka * (K[1]*X - K[2]*K[4])/VT] - Kw,

D = -Ka*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above cubic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Cao	Initial concentration of the acid in moles/L.

Parameters

Parameter	**Name**	**Comments**
P1	pKa	-Log10 of the acid dissociation constant of the weak monoprotic acid.

Sample Applications

- Determining the acid dissociation constant, pKa, of a weak monoprotic acid solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

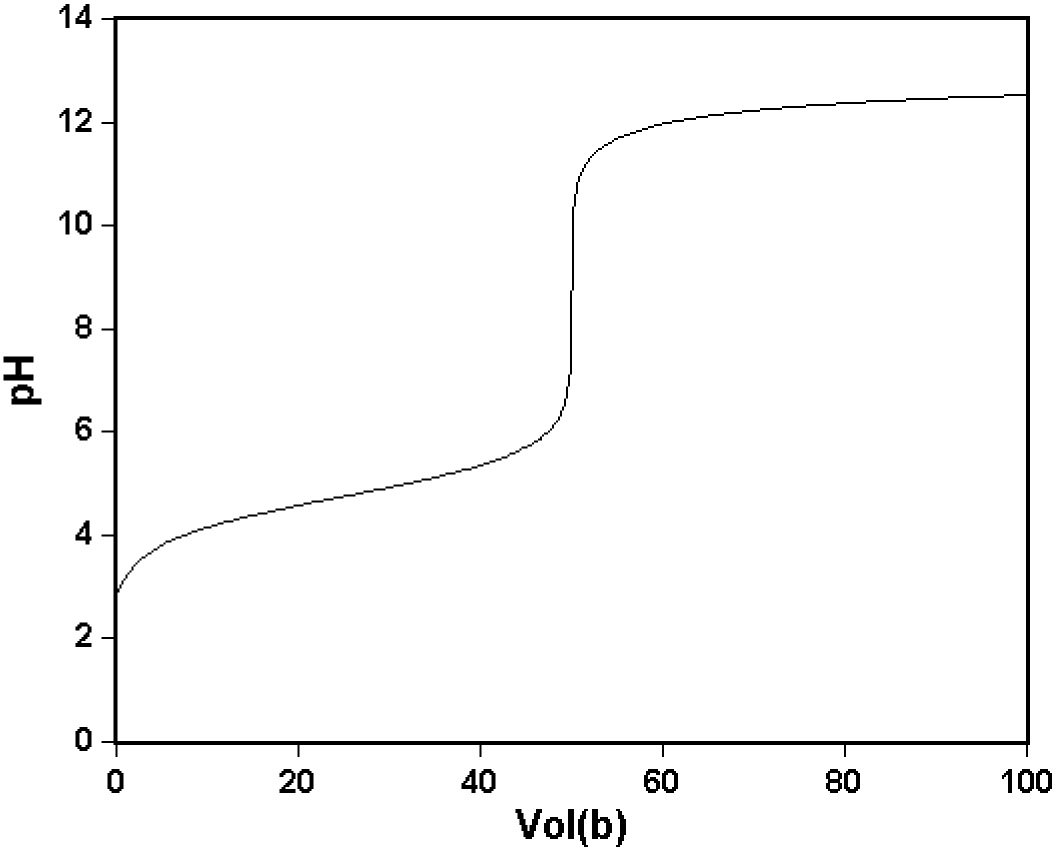
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0426 60

Ftn 0427 63

Ftn 0426: Titration: Weak Monoprotic Acid w/ Strong Base: pKa & Cao



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka = [H^+] * [A^-] / [HA]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^3 + B*[H^+]^2 + C*[H^+] + D = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka = 10^{-P[1]}$,

VT := K[2] + X,

$A = 1.0$,

$B = Ka + K[1]*X/VT$,

$C = [Ka * (K[1]*X - K[2]*P[2])/VT] - Kw$,

$D = -Ka*Kw$,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above cubic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	Name	Comments
P1	pKa	-Log10 of the acid dissociation constant of the weak monoprotic acid.
P2	Cao	Initial concentration of the acid in moles/L.

Sample Applications

- Determining the acid dissociation constant, pKa, and concentration, Cao, of a weak monoprotic acid solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

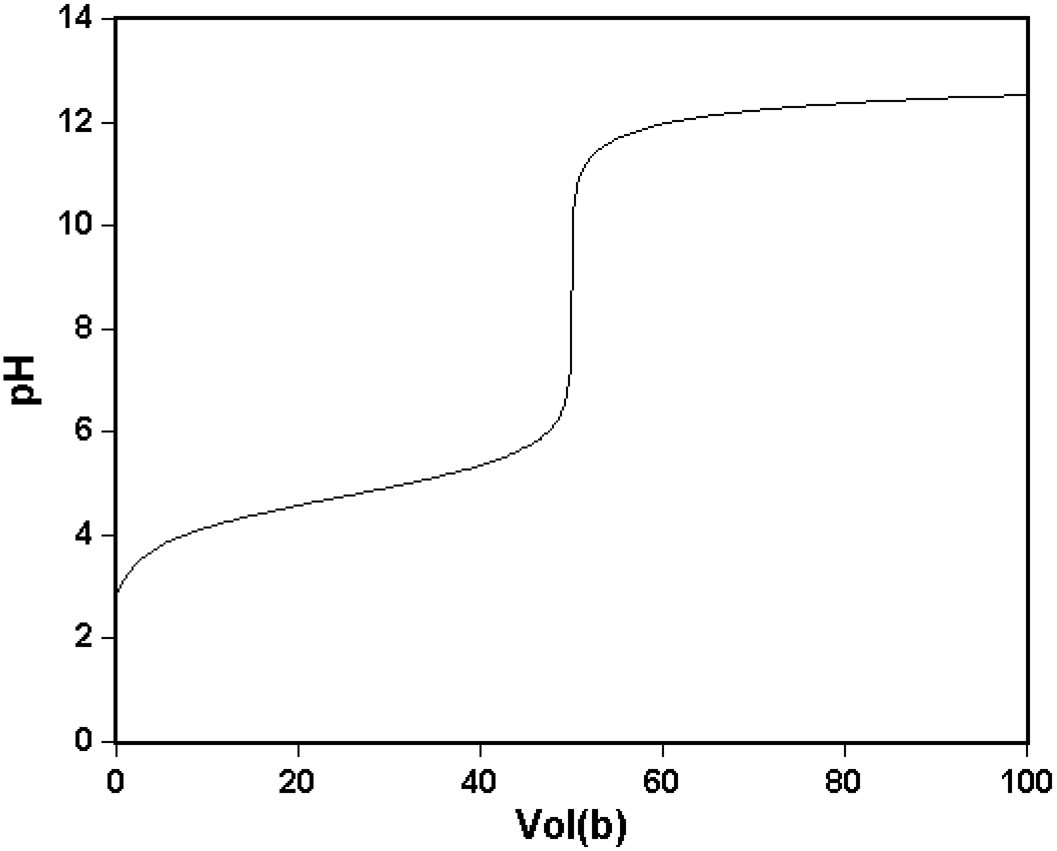
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0425 57

Ftn 0427 63

Ftn 0427: Titration: Weak Monoprotic Acid w/ Strong Base: pKa, Cao & pKw



Equation

HA ⇌ $H^+ + A^-$ with acid dissociation constant Ka = $[H^+] * [A^-] / [HA]$

H_2O ⇌ $H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$A*[H^+]^3 + B*[H^+]^2 + C*[H^+] + D = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[3]}$,

$Ka = 10^{-P[1]}$,

VT := K[2] + X,

A = 1.0,

B = Ka + K[1]*X/VT,

C = [Ka * (K[1]*X - K[2]*P[2])/VT] - Kw,

D = -Ka*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above cubic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	Name	Comments
P1	pKa	-Log10 of the acid dissociation constant of the weak monoprotic acid.
P2	Cao	Initial concentration of the acid in moles/L.
P3	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constant, pKa, and the concentration, Cao, of a weak monoprotic acid solution as well as the water autoprotolysis constant, pKw.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

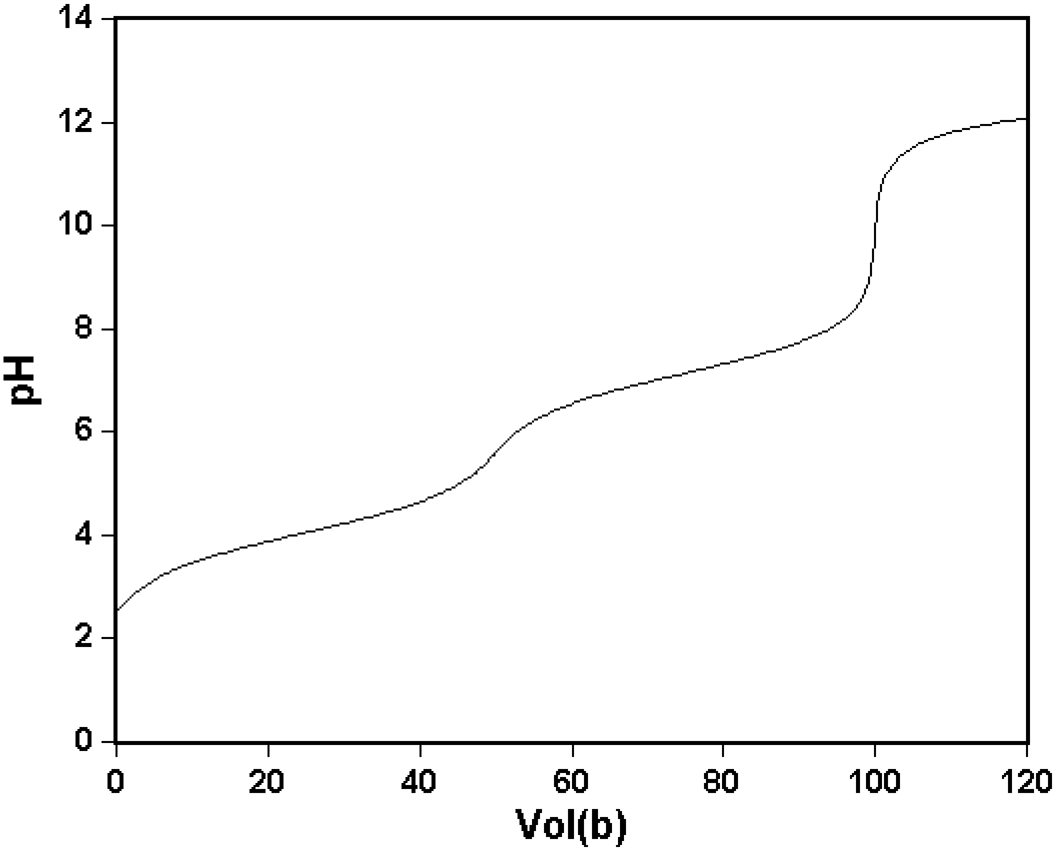
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0425 57

Ftn 0426 60

Ftn 0430: Titration: Weak Diprotic Acid w/ Strong Base: pKa1 & pKa2



Equation

$H_2A \rightleftharpoons H^+ + HA^-$ with acid dissociation constant Ka1 = $[H^+] * [HA^-] / [H_2A]$

$HA^- \rightleftharpoons H^+ + A^{2-}$ with acid dissociation constant Ka2 = $[H^+] * [A^{2-}] / [HA^-]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$$\mathbf{A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0}$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + K[1]*X/VT,

C = Ka1*(Ka2 + K[1]*X/VT - K[2]*K[4])/VT - Kw,

D = Ka1*Ka2*(K[1]*X/VT - 2*K[2]*K[4]/VT) - Ka1*Kw,

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Cao	Initial concentration of the acid in moles/L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the first acid dissociation constant of the weak diprotic acid.
P2	pKa2	-Log10 of the second acid dissociation constant of the weak diprotic acid.

Sample Applications

- Determining the acid dissociation constants, pKa1 & pKa2, of a weak diprotic acid solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

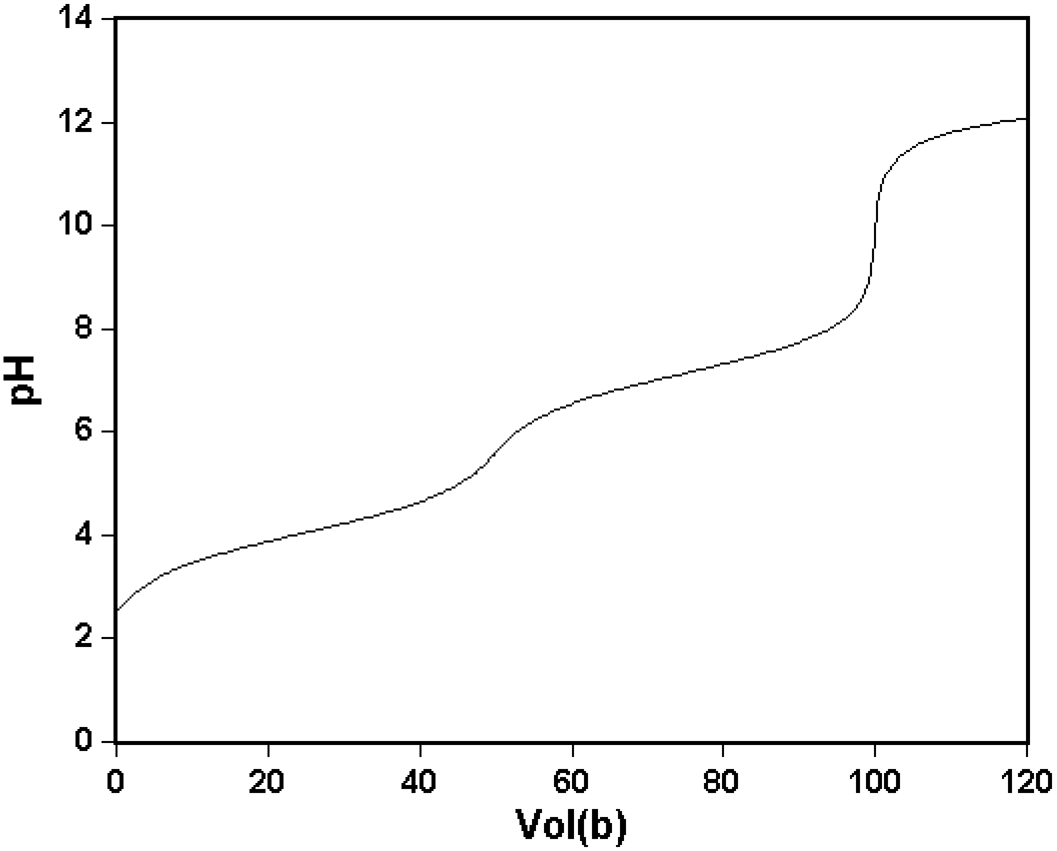
Also see

Ftn 0431 69

Ftn 0432 72

Ftn 0450 93

Ftn 0431: Titration: Weak Diprotic Acid w/ Strong Base: pKa1, pKa2 & Cao



Equation

$H_2A \rightleftharpoons H^+ + HA^-$ with acid dissociation constant $Ka1 = [H^+] * [HA^-] / [H_2A]$

$HA^- \rightleftharpoons H^+ + A^{2-}$ with acid dissociation constant $Ka2 = [H^+] * [A^{2-}] / [HA^-]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$VT := K[2] + X$,

$A = 1.0$,

$B = Ka1 + K[1]*X/VT$,

$C = Ka1*(Ka2 + K[1]*X/VT - K[2]*P[3])/VT - Kw$,

$D = Ka1*Ka2*(K[1]*X/VT - 2*K[2]*P[3]/VT) - Ka1*Kw$,

$E = -Ka1*Ka2*Kw$,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the first acid dissociation constant of the weak diprotic acid.
P2	pKa2	-Log10 of the second acid dissociation constant of the weak diprotic acid.
P3	Cao	Initial concentration of the acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 and the concentration, Cao, of a weak diprotic acid solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

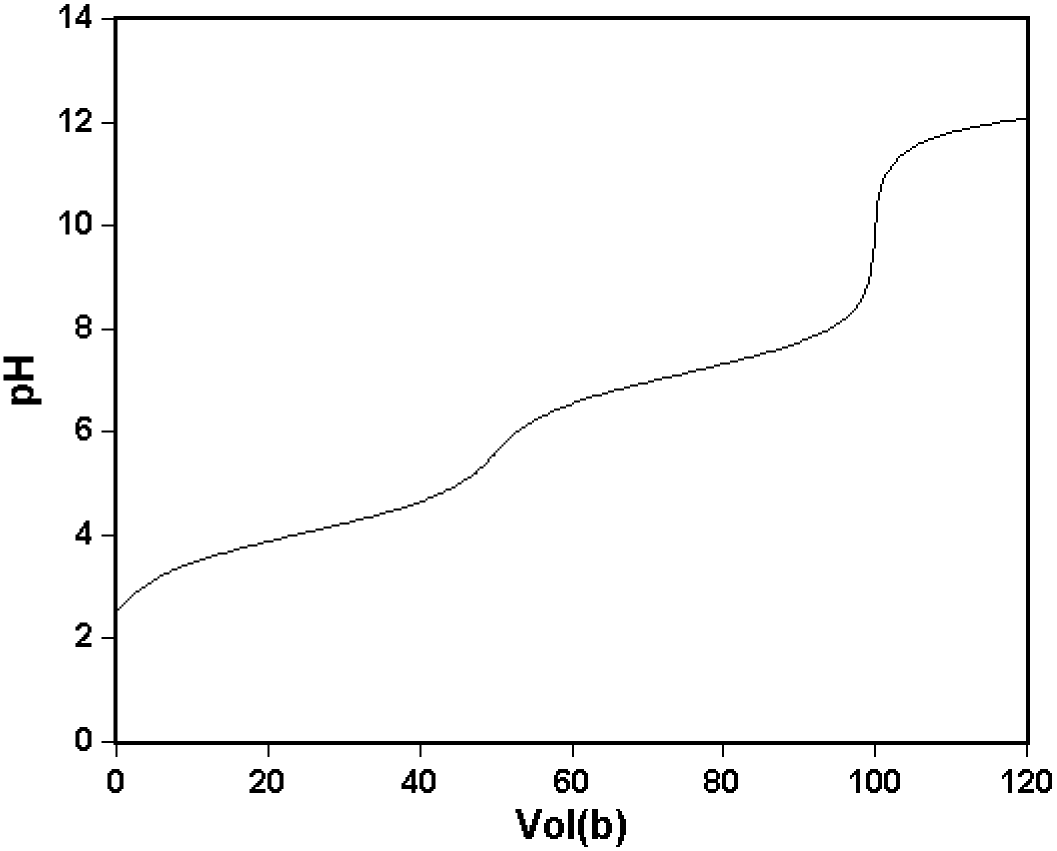
Also see

Ftn 0430 66

Ftn 0432 72

Ftn 0451 96

Ftn 0432: Titration: Weak Diprotic Acid w/ Strong Base: pKa1, pKa2, Cao & pKw



Equation

$H_2A \rightleftharpoons H^+ + HA^-$ with acid dissociation constant $Ka1 = [H^+] * [HA^-] / [H_2A]$

$HA^- \rightleftharpoons H^+ + A^{2-}$ with acid dissociation constant $Ka2 = [H^+] * [A^{2-}] / [HA^-]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$$\mathbf{A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0}$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[4]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + K[1]*X/VT,

C = Ka1*(Ka2 + K[1]*X/VT - K[2]*P[3])/VT - Kw,

D = Ka1*Ka2*(K[1]*X/VT - 2*K[2]*P[3]/VT) - Ka1*Kw,

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the first acid dissociation constant of the weak diprotic acid.
P2	pKa2	-Log10 of the second acid dissociation constant of the weak diprotic acid.
P3	Cao	Initial concentration of the acid in moles/L.
P4	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 and the concentration, Cao, of a weak diprotic acid solution as well as the water autoprotolysis constant.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

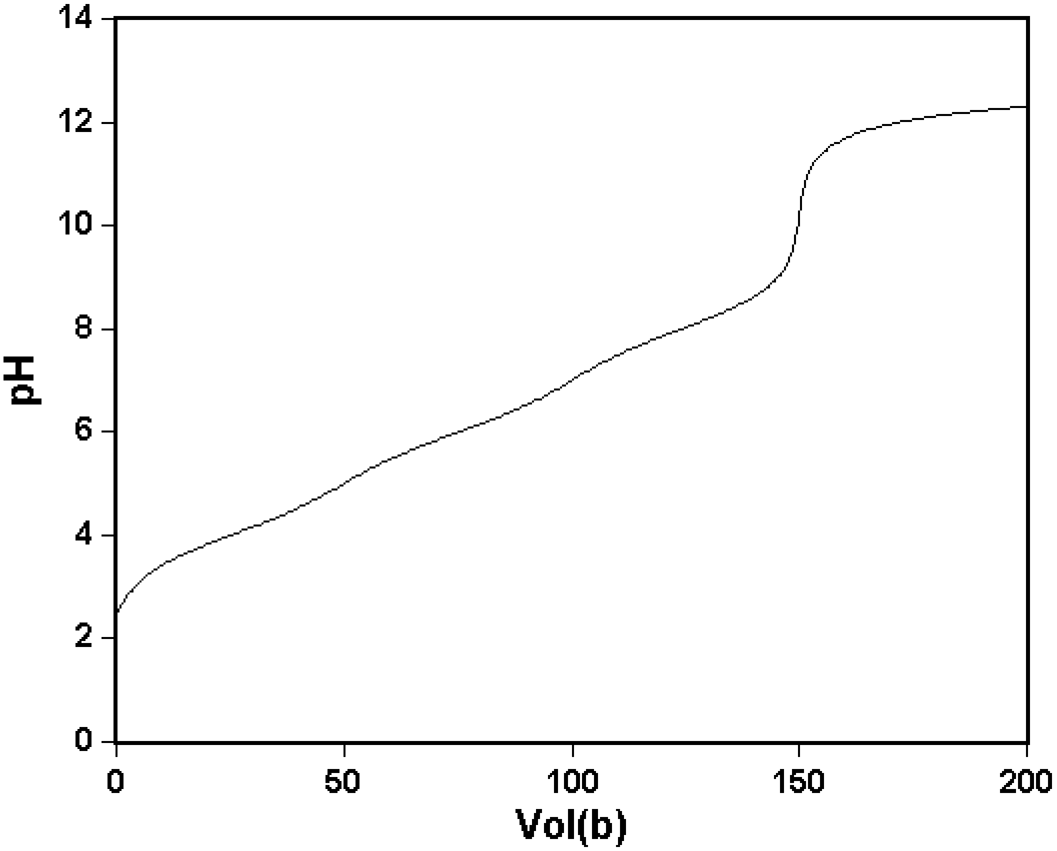
Also see

Ftn 0430 66

Ftn 0431 69

Ftn 0452 99

Ftn 0435: Titration: Weak Triprotic Acid w/ Strong Base: pKa1, pKa2 & pKa3



Equation

$H_3A \rightleftharpoons H^+ + H_2A^-$ with acid dissociation constant $Ka1 = [H^+] * [H_2A^-] / [H_3A]$

$H_2A^- \rightleftharpoons H^+ + HA^{2-}$ with acid dissociation constant $Ka2 = [H^+] * [HA^{2-}] / [H_2A^-]$

$HA^{2-} \rightleftharpoons H^+ + A^{3-}$ with acid dissociation constant $Ka3 = [H^+] * [A^{3-}] / [HA^{2-}]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

$VT := K[2] + X$,

$A = 1.0$,

$B = Ka1 + K[1]*X/VT$,

$C = Ka1*(Ka2 + K[1]*X/VT - K[4]) - Kw$,

$D = Ka1*Ka2*(Ka3 + K[1]*X/VT) - 2*K[4]) - Ka1*Kw$,

$E = Ka1*Ka2*Ka3*(K[1]*X/VT - 3*K[4]) - Ka1*Ka2*Kw$,

$F = -Ka1*Ka2*Ka3*Kw$

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Cao	Initial concentration of the acid in moles/L.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the first acid dissociation constant of the weak triprotic acid.
P2	pKa2	-Log10 of the second acid dissociation constant of the weak triprotic acid.
P3	pKa3	-Log10 of the third acid dissociation constant of the weak triprotic acid.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 & pKa3, of a weak triprotic acid solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

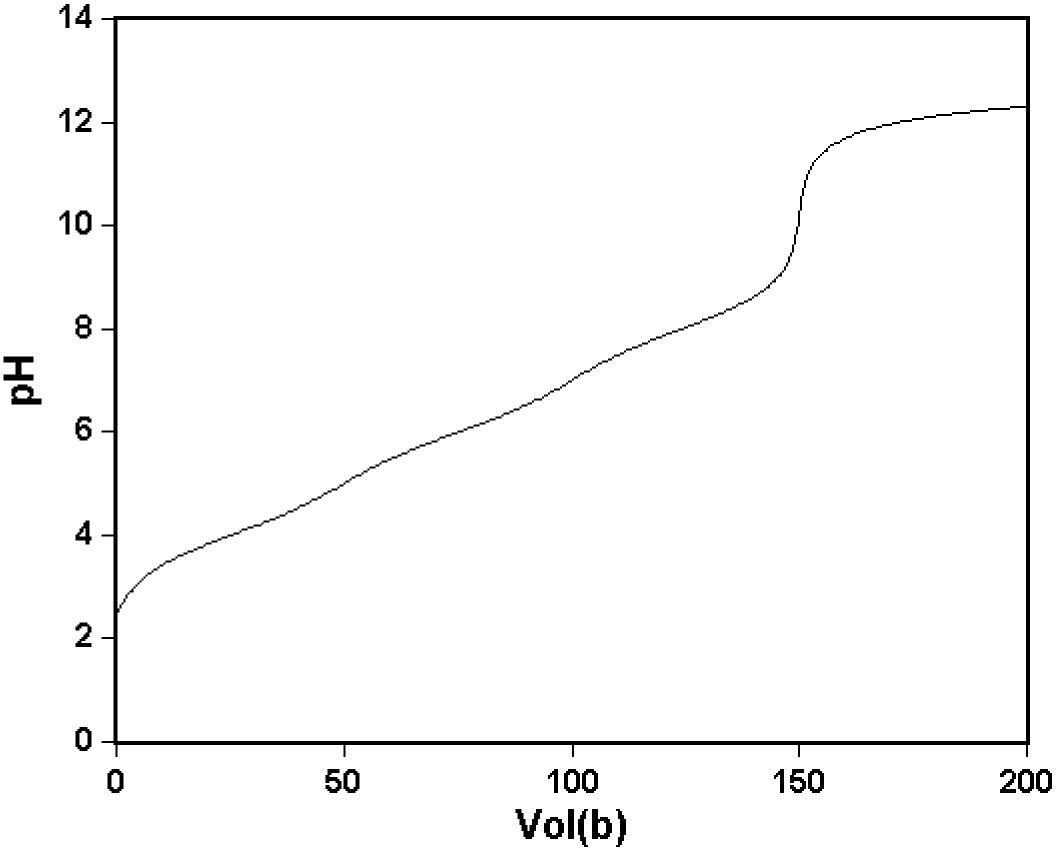
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0436 78

Ftn 0437 81

Ftn 0436: Titration: Weak Triprotic Acid w/ Strong Base: pKa1, pKa2, pKa3 & Cao



Equation

$H_3A \rightleftharpoons H^+ + H_2A^-$ with acid dissociation constant $Ka1 = [H^+] * [H_2A^-] / [H_3A]$

$H_2A^- \rightleftharpoons H^+ + HA^{2-}$ with acid dissociation constant $Ka2 = [H^+] * [HA^{2-}] / [H_2A^-]$

$HA^{2-} \rightleftharpoons H^+ + A^{3-}$ with acid dissociation constant $Ka3 = [H^+] * [A^{3-}] / [HA^{2-}]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + K[1]*X/VT,

C = Ka1*(Ka2 + K[1]*X/VT - P[4]) - Kw,

D = Ka1*Ka2*(Ka3 + K[1]*X/VT) - 2*P[4]) - Ka1*Kw,

E = Ka1*Ka2*Ka3*(K[1]*X/VT - 3*P[4]) - Ka1*Ka2*Kw,

F = -Ka1*Ka2*Ka3*Kw

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the first acid dissociation constant of the weak triprotic acid.

Parameter	**Name**	**Comments**
P2	pKa2	-Log10 of the second acid dissociation constant of the weak triprotic acid.
P3	pKa3	-Log10 of the third acid dissociation constant of the weak triprotic acid.
P4	Cao	Initial concentration of the acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2, pKa3 and concentration, Cao, of a weak triprotic acid solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

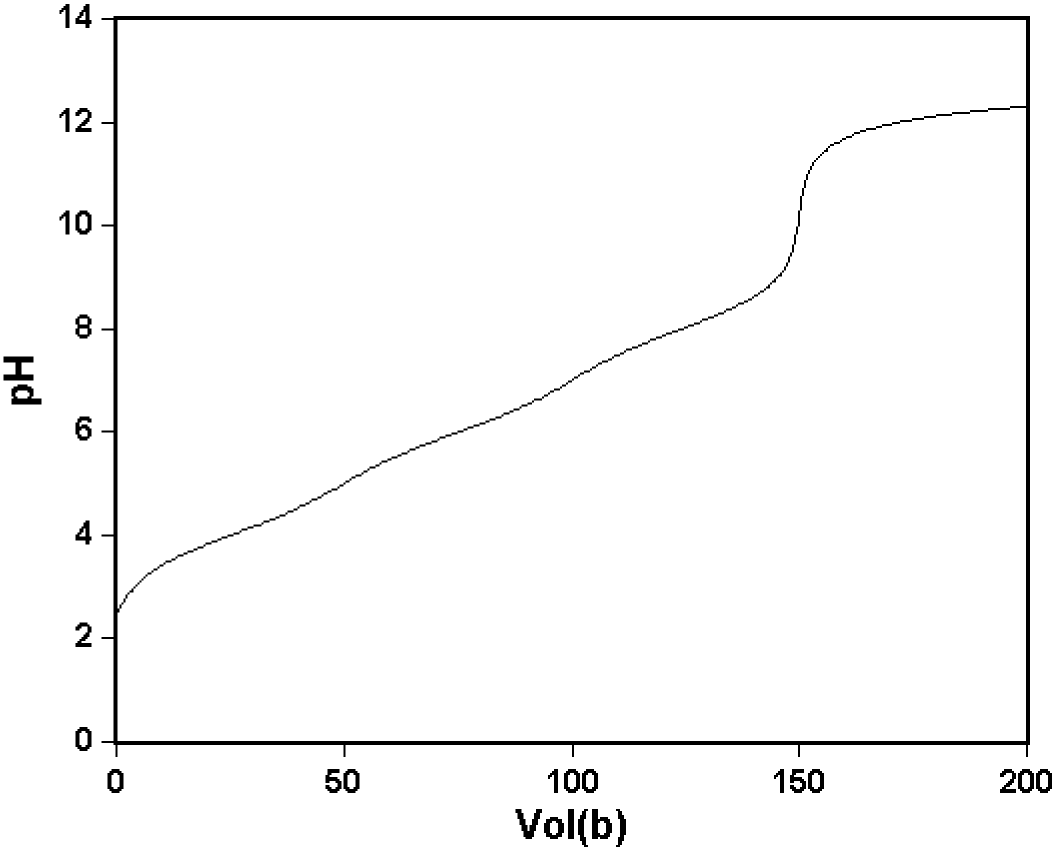
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0435 75

Ftn 0437 81

Ftn 0437: Titration: Weak Triprotic Acid w/ Strong Base: pKa1, pKa2, pKa3, Cao & pKw



Equation

$H_3A \rightleftharpoons H^+ + H_2A^-$ with acid dissociation constant $Ka1 = [H^+] * [H_2A^-] / [H_3A]$

$H_2A^- \rightleftharpoons H^+ + HA^{2-}$ with acid dissociation constant $Ka2 = [H^+] * [HA^{2-}] / [H_2A^-]$

$HA^{2-} \rightleftharpoons H^+ + A^{3-}$ with acid dissociation constant $Ka3 = [H^+] * [A^{3-}] / [HA^{2-}]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$$\mathbf{A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0}$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[5]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + K[1]*X/VT,

C = Ka1*(Ka2 + K[1]*X/VT - P[4]) - Kw,

D = Ka1*Ka2*(Ka3 + K[1]*X/VT) - 2*P[4]) - Ka1*Kw,

E = Ka1*Ka2*Ka3*(K[1]*X/VT - 3*P[4]) - Ka1*Ka2*Kw,

F = -Ka1*Ka2*Ka3*Kw

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the first acid dissociation constant of the weak triprotic acid.

Parameter	Name	Comments
P2	pKa2	-Log10 of the second acid dissociation constant of the weak triprotic acid.
P3	pKa3	-Log10 of the third acid dissociation constant of the weak triprotic acid.
P4	Cao	Initial concentration of the acid in moles/L.
P5	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2, pKa3 and concentration, Cao, of a weak triprotic acid solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

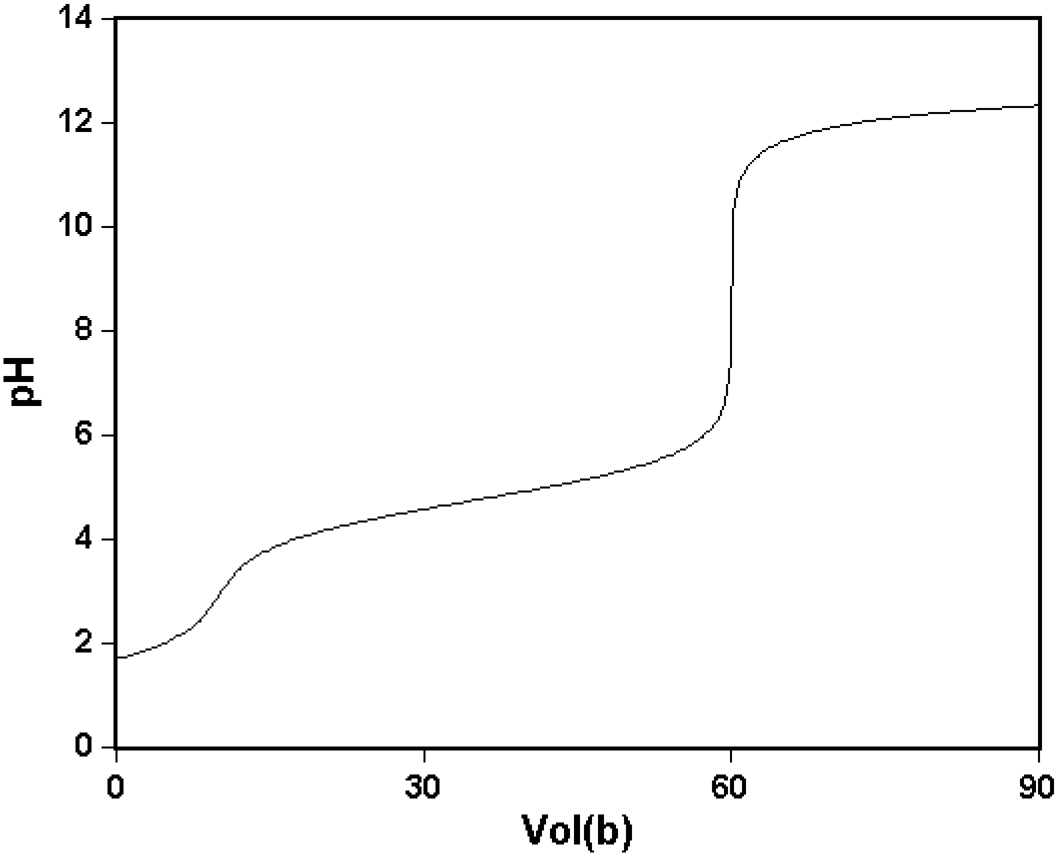
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0435 75

Ftn 0436 78

Ftn 0445: Titration: Strong & Weak Monoprotic Acids w/ Strong Base: pKa & Cso



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka = [H^+] * [A^-] / [HA]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^3 + B*[H^+]^2 + C*[H^+] + D = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka = 10^{-P[1]}$,

VT := K[2] + X,

A = 1.0,

B = Ka + (K[1]*X - K[2]*P[2])/VT,

C = [Ka * (K[1]*X - K[2]*P[2] - K[2]*K[4])/VT] - Kw,

D = -Ka*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above cubic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Cao	Initial concentration of the acid in moles/L.

Parameters

Parameter	**Name**	**Comments**
P1	pKa	-Log10 of the acid dissociation constant of the weak monoprotic acid.
P2	Cso	Initial concentration of the strong acid in moles/L.

Sample Applications

- Determining the acid dissociation constant, pKa, of a weak monoprotic acid and the concentration, Cso, of a strong acid in solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

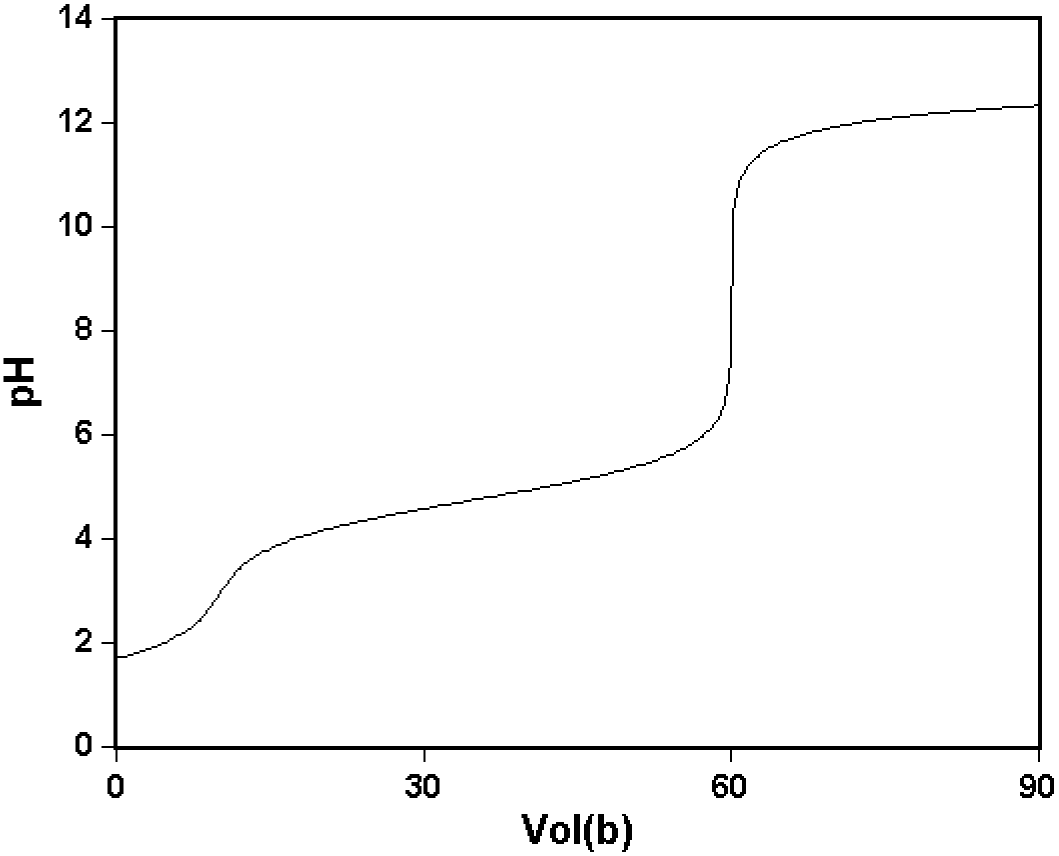
Also see

Ftn 0425 57

Ftn 0446 87

Ftn 0447 90

Ftn 0446: Titration: Strong & Weak Monoprotic Acids w/ Strong Base: pKa, Cso & Cao



Equation

HA ⇌ $H^+ + A^-$ with acid dissociation constant Ka = $[H^+] * [A^-] / [HA]$

H_2O ⇌ $H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$A*[H^+]^3 + B*[H^+]^2 + C*[H^+] + D = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka = 10^{-P[1]}$,

VT := K[2] + X,

A = 1.0,

B = Ka + (K[1]*X - K[2]*P[2])/VT,

C = [Ka * (K[1]*X - K[2]*P[2] - K[2]*P[3])/VT] - Kw,

D = -Ka*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above cubic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	Name	Comments
P1	pKa	-Log10 of the acid dissociation constant of the weak monoprotic acid.
P2	Cso	Initial concentration of the strong acid in moles/L.
P3	Cao	Initial concentration of the acid in moles/L.

Sample Applications

- Determining the acid dissociation constant, pKa, and concentration, Cao, of a weak monoprotic acid and the concentration, Cso, of a strong acid in solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

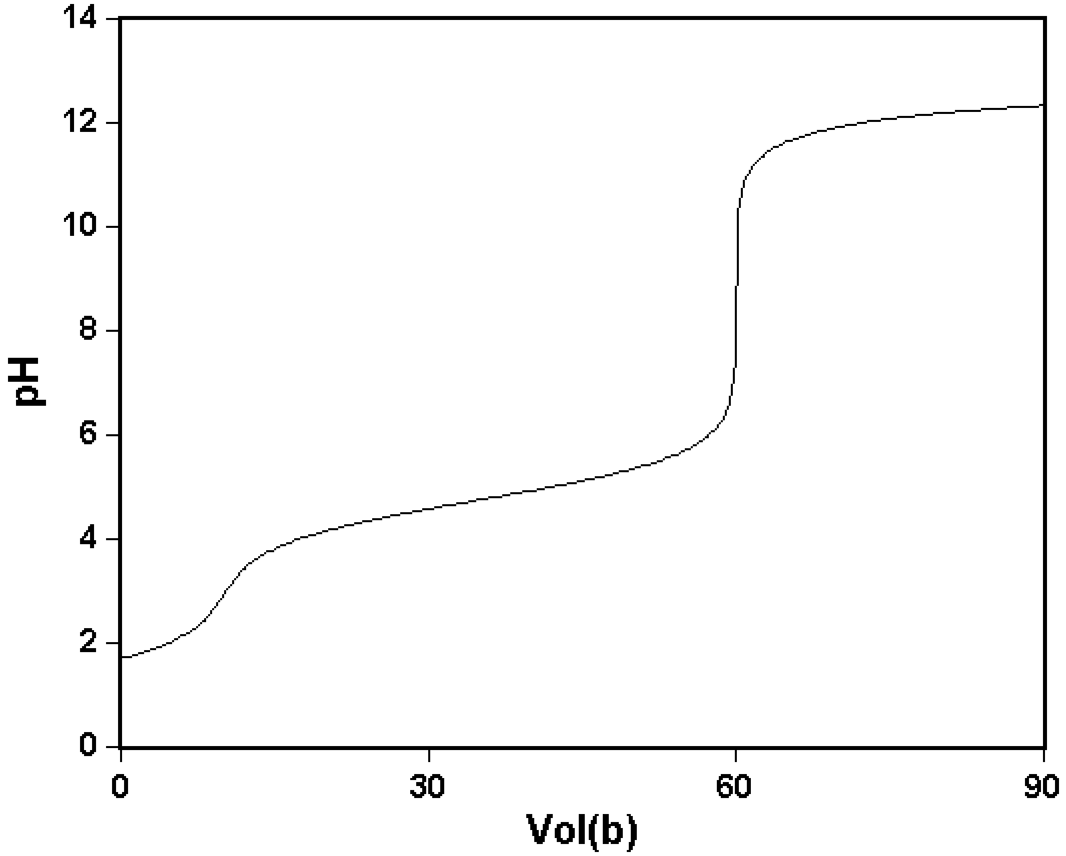
Also see

Ftn 0426 60

Ftn 0445 84

Ftn 0447 90

Ftn 0447: Titration: Strong & Weak Monoprotic Acids w/ Strong Base: pKa, Cso, Cao & pKw



Equation

HA ⇌ $H^+ + A^-$ with acid dissociation constant Ka = $[H^+] * [A^-] / [HA]$

H_2O ⇌ $H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$A*[H^+]^3 + B*[H^+]^2 + C*[H^+] + D = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[4]}$,

$Ka = 10^{-P[1]}$,

VT := K[2] + X,

$A = 1.0,$

$B = Ka + (K[1]*X - K[2]*P[2])/VT,$

$C = [Ka * (K[1]*X - K[2]*P[2] - K[2]*P[3])/VT] - Kw,$

$D = -Ka*Kw,$

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above cubic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	Name	Comments
P1	pKa	-Log10 of the acid dissociation constant of the weak monoprotic acid.
P2	Cso	Initial concentration of the strong acid in moles/L.
P3	Cao	Initial concentration of the acid in moles/L.
P4	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constant, pKa, and concentration, Cao, of a weak monoprotic acid and the concentration, Cso, of a strong acid in solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

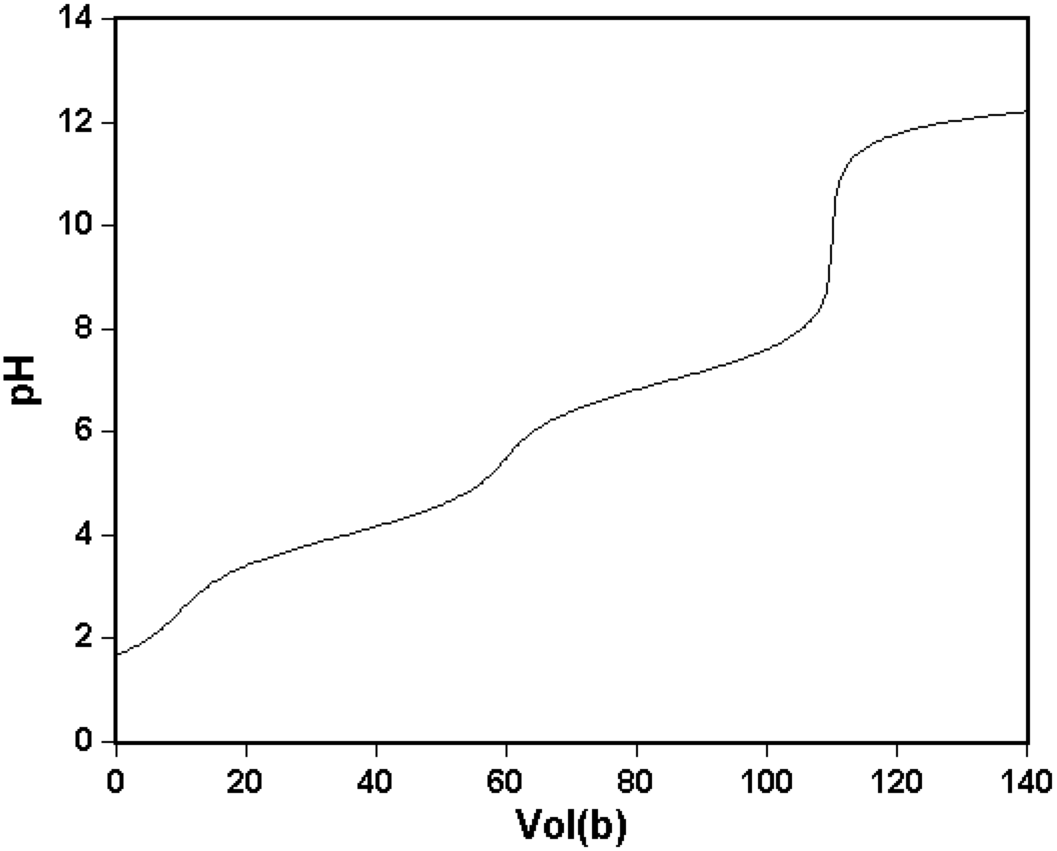
Also see

Ftn 0427 63

Ftn 0445 84

Ftn 0446 87

Ftn 0450: Titration: Strong & Weak Diprotic Acids w/ Strong Base: pKa1, pKa2 & Cso



Equation

$H_2A \rightleftharpoons H^+ + HA^-$ with acid dissociation constant Ka1 = $[H^+] * [HA^-] / [H_2A]$

$HA^- \rightleftharpoons H^+ + A^{2-}$ with acid dissociation constant Ka2 = $[H^+] * [A^{2-}] / [HA^-]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$$\mathbf{A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0}$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + (K[1]*X - K[2]*P[3])/VT,

C = Ka1*(Ka2 + (K[1]*X - K[2]*K[4] - K[2]*P[3])/VT) - Kw,

D = Ka1*Ka2*(K[1]*X - 2*K[2]*K[4] - K[2]*P[3])/VT - Ka1*Kw,

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Cao	Initial concentration of the acid in moles/L.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the first acid dissociation constant of the weak diprotic acid.
P2	pKa2	-Log10 of the second acid dissociation constant of the weak diprotic acid.
P3	Cso	Initial concentration of the strong acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1 & pKa2, of a weak diprotic acid and the concentration, Cso, of a strong acid in solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

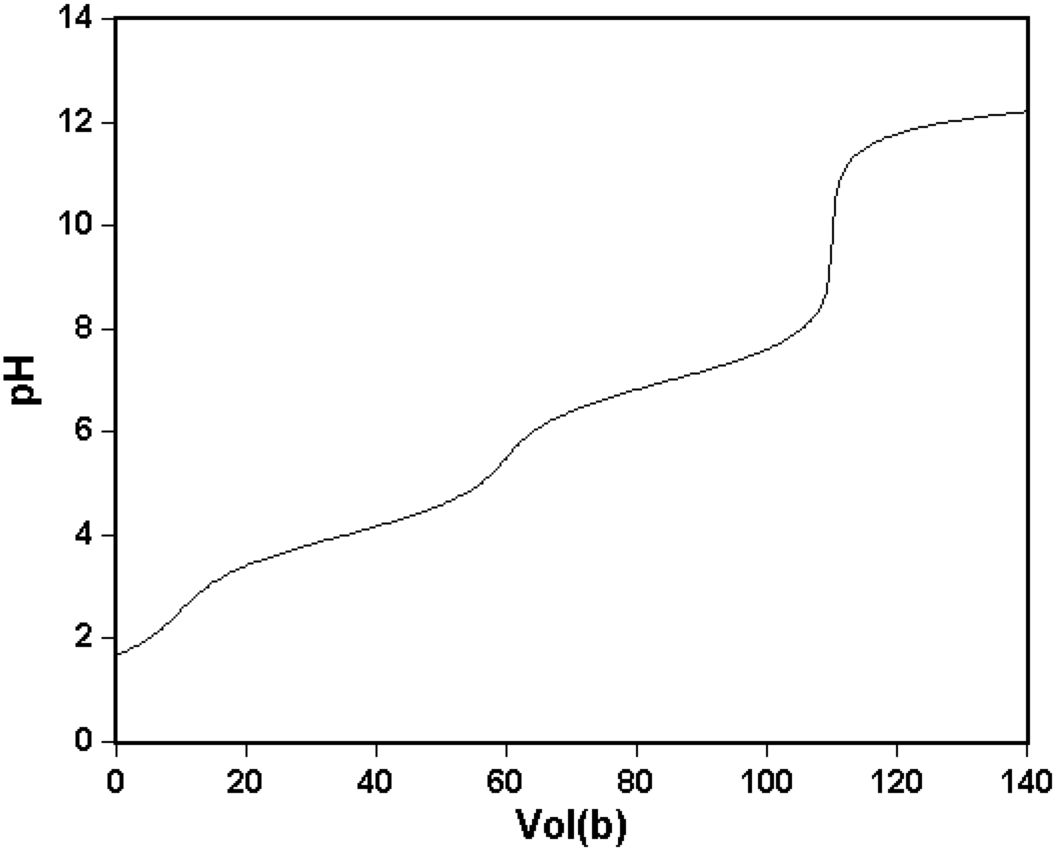
Also see

Ftn 0430 66

Ftn 0451 96

Ftn 0452 99

Ftn 0451: Titration: Strong & Weak Diprotic Acids w/ Strong Base: pKa1, pKa2, Cso & Cao



Equation

$H_2A \rightleftharpoons H^+ + HA^-$ with acid dissociation constant Ka1 = $[H^+] * [HA^-] / [H_2A]$

$HA^- \rightleftharpoons H^+ + A^{2-}$ with acid dissociation constant Ka2 = $[H^+] * [A^{2-}] / [HA^-]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + (K[1]*X - K[2]*P[3])/VT,

C = Ka1*(Ka2 + (K[1]*X - K[2]*P[4] - K[2]*P[3])/VT) - Kw,

D = Ka1*Ka2*(K[1]*X - 2*K[2]*P[4] - K[2]*P[3])/VT - Ka1*Kw,

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the first acid dissociation constant of the weak diprotic acid.
P2	pKa2	-Log10 of the second acid dissociation constant of the weak diprotic acid.
P3	Cso	Initial concentration of the strong acid in moles/L.
P4	Cao	Initial concentration of the acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1 & pKa2, and concentration, Cao, of a weak diprotic acid as well as the concentration, Cso, a strong acid in solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

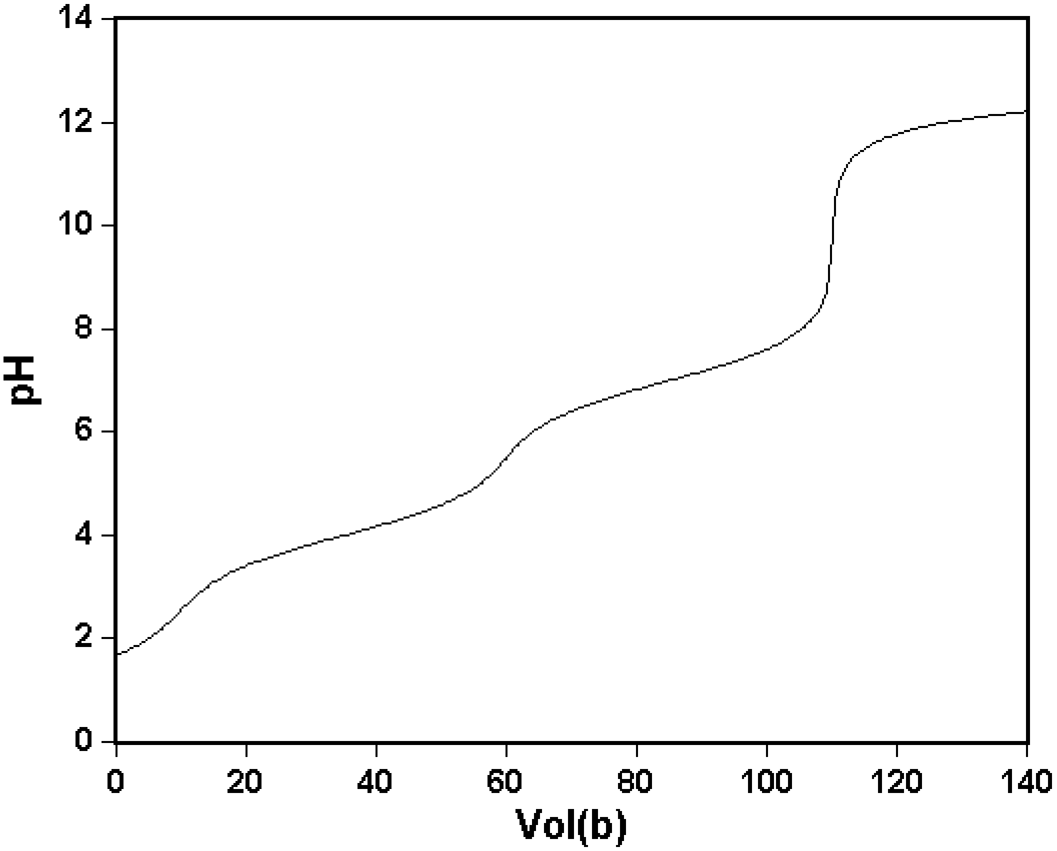
Also see

Ftn 0431 69

Ftn 0450 93

Ftn 0452 99

Ftn 0452: Titration: Strong & Weak Diprotic Acids w/ Strong Base: pKa1, pKa2, Cso, Cao & pKw



Equation

$H_2A \rightleftharpoons H^+ + HA^-$ with acid dissociation constant $Ka1 = [H^+] * [HA^-] / [H_2A]$

$HA^- \rightleftharpoons H^+ + A^{2-}$ with acid dissociation constant $Ka2 = [H^+] * [A^{2-}] / [HA^-]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$$A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[5]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + (K[1]*X - K[2]*P[3])/VT,

C = Ka1*(Ka2 + (K[1]*X - K[2]*P[4] - K[2]*P[3])/VT) - Kw,

D = Ka1*Ka2*(K[1]*X - 2*K[2]*P[4] - K[2]*P[3])/VT - Ka1*Kw,

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the first acid dissociation constant of the weak diprotic acid.
P2	pKa2	-Log10 of the second acid dissociation constant of the weak diprotic acid.
P3	Cso	Initial concentration of the strong acid in moles/L.
P4	Cao	Initial concentration of the acid in moles/L.
P5	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constants, pKa1 & pKa2, and concentration, Cao, of a weak diprotic acid as well as the concentration, Cso, of a strong acid in solution and the water autoprotolysis constant.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

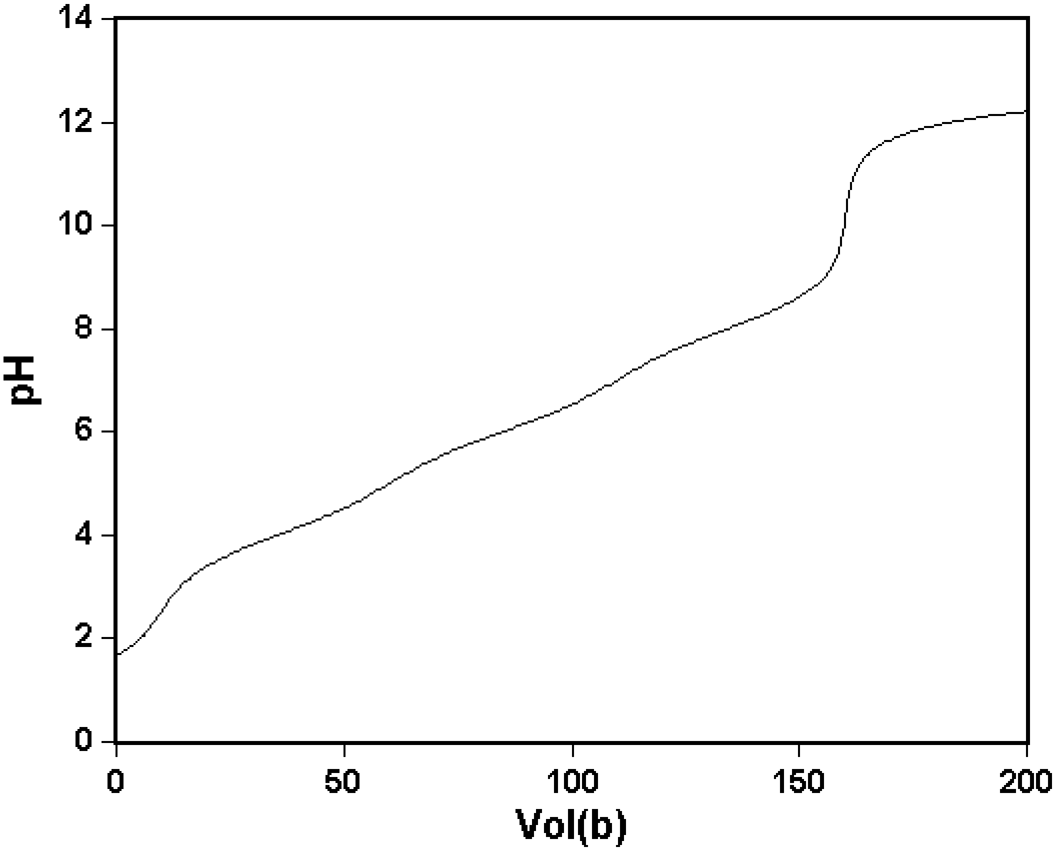
Also see

Ftn 0432 72

Ftn 0450 93

Ftn 0451 96

Ftn 0455: Titration: Strong & Weak Triprotic Acids w/ Strong Base: pKa1, pKa2, pKa3 & Cso



Equation

$H_3A \rightleftharpoons H^+ + H_2A^-$ with acid dissociation constant Ka1 = $[H^+] * [H_2A^-] / [H_3A]$

$H_2A^- \rightleftharpoons H^+ + HA^{2-}$ with acid dissociation constant Ka2 = $[H^+] * [HA^{2-}] / [H_2A^-]$

$HA^{2-} \rightleftharpoons H^+ + A^{3-}$ with acid dissociation constant Ka3 = $[H^+] * [A^{3-}] / [HA^{2-}]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + (K[1]*X - K[2]*P[4])/VT,

C = Ka1*(Ka2 - K[4] + (K[1]*X - K[2]*P[4])/VT) - Kw,

D = Ka1*Ka2*(Ka3 + (K[1]*X - K[2]*P[4])/VT - 2*K[4]) - Ka1*Kw,

E = Ka1*Ka2*Ka3*((K[1]*X - K[2]*P[4])/VT - 3*K[4]) - Ka1*Ka2*Kw,

F = -Ka1*Ka2*Ka3*Kw

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Cao	Initial concentration of the acid in moles/L.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the first acid dissociation constant of the weak triprotic acid.
P2	pKa2	-Log10 of the second acid dissociation constant of the weak triprotic acid.
P3	pKa3	-Log10 of the third acid dissociation constant of the weak triprotic acid.
P4	Cso	Initial concentration of the strong acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 & pKa3, of a weak triprotic acid and the concentration, Cso, of the strong acid.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

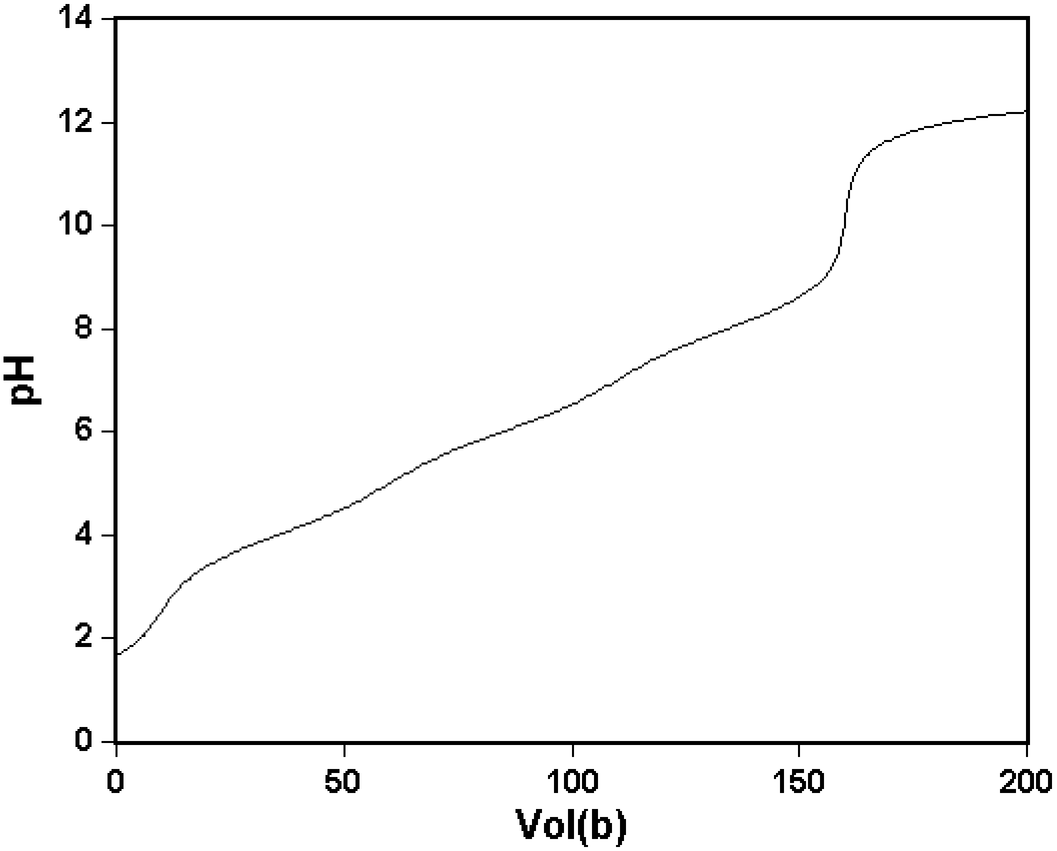
Also see

Ftn 0435 75

Ftn 0456 105

Ftn 0457 108

Ftn 0456: Titration: Strong & Weak Triprotic Acids w/ Strong Base: pKa1, pKa2, pKa3, Cso & Cao



Equation

$H_3A \rightleftharpoons H^+ + H_2A^-$ with acid dissociation constant $Ka1 = [H^+] * [H_2A^-] / [H_3A]$

$H_2A^- \rightleftharpoons H^+ + HA^{2-}$ with acid dissociation constant $Ka2 = [H^+] * [HA^{2-}] / [H_2A^-]$

$HA^{2-} \rightleftharpoons H^+ + A^{3-}$ with acid dissociation constant $Ka3 = [H^+] * [A^{3-}] / [HA^{2-}]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + (K[1]*X - K[2]*P[4])/VT,

C = Ka1*(Ka2 - P[5] + (K[1]*X - K[2]*P[4])/VT) - Kw,

D = Ka1*Ka2*(Ka3 + (K[1]*X - K[2]*P[4])/VT - 2*P[5]) - Ka1*Kw,

E = Ka1*Ka2*Ka3*((K[1]*X - K[2]*P[4])/VT - 3*P[5]) - Ka1*Ka2*Kw,

F = -Ka1*Ka2*Ka3*Kw

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the first acid dissociation constant of the weak triprotic acid.

Parameter	**Name**	**Comments**
P2	pKa2	-Log10 of the second acid dissociation constant of the weak triprotic acid.
P3	pKa3	-Log10 of the third acid dissociation constant of the weak triprotic acid.
P4	Cso	Initial concentration of the strong acid in moles/L.
P5	Cao	Initial concentration of the acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 & pKa3, and concentration, Cao, of a weak triprotic acid as well as the concentration, Cso, of the strong acid.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.
- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

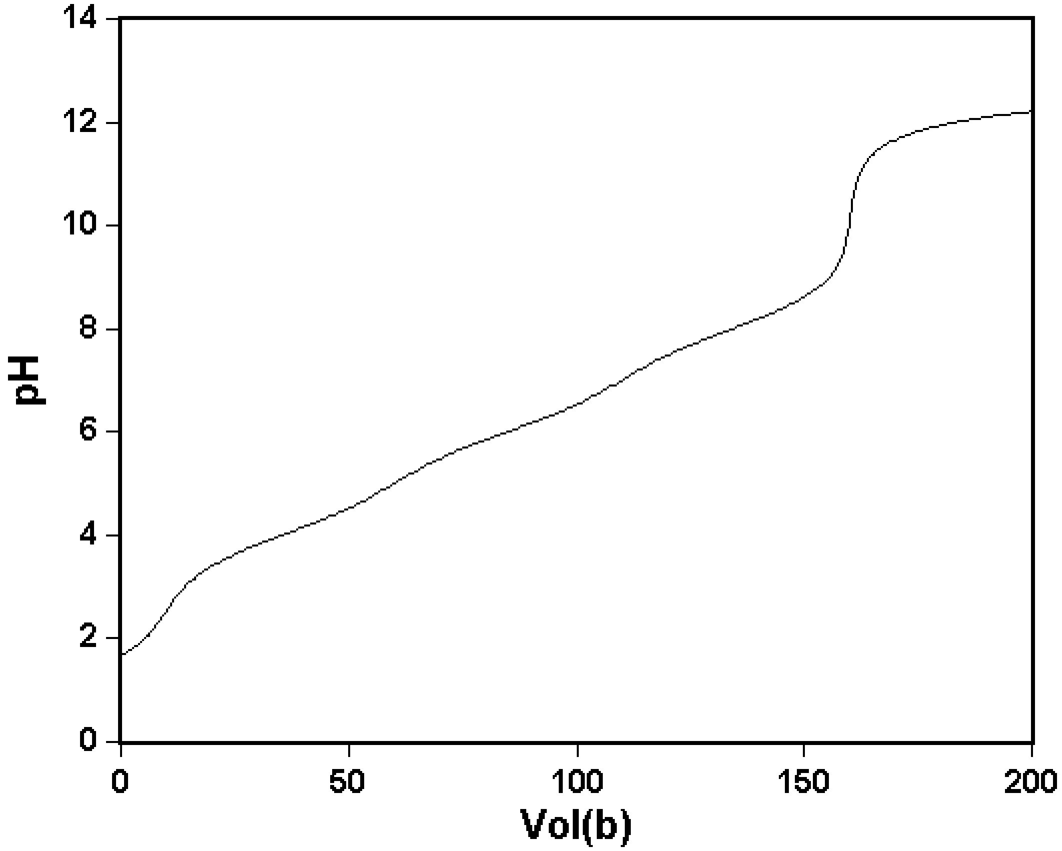
Also see

Ftn 0436 78

Ftn 0455 102

Ftn 0457 108

Ftn 0457: Titration: Strong & Weak Triprotic Acids w/ Strong Base: pKa1, pKa2, pKa3, Cso, Cao & pKw



Equation

$H_3A \rightleftharpoons H^+ + H_2A^-$ with acid dissociation constant Ka1 = $[H^+] * [H_2A^-] / [H_3A]$

$H_2A^- \rightleftharpoons H^+ + HA^{2-}$ with acid dissociation constant Ka2 = $[H^+] * [HA^{2-}] / [H_2A^-]$

$HA^{2-} \rightleftharpoons H^+ + A^{3-}$ with acid dissociation constant Ka3 = $[H^+] * [A^{3-}] / [HA^{2-}]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[6]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + (K[1]*X - K[2]*P[4])/VT,

C = Ka1*(Ka2 - P[5] + (K[1]*X - K[2]*P[4])/VT) - Kw,

D = Ka1*Ka2*(Ka3 + (K[1]*X - K[2]*P[4])/VT - 2*P[5]) - Ka1*Kw,

E = Ka1*Ka2*Ka3*((K[1]*X - K[2]*P[4])/VT - 3*P[5]) - Ka1*Ka2*Kw,

F = -Ka1*Ka2*Ka3*Kw

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.

- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the first acid dissociation constant of the weak triprotic acid.
P2	pKa2	-Log10 of the second acid dissociation constant of the weak triprotic acid.

Parameter	Name	Comments
P3	pKa3	-Log10 of the third acid dissociation constant of the weak triprotic acid.
P4	Cso	Initial concentration of the strong acid in moles/L.
P5	Cao	Initial concentration of the acid in moles/L.
P6	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 & pKa3, and concentration, Cao, of a weak triprotic acid as well as the concentration, Cso, of the strong acid and the water autoprotolysis constant, pKw.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

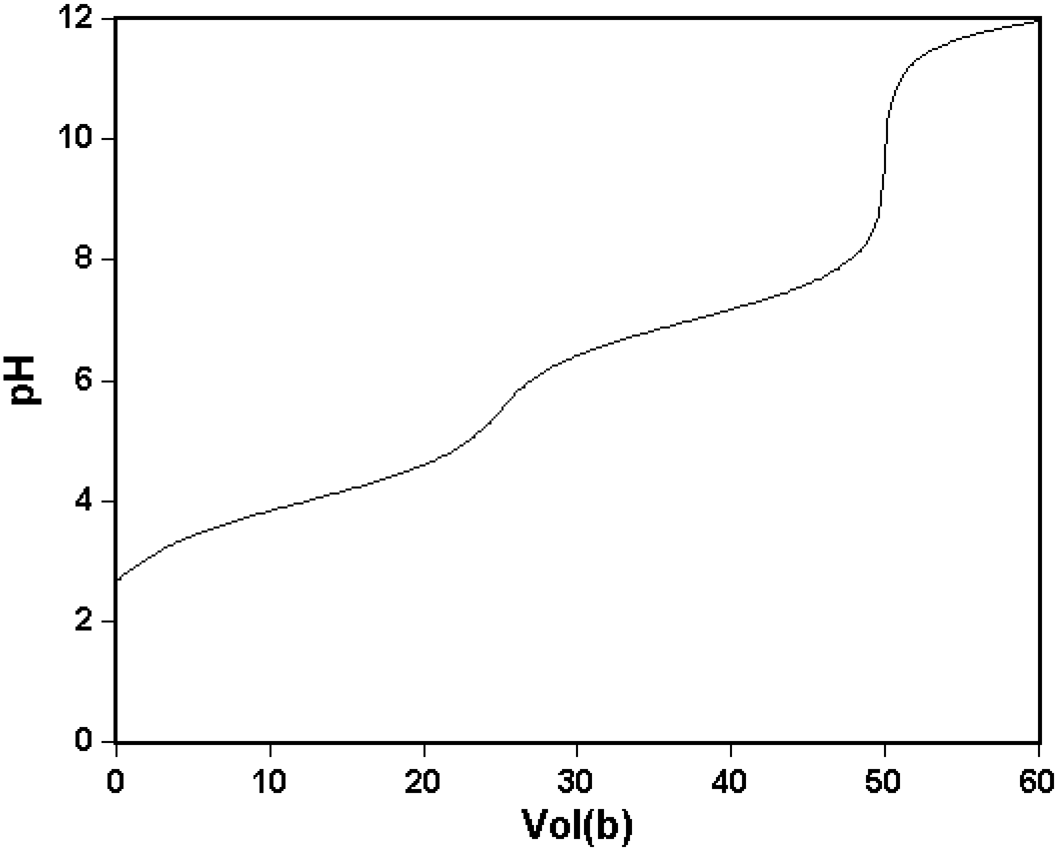
Also see

Ftn 0437 81

Ftn 0455 102

Ftn 0456 105

Ftn 0465: Titration: Two Weak Monoprotic Acids w/ Strong Base: pKa1 & pKa2



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka1 = [H^+] * [A^-] / [HA]$

$HB \rightleftharpoons H^+ + B^-$ with acid dissociation constant $Ka2 = [H^+] * [B^-] / [HB]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + K[1]*X/VT,

C = (Ka1+Ka2)*(K[1]*X - Ka1*K[2]*K[4] - Ka2*K[2]*K[5])/VT + Ka1*Ka2 - Kw,

D = (K[1]*X - K[2]*K[4] - K[2]*K[5])*Ka1*Ka2/VT - Kw*(Ka1+Ka2)

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
K5	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.

Parameter	Name	Comments
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.

Sample Applications

- Determining the acid dissociation constants, pKa1 and pKa2, of a mixture of two weak monoprotic acids.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

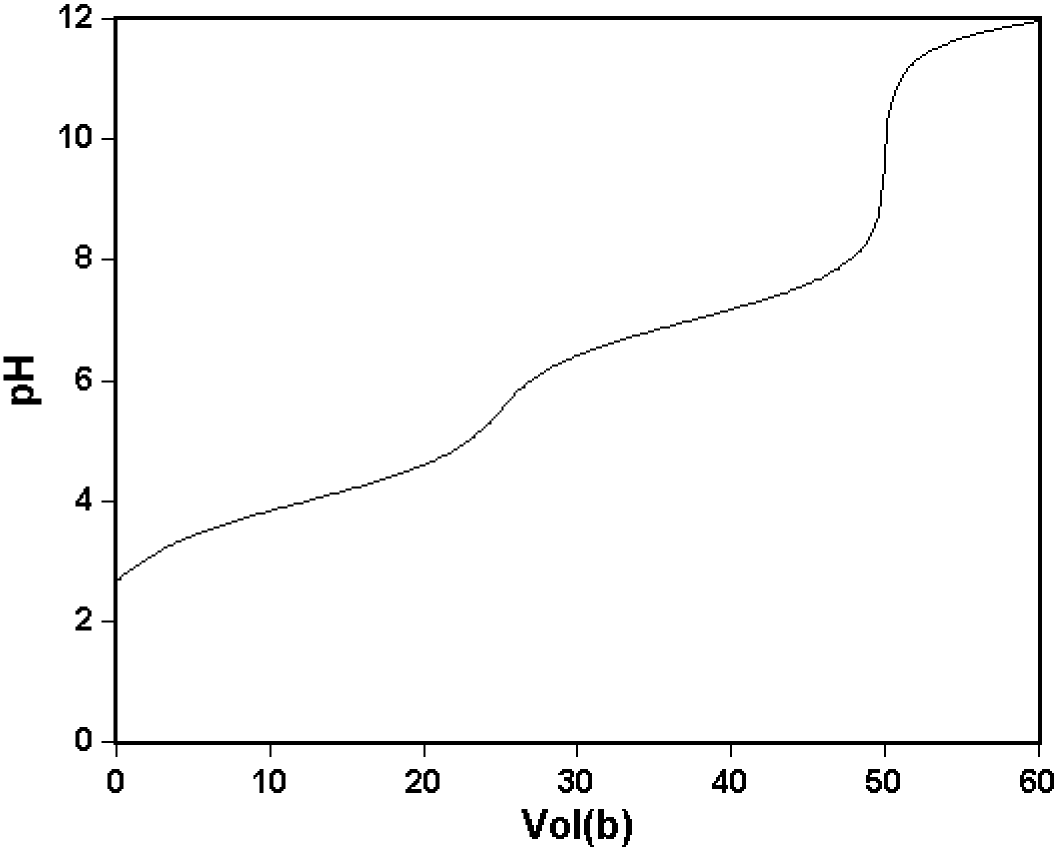
- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

Also see

Ftn 0426 60

Ftn 0427 63

Ftn 0466: Titration: Two Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2, Ca1o & Ca2o



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka1 = [H^+] * [A^-] / [HA]$

$HB \rightleftharpoons H^+ + B^-$ with acid dissociation constant $Ka2 = [H^+] * [B^-] / [HB]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + K[1]*X/VT,

C = (Ka1+Ka2)*(K[1]*X - Ka1*K[2]*P[3] - Ka2*K[2]*P[4])/VT + Ka1*Ka2 - Kw,

D = (K[1]*X - K[2]*P[3] - K[2]*P[4])*Ka1*Ka2/VT - Kw*(Ka1+Ka2)

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.

Parameter	Name	Comments
P4	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1 and pKa2, of a mixture of two weak monoprotic acids.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

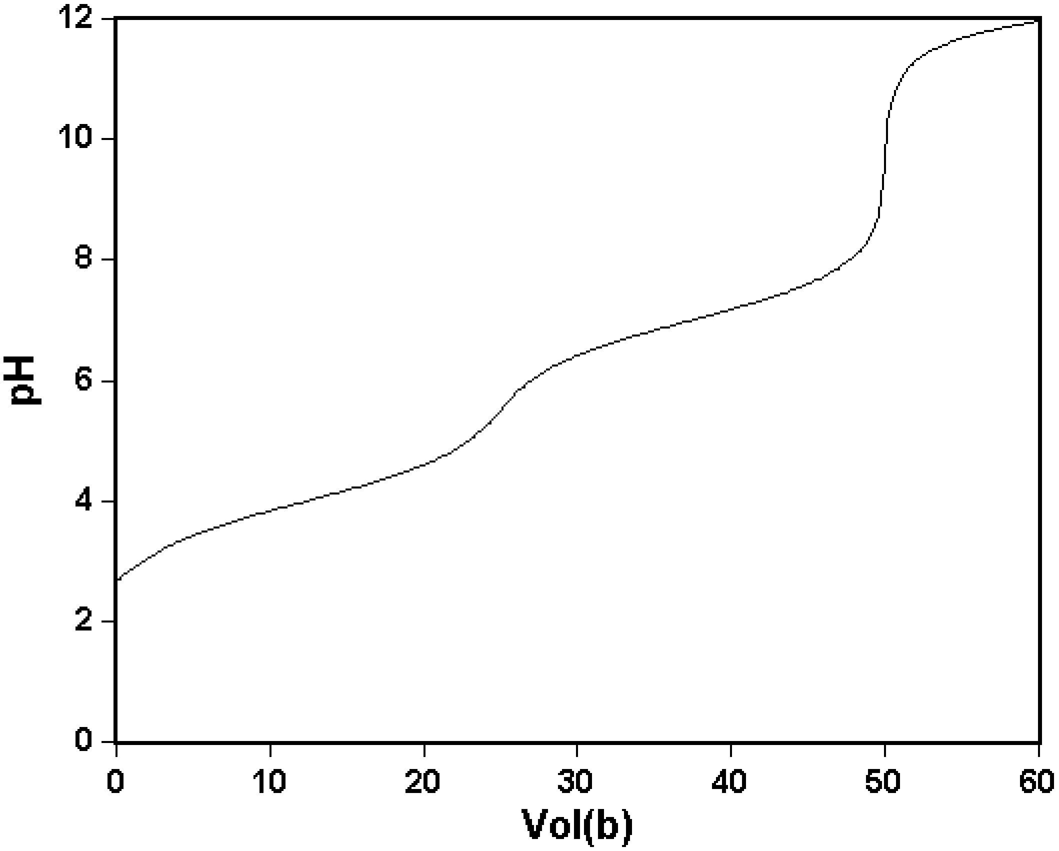
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0426 60

Ftn 0427 63

Ftn 0467: Titration: Two Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2, Ca1o, Ca2o & pKw



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka1 = [H^+] * [A^-] / [HA]$

$HB \rightleftharpoons H^+ + B^-$ with acid dissociation constant $Ka2 = [H^+] * [B^-] / [HB]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[5]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + K[1]*X/VT,

C = (Ka1+Ka2)*(K[1]*X - Ka1*K[2]*P[3] - Ka2*K[2]*P[4])/VT + Ka1*Ka2 - Kw,

D = (K[1]*X - K[2]*P[3] - K[2]*P[4])*Ka1*Ka2/VT - Kw*(Ka1+Ka2)

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
P4	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.

Parameter	Name	Comments
P5	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constants, pKa1 and pKa2, of a mixture of two weak monoprotic acids.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

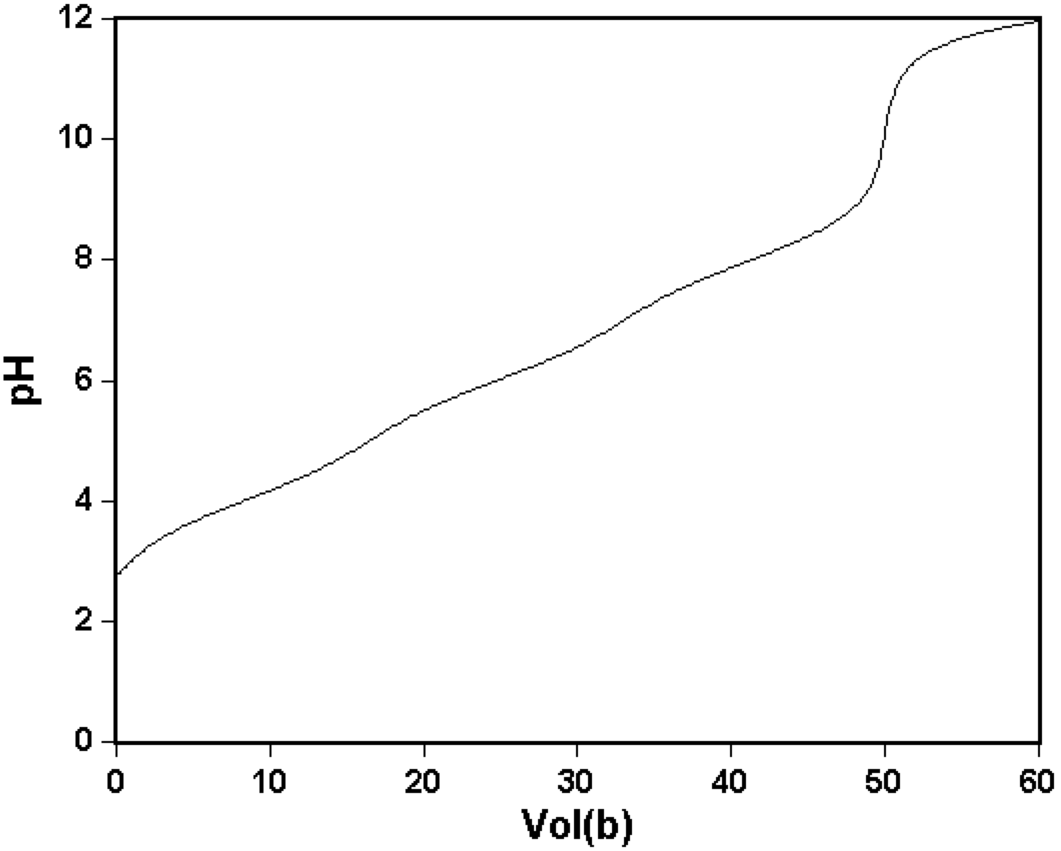
- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

Also see

Ftn 0426 60

Ftn 0427 63

Ftn 0470: Titration: Three Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2 & pKa3



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka1 = [H^+] * [A^-] / [HA]$

$HB \rightleftharpoons H^+ + B^-$ with acid dissociation constant $Ka2 = [H^+] * [B^-] / [HB]$

$HC \rightleftharpoons H^+ + C^-$ with acid dissociation constant $Ka3 = [H^+] * [C^-] / [HC]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

Ka1 = $10^{-P[1]}$,

Ka2 = $10^{-P[2]}$,

Ka3 = $10^{-P[3]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + Ka3+ K[1]*X/VT,

C = (Ka1+Ka2+Ka3)*K[1]*X/VT + Ka1*(Ka2+Ka3-K[2]*K[4]/VT) - Ka2*K[2]*K[5]//VT - Ka3*K[2]*K[6]/VT - Kw,

D = (Ka1*Ka2 + Ka1*Ka3 + Ka2*Ka3)*K[1]*X/VT

- Ka1*(Ka2+Ka3)*K[2]*K[4]/VT

- Ka2*(Ka1+Ka3)*K[2]*K[5]/VT

- Ka3*(Ka1+Ka2)*K[2]*K[6]/VT

- Kw*(Ka1+Ka2+Ka3)

+ Ka1*Ka2*Ka3

E = Ka1*Ka2*Ka3*(K[1]*X - K[2]*K[4] - K[2]*K[5] - K[2]*K[6])/VT

- Kw*(Ka1*Ka2+Ka1*Ka3+Ka2*Ka3)

F = -Ka1*Ka2*Ka3*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Constant	Name	Comments
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
K5	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.
K6	Ca3o	Initial concentration of the third monoprotic weak acid in moles/L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	pKa3	-Log10 of the acid dissociation constant of the third weak monoprotic acid.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 and pKa3, of a mixture of three weak monoprotic acids.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

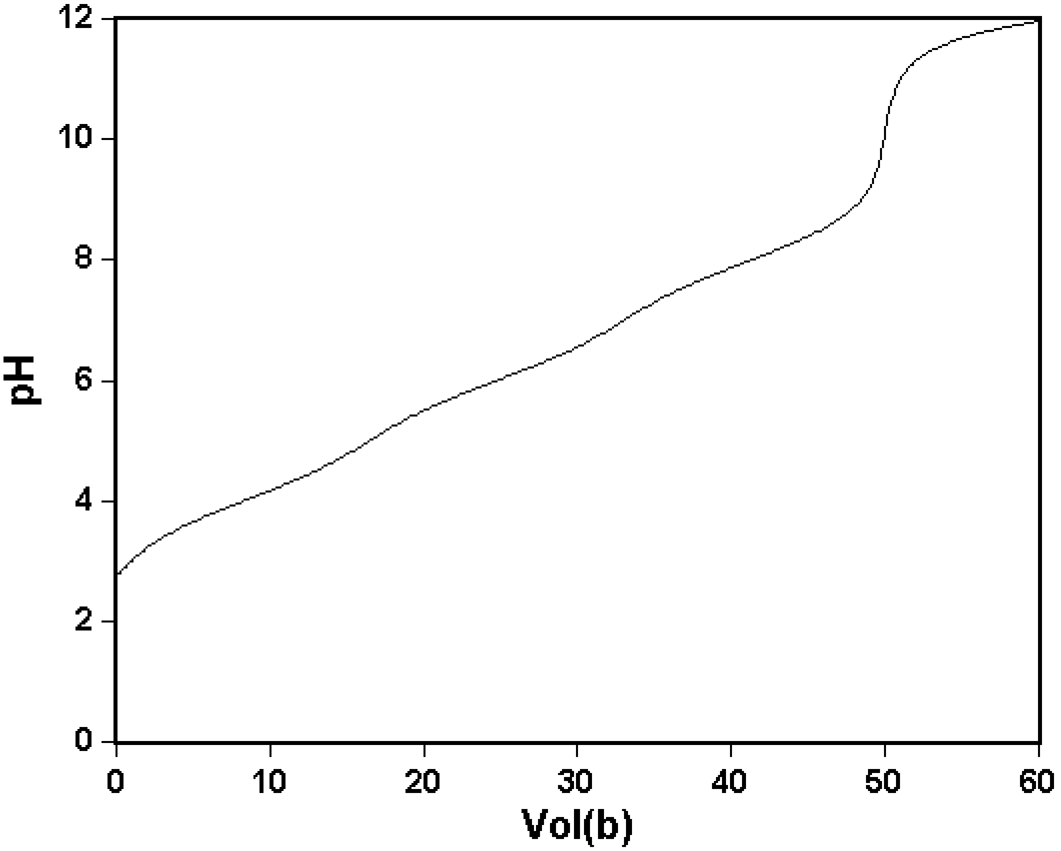
Also see

Ftn 0435 75

Ftn 0471 123

Ftn 0472 126

Ftn 0471: Titration: Three Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2, pKa3, Ca1o, Ca2o & Ca3o



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka1 = [H^+] * [A^-] / [HA]$

$HB \rightleftharpoons H^+ + B^-$ with acid dissociation constant $Ka2 = [H^+] * [B^-] / [HB]$

$HC \rightleftharpoons H^+ + C^-$ with acid dissociation constant $Ka3 = [H^+] * [C^-] / [HC]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + Ka3+ K[1]*X/VT,

C = (Ka1+Ka2+Ka3)*K[1]*X/VT + Ka1*(Ka2+Ka3-K[2]*P[4]/VT) - Ka2*K[2]*P[5]//VT - Ka3*K[2]*P[6]/VT - Kw,

D = (Ka1*Ka2 + Ka1*Ka3 + Ka2*Ka3)*K[1]*X/VT

- Ka1*(Ka2+Ka3)*K[2]*P[4]/VT

- Ka2*(Ka1+Ka3)*K[2]*P[5]/VT

- Ka3*(Ka1+Ka2)*K[2]*P[6]/VT

- Kw*(Ka1+Ka2+Ka3)

+ Ka1*Ka2*Ka3

E = Ka1*Ka2*Ka3*(K[1]*X - K[2]*P[4] - K[2]*P[5] - K[2]*P[6])/VT

- Kw*(Ka1*Ka2+Ka1*Ka3+Ka2*Ka3)

F = -Ka1*Ka2*Ka3*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Constant	**Name**	**Comments**
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	pKa3	-Log10 of the acid dissociation constant of the third weak monoprotic acid.
P4	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
P5	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.
P6	Ca3o	Initial concentration of the third monoprotic weak acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 and pKa3, and the concentrations, Ca1o, Ca2o and Ca3o, of the acids in a mixture of three weak monoprotic acids.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

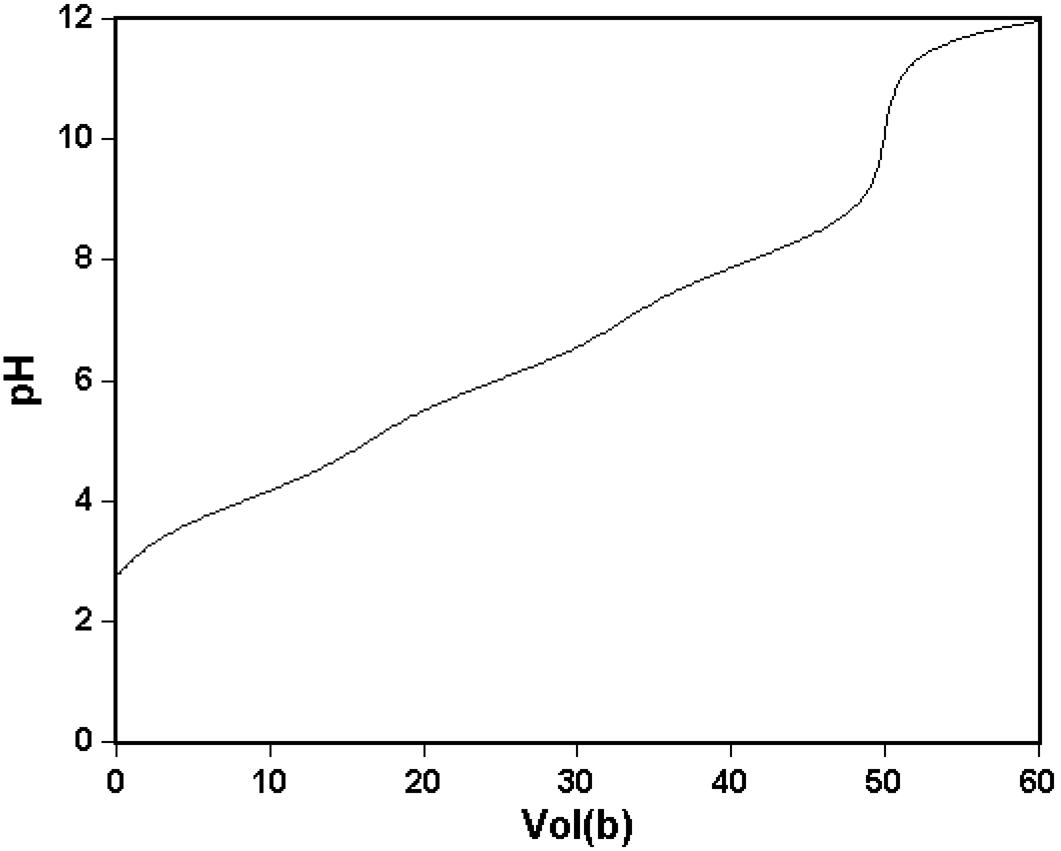
Also see

Ftn 0436 78

Ftn 0470 120

Ftn 0472 126

Ftn 0472: Titration: Three Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2, pKa3, Ca1o, Ca2o, Ca3o & pKw



Equation

HA ⇌ $H^+ + A^-$ with acid dissociation constant Ka1 = $[H^+] * [A^-] / [HA]$

HB ⇌ $H^+ + B^-$ with acid dissociation constant Ka2 = $[H^+] * [B^-] / [HB]$

HC ⇌ $H^+ + C^-$ with acid dissociation constant Ka3 = $[H^+] * [C^-] / [HC]$

H_2O ⇌ $H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[7]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

$VT := K[2] + X$,

$A = 1.0$,

$B = Ka1 + Ka2 + Ka3+ K[1]*X/VT$,

$C = (Ka1+Ka2+Ka3)*K[1]*X/VT + Ka1*(Ka2+Ka3-K[2]*P[4]/VT) - Ka2*K[2]*P[5]//VT - Ka3*K[2]*P[6]/VT - Kw$,

$D = (Ka1*Ka2 + Ka1*Ka3 + Ka2*Ka3)*K[1]*X/VT$

$- Ka1*(Ka2+Ka3)*K[2]*P[4]/VT$

$- Ka2*(Ka1+Ka3)*K[2]*P[5]/VT$

$- Ka3*(Ka1+Ka2)*K[2]*P[6]/VT$

$- Kw*(Ka1+Ka2+Ka3)$

$+ Ka1*Ka2*Ka3$

$E = Ka1*Ka2*Ka3*(K[1]*X - K[2]*P[4] - K[2]*P[5] - K[2]*P[6])/VT$

$- Kw*(Ka1*Ka2+Ka1*Ka3+Ka2*Ka3)$

$F = -Ka1*Ka2*Ka3*Kw$,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	pKa3	-Log10 of the acid dissociation constant of the third weak monoprotic acid.
P4	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
P5	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.
P6	Ca3o	Initial concentration of the third monoprotic weak acid in moles/L.
P7	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 and pKa3, and the concentrations, Ca1o, Ca2o and Ca3o, of the acids of a mixture of three weak monoprotic acids as well as the water autoprotolysis constant, pKw.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

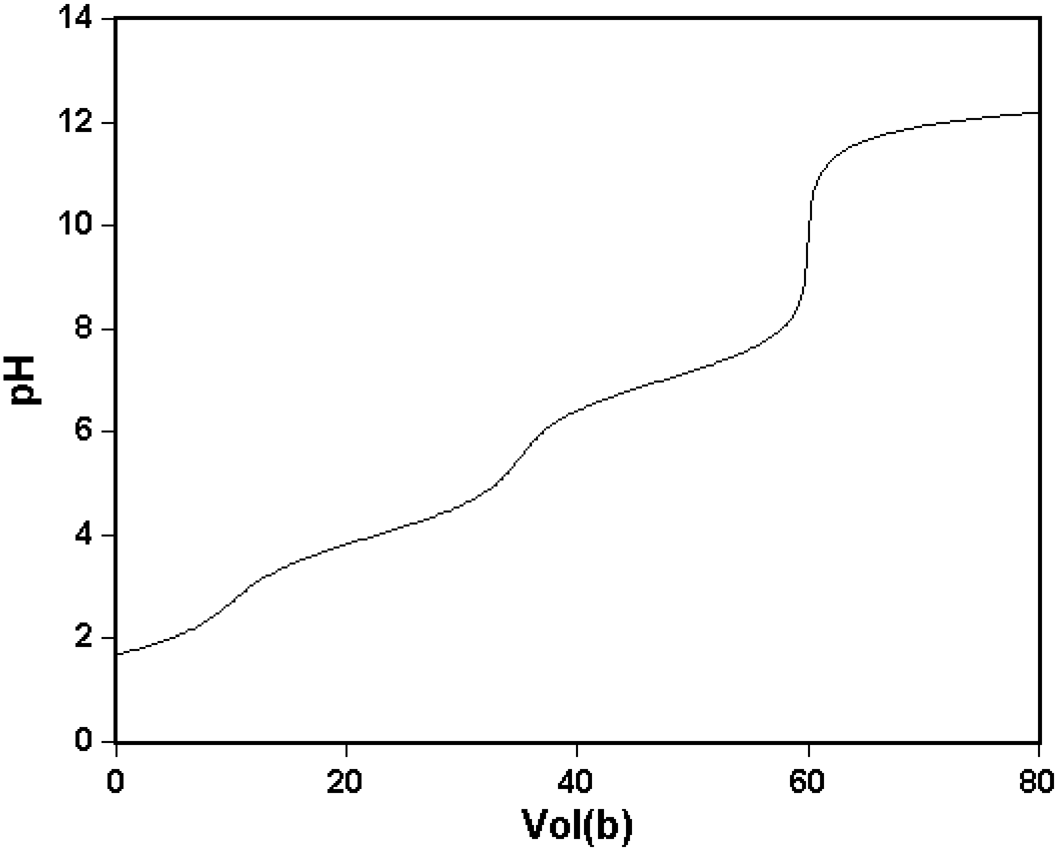
Also see

Ftn 0437 81

Ftn 0470 120

Ftn 0471 123

Ftn 0485: Titration: Strong Acid + Two Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2 & Cso



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka1 = [H^+] * [A^-] / [HA]$

$HB \rightleftharpoons H^+ + B^-$ with acid dissociation constant $Ka2 = [H^+] * [B^-] / [HB]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$$A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + (K[1]*X - K[2]*P[3])/VT,

C = (Ka1+Ka2)*(K[1]*X - K[2]*P[3])/VT - K[2]*(Ka1*K[4] - Ka2*K[5])/VT + Ka1*Ka2 - Kw;

D = (K[1]*X - K[2]*K[4] - K[2]*K[5])*Ka1*Ka2/VT - Kw*(Ka1+Ka2),

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
K5	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.

Parameter	Name	Comments
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	Cso	Initial concentration of the strong acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1 and pKa2, of a mixture of two weak monoprotic acids and the concentration, Cso, of a strong acid in solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

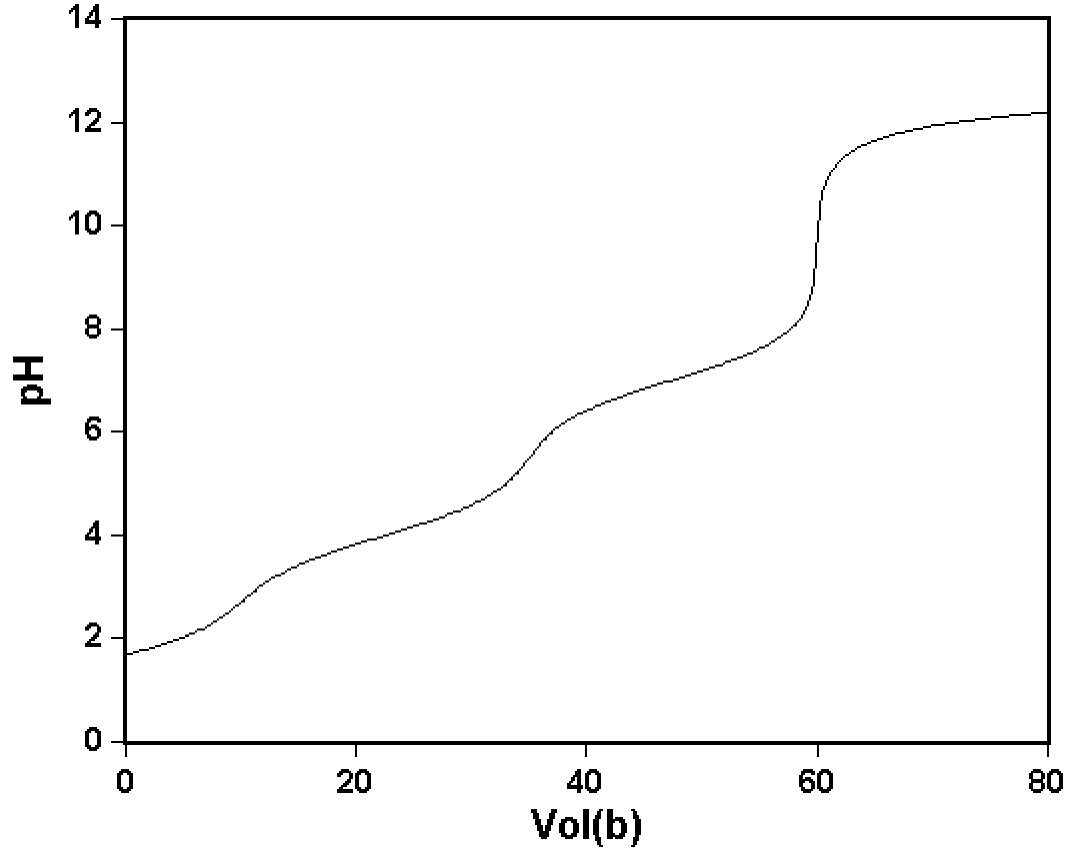
Also see

Ftn 0465 111

Ftn 0486 132

Ftn 0487 135

Ftn 0486: Titration: Strong Acid + Two Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2, Cso, Ca1o & Ca2o



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka1 = [H^+] * [A^-] / [HA]$

$HB \rightleftharpoons H^+ + B^-$ with acid dissociation constant $Ka2 = [H^+] * [B^-] / [HB]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$$\mathbf{A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0}$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + (K[1]*X - K[2]*P[3])/VT,

C = (Ka1+Ka2)*(K[1]*X - K[2]*P[3])/VT - K[2]*(Ka1*P[4] - Ka2*P[5])/VT + Ka1*Ka2 - Kw;

D = (K[1]*X - K[2]*P[4] - K[2]*P[5])*Ka1*Ka2/VT - Kw*(Ka1+Ka2),

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	Cso	Initial concentration of the strong acid in moles/L.

Parameter	Name	Comments
P4	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
P5	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1 and pKa2, and concentrations of a mixture of two weak monoprotic acids as well as the concentration, Cso, of a strong acid in solution..

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

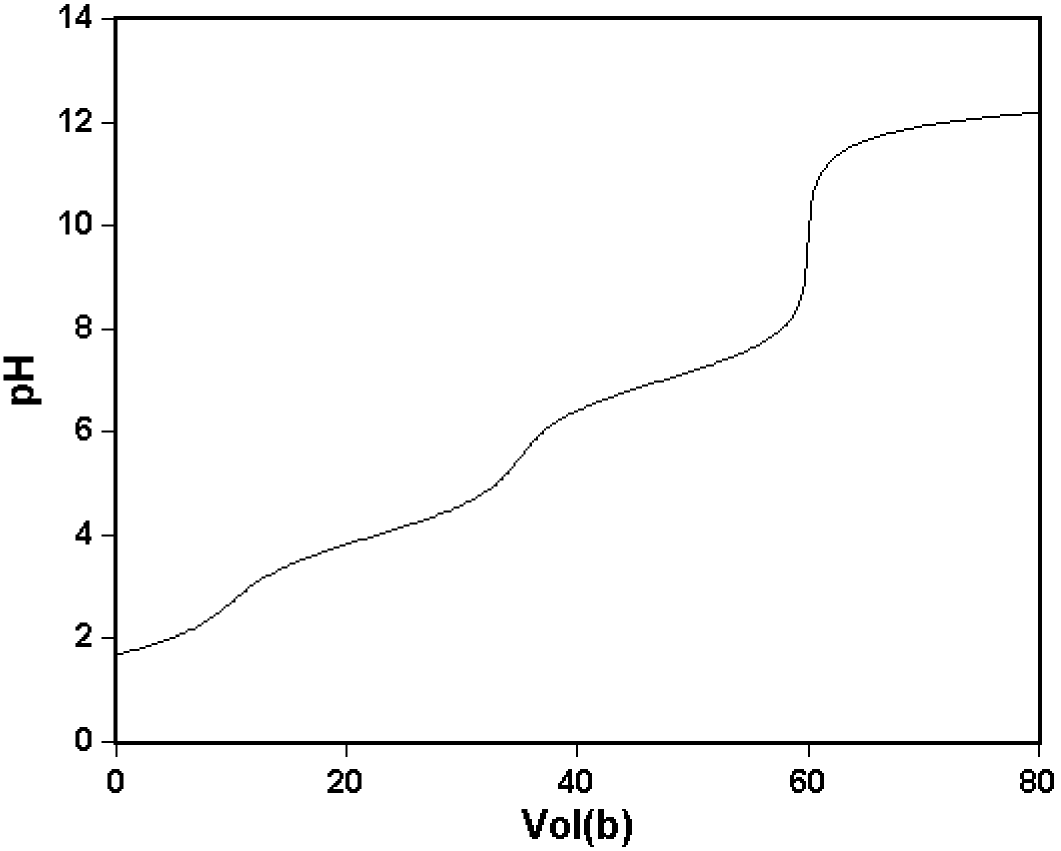
Also see

Ftn 0466 114

Ftn 0485 129

Ftn 0487 135

Ftn 0487: Titration: Strong Acid + Two Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2, Cso, Ca1o, Ca2o & pKw



Equation

HA $\rightleftharpoons$ $H^+ + A^-$ with acid dissociation constant Ka1 = $[H^+] * [A^-] / [HA]$

HB $\rightleftharpoons$ $H^+ + B^-$ with acid dissociation constant Ka2 = $[H^+] * [B^-] / [HB]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$A*[H^+]^4 + B*[H^+]^3 + C*[H^+]^2 + D*[H^+] + E = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[6]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + (K[1]*X - K[2]*P[3])/VT,

C = (Ka1+Ka2)*(K[1]*X - K[2]*P[3])/VT - K[2]*(Ka1*P[4] - Ka2*P[5])/VT + Ka1*Ka2 - Kw;

D = Ka1*Ka2*(K[1]*X - K[2]*P[4] - K[2]*P[5])/VT - Kw*(Ka1+Ka2),

E = -Ka1*Ka2*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quartic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	Cso	Initial concentration of the strong acid in moles/L.
P4	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.

Parameter	Name	Comments
P5	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.
P6	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constants, pKa1 and pKa2, and concentrations of a mixture of two weak monoprotic acids as well as the concentration, Cso, of a strong acid in solution and the water autoprotolysis constant, pKw.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

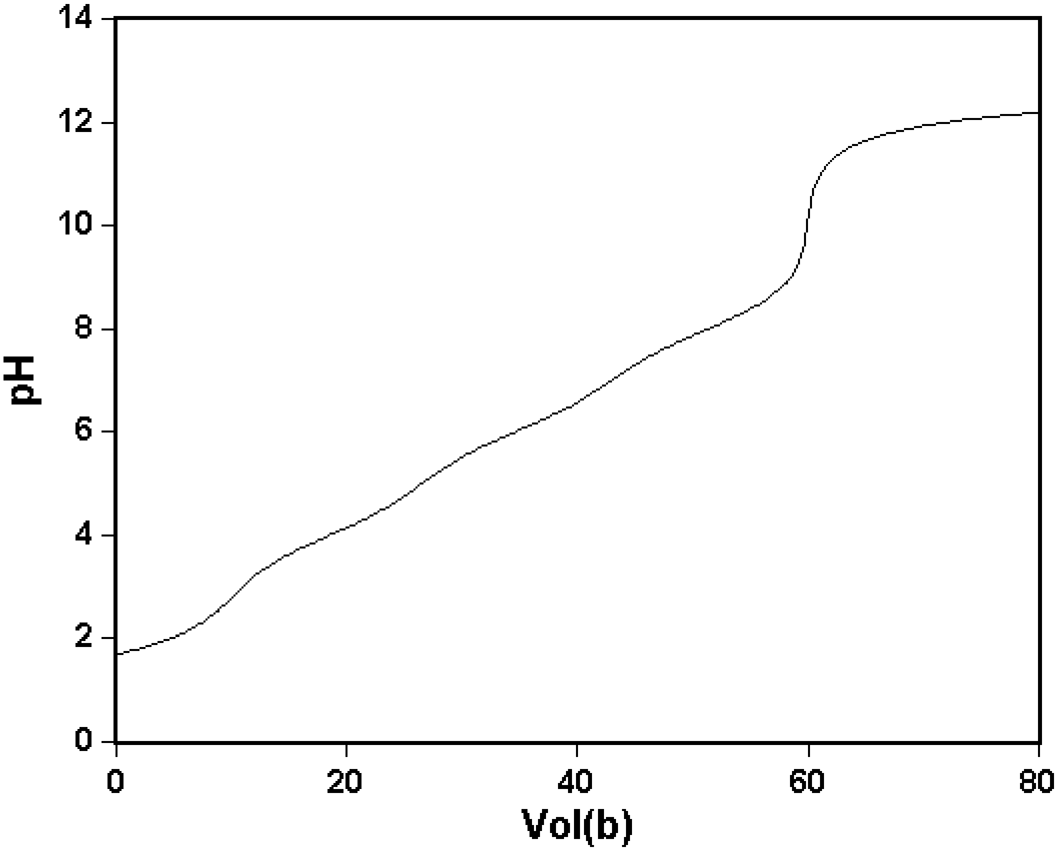
Also see

Ftn 0467 117

Ftn 0485 129

Ftn 0486 132

Ftn 0490: Titration: Strong Acid + Three Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2, pKa3 & Cso



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka1 = [H^+] * [A^-] / [HA]$

$HB \rightleftharpoons H^+ + B^-$ with acid dissociation constant $Ka2 = [H^+] * [B^-] / [HB]$

$HC \rightleftharpoons H^+ + C^-$ with acid dissociation constant $Ka3 = [H^+] * [C^-] / [HC]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

$VT := K[2] + X$,

$A = 1.0$,

$B = Ka1 + Ka2 + Ka3+ (K[1]*X - K[2]*P[4])/VT$,

$C = (Ka1+Ka2+Ka3)*(K[1]*X - K[2]*P[4])/VT + Ka1*(Ka2+Ka3-K[2]*K[4]/VT) - Ka2*K[2]*K[5]//VT - Ka3*K[2]*K[6]/VT - Kw$,

$D = (Ka1*Ka2 + Ka1*Ka3 + Ka2*Ka3)*(K[1]*X - K[2]*P[4])/VT$

$- Ka1*(Ka2+Ka3)*K[2]*K[4]/VT$

$- Ka2*(Ka1+Ka3)*K[2]*K[5]/VT$

$- Ka3*(Ka1+Ka2)*K[2]*K[6]/VT$

$- Kw*(Ka1+Ka2+Ka3)$

$+ Ka1*Ka2*Ka3$

$E = Ka1*Ka2*Ka3*(K[1]*X - K[2]*P[4] - K[2]*K[4] - K[2]*K[5] - K[2]*K[6])/VT$

$- Kw*(Ka1*Ka2+Ka1*Ka3+Ka2*Ka3)$

$F = -Ka1*Ka2*Ka3*Kw$,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	Name	Comments
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that used for the volume of strong base titrant, e.g. mL or L.

Constant	**Name**	**Comments**
K3	pKw	-Log10 of the water autoprotolysis constant.
K4	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
K5	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.
K6	Ca3o	Initial concentration of the third monoprotic weak acid in moles/L.

Parameters

Parameter	**Name**	**Comments**
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	pKa3	-Log10 of the acid dissociation constant of the third weak monoprotic acid.
P4	Cso	Initial concentration of the strong acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 and pKa3, of a mixture of three weak monoprotic acids and the concentration, Cso, of a strong acid in solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

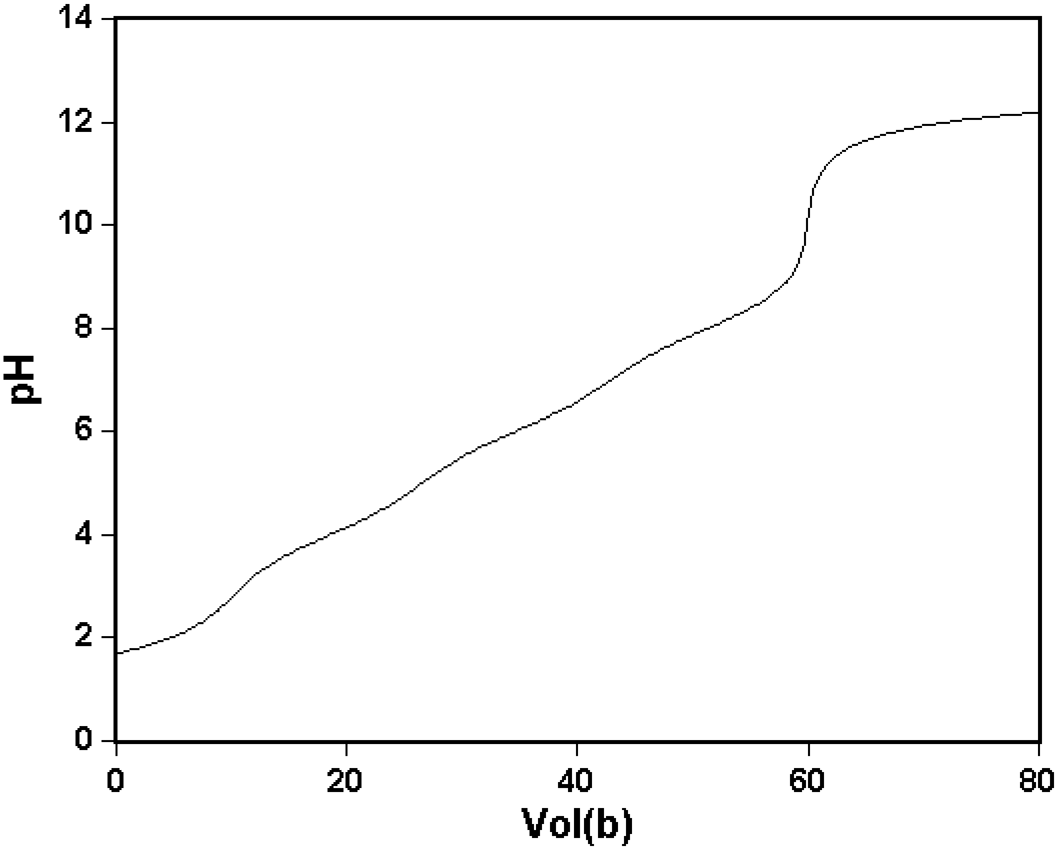
Also see

Ftn 0470 120

Ftn 0491 142

Ftn 0492 146

Ftn 0491: Titration: Strong Acid + Three Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2, pKa3, Cso, Ca1o, Ca2o & Ca3o



Equation

HA ⇌ $H^+ + A^-$ with acid dissociation constant Ka1 = $[H^+] * [A^-] / [HA]$

HB ⇌ $H^+ + B^-$ with acid dissociation constant Ka2 = $[H^+] * [B^-] / [HB]$

HC ⇌ $H^+ + C^-$ with acid dissociation constant Ka3 = $[H^+] * [C^-] / [HC]$

H_2O ⇌ $H^+ + OH^-$ with water autoprotolysis constant Kw = $[H^+] * [OH^-]$

$$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-K[3]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + Ka3+ (K[1]*X - K[2]*P[4])/VT,

C = (Ka1+Ka2+Ka3)*(K[1]*X - K[2]*P[4])/VT + Ka1*(Ka2+Ka3-K[2]*P[5]/VT) - Ka2*K[2]*P[6]//VT - Ka3*K[2]*P[7]/VT - Kw,

D = (Ka1*Ka2 + Ka1*Ka3 + Ka2*Ka3)*(K[1]*X - K[2]*P[4])/VT

- Ka1*(Ka2+Ka3)*K[2]*P[5]/VT

- Ka2*(Ka1+Ka3)*K[2]*P[6]/VT

- Ka3*(Ka1+Ka2)*K[2]*P[7]/VT

- Kw*(Ka1+Ka2+Ka3)

+ Ka1*Ka2*Ka3

E = Ka1*Ka2*Ka3*(K[1]*X - K[2]*P[4] - K[2]*P[5] - K[2]*P[6] - K[2]*P[7])/VT

- Kw*(Ka1*Ka2+Ka1*Ka3+Ka2*Ka3)

F = -Ka1*Ka2*Ka3*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that

Constant	Name	Comments
		used for the volume of strong base titrant, e.g. mL or L.
K3	pKw	-Log10 of the water autoprotolysis constant.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	pKa3	-Log10 of the acid dissociation constant of the third weak monoprotic acid.
P4	Cso	Initial concentration of the strong acid in moles/L.
P5	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
P6	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.
P7	Ca3o	Initial concentration of the third monoprotic weak acid in moles/L.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 & pKa3, and concentrations, Ca1o, Ca2o & Ca3o of a mixture of three weak monoprotic acids as well as the concentration, Cso, of a strong acid in solution.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

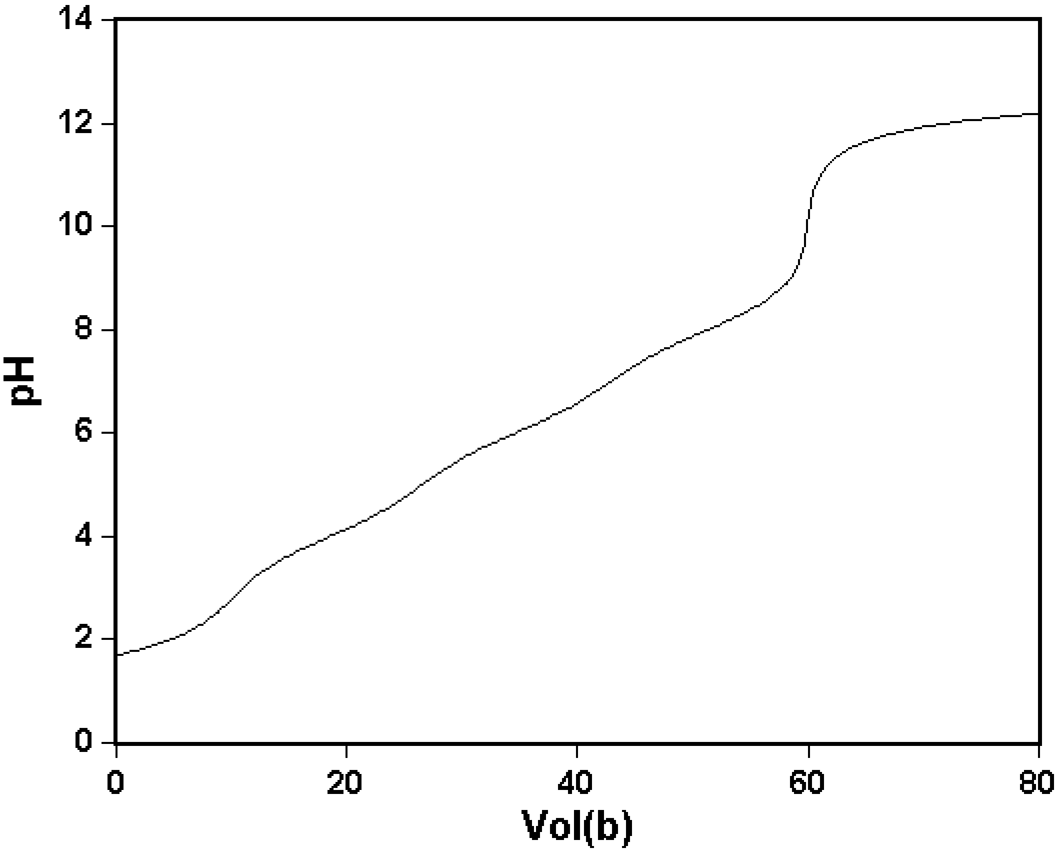
Also see

Ftn 0471 123

Ftn 0490 138

Ftn 0492 146

Ftn 0492: Titration: Strong Acid + Three Weak Monoprotic Acids w/ Strong Base: pKa1, pKa2, pKa3, Cso, Ca1o, Ca2o, Ca3o & pKw



Equation

$HA \rightleftharpoons H^+ + A^-$ with acid dissociation constant $Ka1 = [H^+] * [A^-] / [HA]$

$HB \rightleftharpoons H^+ + B^-$ with acid dissociation constant $Ka2 = [H^+] * [B^-] / [HB]$

$HC \rightleftharpoons H^+ + C^-$ with acid dissociation constant $Ka3 = [H^+] * [C^-] / [HC]$

$H_2O \rightleftharpoons H^+ + OH^-$ with water autoprotolysis constant $Kw = [H^+] * [OH^-]$

$$A*[H^+]^5 + B*[H^+]^4 + C*[H^+]^3 + D*[H^+]^2 + E*[H^+] + F = 0$$

in which

$[H^+] = 10^{-Y}$,

$Kw = 10^{-P[8]}$,

$Ka1 = 10^{-P[1]}$,

$Ka2 = 10^{-P[2]}$,

$Ka3 = 10^{-P[3]}$,

VT := K[2] + X,

A = 1.0,

B = Ka1 + Ka2 + Ka3+ (K[1]*X - K[2]*P[4])/VT,

C = (Ka1+Ka2+Ka3)*(K[1]*X - K[2]*P[4])/VT + Ka1*(Ka2+Ka3-K[2]*P[5]/VT) - Ka2*K[2]*P[6]//VT - Ka3*K[2]*P[7]/VT - Kw,

D = (Ka1*Ka2 + Ka1*Ka3 + Ka2*Ka3)*(K[1]*X - K[2]*P[4])/VT

- Ka1*(Ka2+Ka3)*K[2]*P[5]/VT

- Ka2*(Ka1+Ka3)*K[2]*P[6]/VT

- Ka3*(Ka1+Ka2)*K[2]*P[7]/VT

- Kw*(Ka1+Ka2+Ka3)

+ Ka1*Ka2*Ka3

E = Ka1*Ka2*Ka3*(K[1]*X - K[2]*P[4] - K[2]*P[5] - K[2]*P[6] - K[2]*P[7])/VT

- Kw*(Ka1*Ka2+Ka1*Ka3+Ka2*Ka3)

F = -Ka1*Ka2*Ka3*Kw,

and

- Y is the measured response, the pH, which is defined as -Log10 of the hydrogen ion, H^+, concentration. Its calculated value is -Log10 of the *largest real root* of the above quintic equation.
- X is the independent variable, the volume of added strong base titrant.

Constants

Constant	**Name**	**Comments**
K1	Cbo	Concentration of the strong base titrant, such as NaOH, in moles/L
K2	Vao	Initial volume of the acid solution. The unit of measurement must be the same as that

Constant	Name	Comments
		used for the volume of strong base titrant, e.g. mL or L.

Parameters

Parameter	Name	Comments
P1	pKa1	-Log10 of the acid dissociation constant of the first weak monoprotic acid.
P2	pKa2	-Log10 of the acid dissociation constant of the second weak monoprotic acid.
P3	pKa3	-Log10 of the acid dissociation constant of the third weak monoprotic acid.
P4	Cso	Initial concentration of the strong acid in moles/L.
P5	Ca1o	Initial concentration of the first monoprotic weak acid in moles/L.
P6	Ca2o	Initial concentration of the second monoprotic weak acid in moles/L.
P7	Ca3o	Initial concentration of the third monoprotic weak acid in moles/L.
P8	pKw	-Log10 of the water autoprotolysis constant.

Sample Applications

- Determining the acid dissociation constants, pKa1, pKa2 & pKa3, and concentrations, Ca1o, Ca2o & Ca3o of a mixture of three weak monoprotic acids as well as the concentration, Cso, of a strong acid in solution and the water autoprotolysis constant, pKw.

Remarks

- When automatic initial estimates are made, ***FitAll*** assumes that the data are sorted on column number 1; that is, the X-values.

- The derivation assumes that the activity coefficients do not change during the titration. This means that the ionic strength of the original acid solution and that of the base titrant are the same. Experimentally, this is usually accomplished by having an excess of an inert salt, such as $NaClO_4$, in each solution.

- A negative value for the concentration of the strong acid indicates that initially there was some strong base in the solution and the concentration of the strong base is equal to the absolute value of the calculated value of the strong acid concentration

Also see

Ftn 0472 126

Ftn 0490 138

Ftn 0491 142

Appendix

Getting Help

To get technical or other assistance from MTR Software you can:

Visit MTR Software's website at:

www.fitall.com

Email MTR Software at:

support@fitall.com

Write to MTR Software at:

MTR Software

77 Carlton Street, Suite 808

Toronto ON Canada

M5B 2J7

Telephone MTR Software at:

416-596-1499

Describe your problem or difficulty as completely as you can. We will try to answer your query quickly and completely.

You should also include your email address as well as your daytime, evening and weekend telephone numbers.

Adding Functions to FitAll

There are four ways to add your own specialized functions to ***FitAll***.

1. In ***FitAll*** version 10 you can use the new "Scripted Function" feature to add functions that can be defined by a one-line expression and contains one independent variable, X. and up to ten parameters, P.

2. You can contact ***MTR*** **Software** to get a quotation on the cost of creating a custom ***FitAll*** **Function Library** for you.

3. The ***FitAll*** **Programmer's Guide**, which is included with ***FitAll*** **Research Edition**, explains:

    - how to modify the supplied source code for the User Defined ***FitAll*** **Function Libraries** and

    - how to compile them using Embarcadero / CodeGear / Borland Delphi version 5 to XE2, **FreePascal** version 2.2 or later and **Lazarus** version 1.0 or later. FreePascal and Lazarus are open source Pascal compilers available from www.freepascal.org and www.lazarus.freepascal.org . Lazarus is highly recommended.

4. You can contact ***MTR*** **Software** and request that the function be added to one of ***FitAll***'s **Function Libraries**.

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