User's Manual

ABEW
Version 1.9.0

Chemical software
Acid-base equilibria for Windows

Windows XP ® - Windows Vista ® - Windows 7 ® - Windows 8 ® - Windows 10 ®

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Introduction

ABEW is a Windows application to solve acid-base chemical equilibrium.

This manual isn't about acid-base reactions theory.

Please, read this manual carefully in order to learn all the capabilities of the application.

Terms of use

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Before the installation we recommended to make backup of your data and create a restoration point.

You will be able freely to evaluate the software during the time that considers necessary. Passed this period of evaluation you would have or to register it or uninstall it.

To register the software, please see the option "REGISTER APPLICATION" in the help menu of the software.

After paying the registry fee you will receive by email the REGISTRATION KEY of the software.
Once registered the software, it will be able to use the options that were disabled until that moment.

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You cannot use the same REGISTRATION KEY for multiple computers.

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It is possible that the shared file already exists and whether or not previously replaced by a different version during the installation of the VaxaSoftware's software.

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Main window

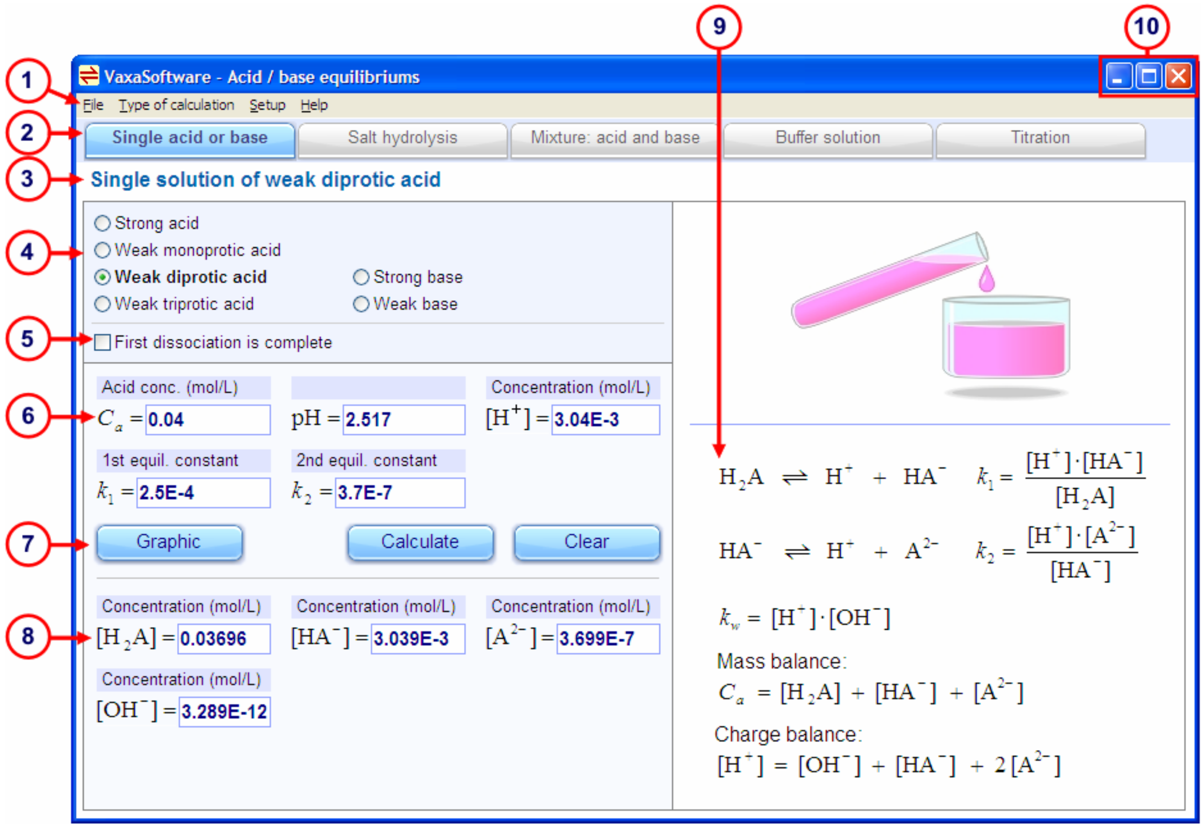


Fig. 1
Main window

(1) Menu bar

It contains the menus *File*, *Type of calculation*, *Setup,* and *Help*.

File menu

Exit
Close the application.

Type of calculation menu

Single acid-base
To perform equilibriums of single solutions of acids or bases.

Salt hydrolysis
To perform equilibriums of salts hydrolysis.

Mixture: acid and base
To perform equilibriums of mixtures of acids and bases.

Buffer solution
To perform equilibriums of buffer solutions.

Titration
To perform titrations of acids and bases.

Setup menu

Decimal separator:
We can select either point **.** or comma **,** as decimal separator.
The output values are shown using the selected decimal separator.

Significant digits

We can select between 4 and 12 significant digits for the output values.

Ionic product of water Kw
Allow us to select the value of the ionic product of water Kw.
We can select either pK_W = 14.00 (25 °C) or pK_W = 13.59 (37 °C)

◆ ***Note:***
$pKw = - \log_{10}K_W$ therefore $K_W = 10^{-pKw}$ thus: $pKw = 14.00 \rightarrow K_W = 10^{-14}$
$pKw = 13.59 \rightarrow K_W = 2.57 \cdot 10^{-14}$

Help menu

User's manual (PDF document)...
Show this manual.

Application registration...
Show the registration form window to register the application.

Disabled functions in the unregistered version
Show the list of disabled functions when the application is not registered.

Home page (www.vaxasoftware.com)...
Connect to VaxaSoftware home page.
An active Internet connection and a browser are required.

About...
Show the *Splash* window with the version and description of the application.

(2) Tab bar

Single acid-base
To perform equilibriums of single solutions of acids or bases.

Salt hydrolysis
To perform equilibriums of salts hydrolysis.

Mixture: acid and base
To perform equilibriums of mixtures of acids and bases.

Buffer solution
To perform equilibriums of buffer solutions.

Titration
To perform titrations of acids and bases.

(3) Current calculation title

Shows the title of the current equilibrium calculation.

(4) Option buttons

Allow us to select a more specific calculation.

(5) *First dissociation complete* checkbox

Allows us indicate when a diprotic or tripotic acid has its first dissociation is complete.
(It's mean the first acidity constant is infinity: $k_1 = \infty$).

(6) Input textboxes

Allow us to enter the input values.

The numeric values can be entered in the following formats:

- Standard numbers: 0.24; 15.23
- Percentage: 90%; 12%
- Fractions: 2/3; 5/8
- Scientific notation: 2E-4 (equal to $2x10^{-4} = 0.0002$)

◆ ***Note 1:***

Decimal separator:

We can use either point **.** or comma **,** as decimal separator. The output value is shown using the same decimal separator.

◆ ***Note 2:***

Scientific notation:

The scientific notation is used to show very big or very small numbers.
A scientific notation number has a mantissa and a power of 10.
In order to enter a scientific notation number we use letter E to input the exponent of 10.

Examples:

5.67×10^{89}	is entered as	5.67 E 89
1.23×10^{-34}	is entered as	1.23 E-34

(7) *Calculate*, *Graphic* and *Clear buttons*

Calculate

Calculate output values from input values.

Graphic

Show *Edit type of graphic* window.

Clear

Clear all the input/output values.

(8) Output textboxes

Shows the output values.

(9) Formulas

Shows the formulas of the current equilibrium.

(10) Window control buttons

These are the classics buttons of the windows of MS-Windows ®.

Minimize button
Minimize the application to an icon on the desktop.

Maximize / Restore button
Maximize / restore the application's window size.

Close button
Close the application. Also we can press Alt + F4 keys on our keyboard.

Types of equilibrium calculations

This application can perform 5 main types of equilibrium calculations.
We'll do click the appropriate tab to select the desired type of calculation.

Single acid or base solution equilibrium

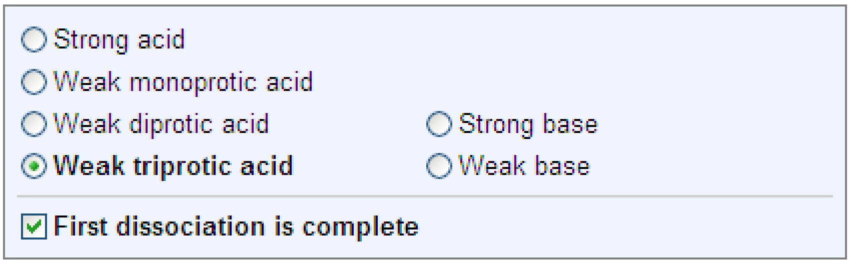


Fig. 2

The following calculations are available:

- Strong acid.
- Weak monoprotic acid.
- Weak diprotic acid.
- Weak triprotic acid.
- Strong base
- Weak base.

◆ ***Note:***
If the acid is diprotic or tripotic and its first dissociation stage is complete then we press the *First dissociation is complete* checkbox.
(It's mean the first acidity constant is infinity: $k_1 = \infty$).

Salt hydrolysis equilibrium

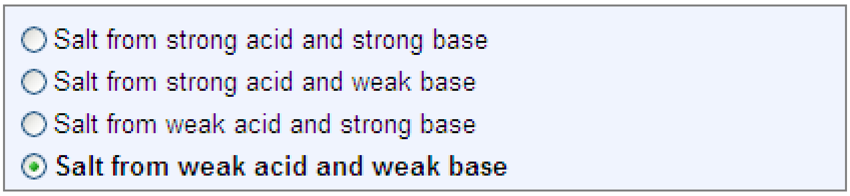


Fig. 3

The following calculations are available:

- Salt from strong acid and strong base.
- Salt from strong acid and weak base.
- Salt from weak acid and strong base.
- Salt from weak acid and weak base.

Mixture of acid + base equilibrium

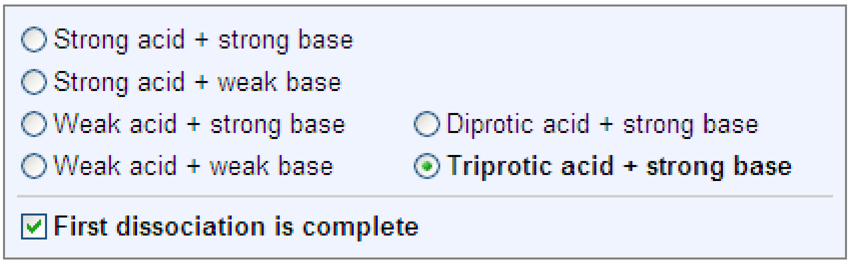


Fig. 4

The following calculations are available:

- Strong acid + strong base.
- Strong acid + weak base.
- Weak (monoprotic) acid + strong base.
- Weak (monoprotic) acid + weak base.
- Diprotic acid + strong base.
- Triprotic acid + strong base.

◆ ***Note:***
If the acid is diprotic or tripotic and its first dissociation stage is complete then we press the *First dissociation is complete* checkbox.
(It's mean the first acidity constant is infinity: $k_1 = \infty$).

Buffer solution equilibrium

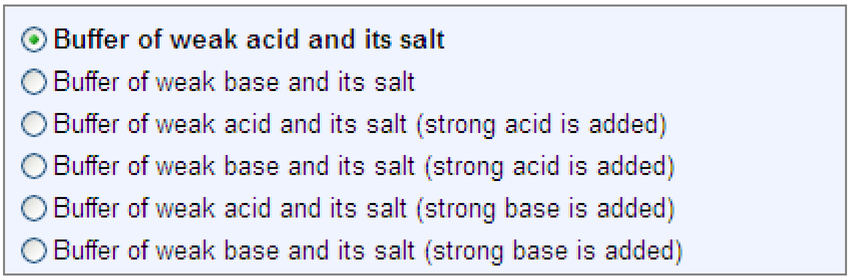


Fig. 5

The following calculations are available:

- Buffer of weak acid and its salt.
- Buffer of weak base and its salt.
- Buffer of weak acid and its salt (strong acid is added).
- Buffer of weak base and its salt (strong acid is added).
- Buffer of weak acid and its salt (strong base is added).
- Buffer of weak base and its salt (strong base is added).

Acid-base titration equilibrium

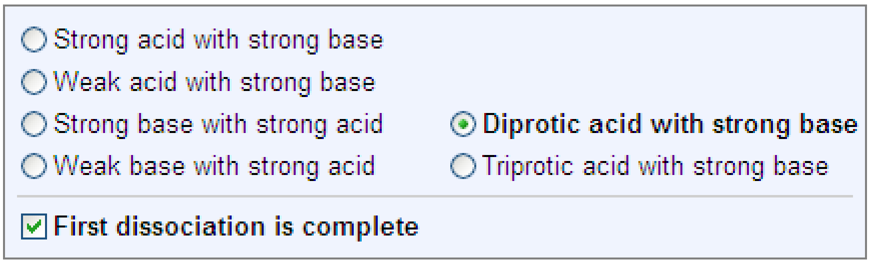


Fig. 6

The following calculations are available:

- Titration of strong acid with strong base.
- Titration of weak (monoprotic) acid with strong base.
- Titration of strong base with strong acid.
- Titration of weak base with strong acid.
- Titration of diprotic acid with strong base.
- Titration of triprotic acid with strong base.

◆ ***Note:***
If the acid is diprotic or tripotic and its first dissociation stage is complete then we press the *First dissociation is complete* checkbox.
(It's mean the first acidity constant is infinity: $k_1 = \infty$).

Edit type of graphic window

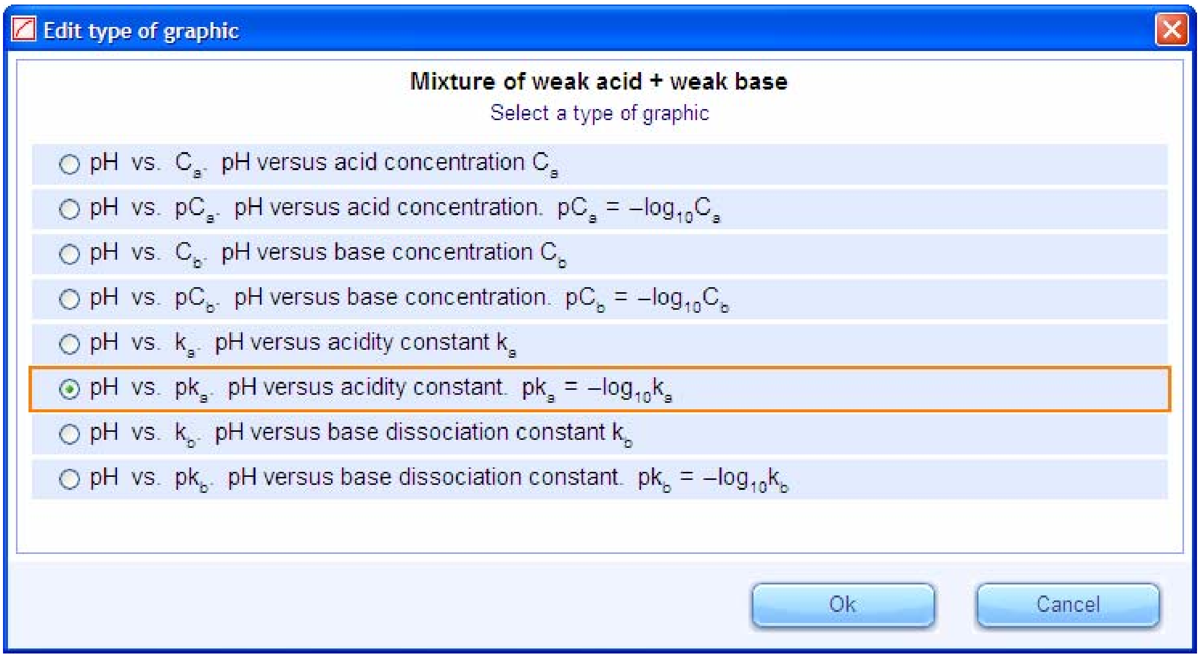


Fig. 7
Selecting type of graphic window

This window allows us to select the graph type to represent the equilibrium calculation.

Graphic window

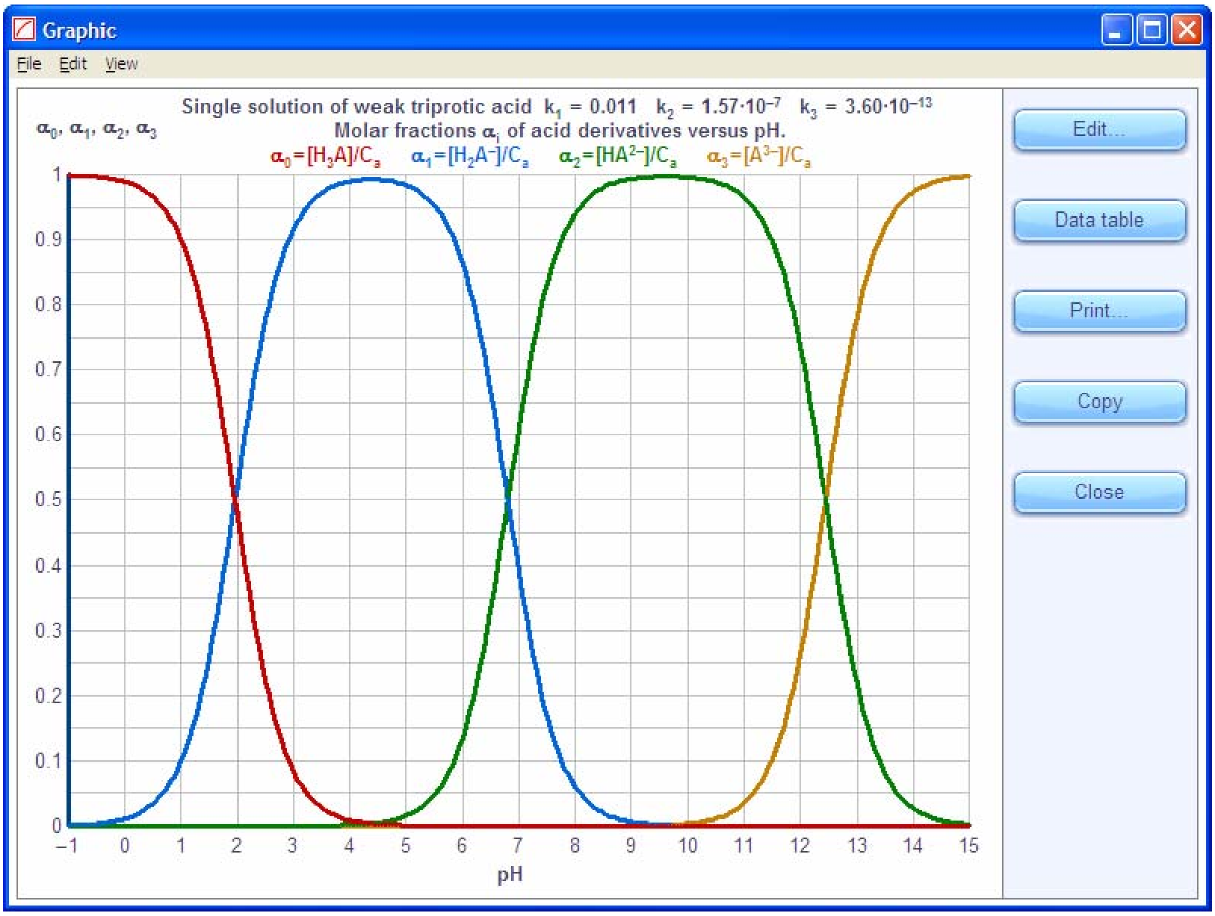


Fig. 8
Graphic window

The *graphic* window shows the graph for the selected type of equilibrium calculation.

This window has the following menus and buttons:

File menu

Edit type of graphic...
Open the *Edit type of graphic* window.

Save image as...
Save the graph as a Bitmap file.

Print...
Open the *Print* window. In it we can select the printer destination and specify the number of copies.

Close
Close the window.

Edit menu

Copy
Copy the graph to the clipboard.

View menu

> ***Data table***
> Open the *Data table* window.

Buttons:

Edit...
Open the *Edit type of graphic* window.

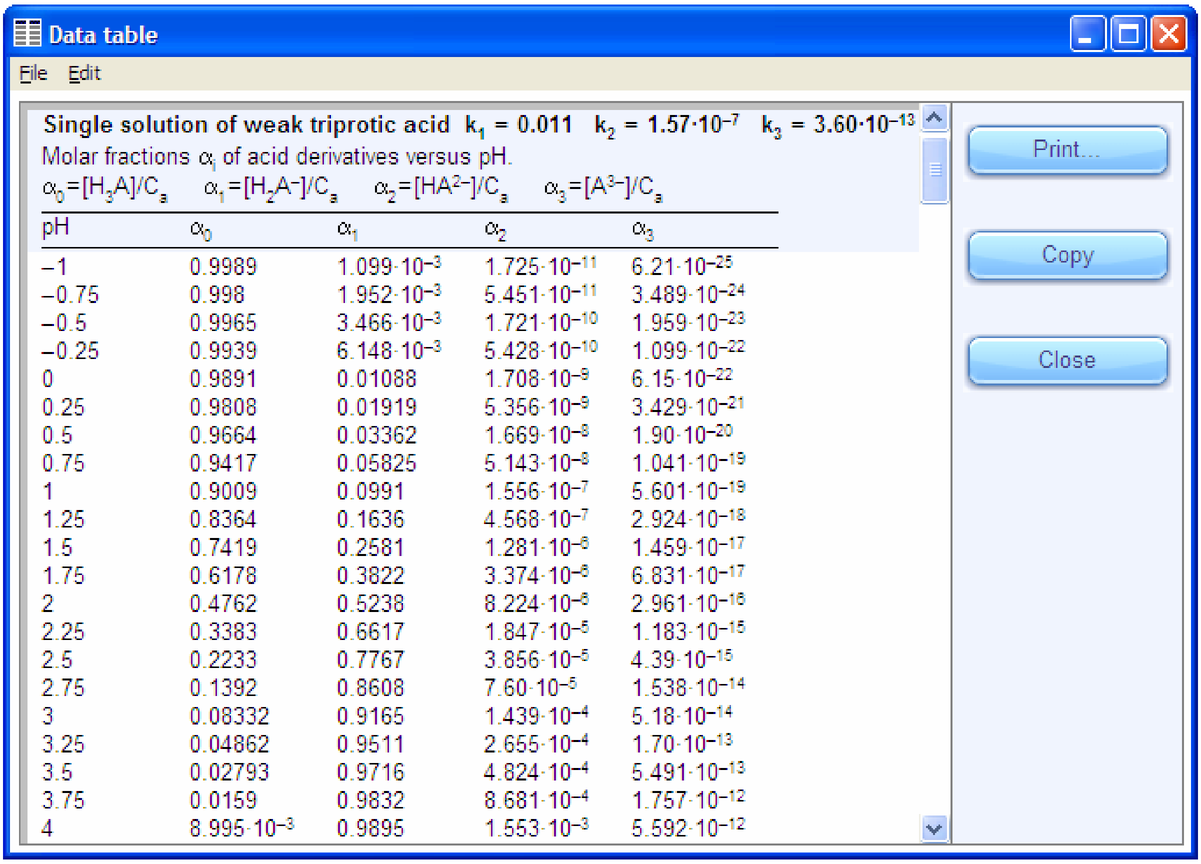
Data table
Open the *Data table* window.

Print...
Open the *Print* window. In it we can select the printer destination and specify the number of copies.

Copy
Copy the graph to the clipboard.

Close
Close the window.

Data table **window**



Single solution of weak triprotic acid $k_1 = 0.011$ $k_2 = 1.57 \cdot 10^{-7}$ $k_3 = 3.60 \cdot 10^{-13}$

Molar fractions α_i of acid derivatives versus pH.

$\alpha_0=[H_3A]/C_a$ $\alpha_1=[H_2A^-]/C_a$ $\alpha_2=[HA^{2-}]/C_a$ $\alpha_3=[A^{3-}]/C_a$

pH	α_0	α_1	α_2	α_3
−1	0.9989	$1.099 \cdot 10^{-3}$	$1.725 \cdot 10^{-11}$	$6.21 \cdot 10^{-25}$
−0.75	0.998	$1.952 \cdot 10^{-3}$	$5.451 \cdot 10^{-11}$	$3.489 \cdot 10^{-24}$
−0.5	0.9965	$3.466 \cdot 10^{-3}$	$1.721 \cdot 10^{-10}$	$1.959 \cdot 10^{-23}$
−0.25	0.9939	$6.148 \cdot 10^{-3}$	$5.428 \cdot 10^{-10}$	$1.099 \cdot 10^{-22}$
0	0.9891	0.01088	$1.708 \cdot 10^{-9}$	$6.15 \cdot 10^{-22}$
0.25	0.9808	0.01919	$5.356 \cdot 10^{-9}$	$3.429 \cdot 10^{-21}$
0.5	0.9664	0.03362	$1.669 \cdot 10^{-8}$	$1.90 \cdot 10^{-20}$
0.75	0.9417	0.05825	$5.143 \cdot 10^{-8}$	$1.041 \cdot 10^{-19}$
1	0.9009	0.0991	$1.556 \cdot 10^{-7}$	$5.601 \cdot 10^{-19}$
1.25	0.8364	0.1636	$4.568 \cdot 10^{-7}$	$2.924 \cdot 10^{-18}$
1.5	0.7419	0.2581	$1.281 \cdot 10^{-6}$	$1.459 \cdot 10^{-17}$
1.75	0.6178	0.3822	$3.374 \cdot 10^{-6}$	$6.831 \cdot 10^{-17}$
2	0.4762	0.5238	$8.224 \cdot 10^{-6}$	$2.961 \cdot 10^{-16}$
2.25	0.3383	0.6617	$1.847 \cdot 10^{-5}$	$1.183 \cdot 10^{-15}$
2.5	0.2233	0.7767	$3.856 \cdot 10^{-5}$	$4.39 \cdot 10^{-15}$
2.75	0.1392	0.8608	$7.60 \cdot 10^{-5}$	$1.538 \cdot 10^{-14}$
3	0.08332	0.9165	$1.439 \cdot 10^{-4}$	$5.18 \cdot 10^{-14}$
3.25	0.04862	0.9511	$2.655 \cdot 10^{-4}$	$1.70 \cdot 10^{-13}$
3.5	0.02793	0.9716	$4.824 \cdot 10^{-4}$	$5.491 \cdot 10^{-13}$
3.75	0.0159	0.9832	$8.681 \cdot 10^{-4}$	$1.757 \cdot 10^{-12}$
4	$8.995 \cdot 10^{-3}$	0.9895	$1.553 \cdot 10^{-3}$	$5.592 \cdot 10^{-12}$

Fig. 9
Data table window

The *Data table* window displays the data table of the current graphic.

This window has the following menus and buttons:

File menu

Save data table as...
Save the data table as text file.

◆ ***Note:***
Some formats might get lost.

Print...
Open the *Print* window. In it we can select the printer destination and specify the number of copies.

Close
Close the window.

Edit menu

Copy
Copy the data table to the clipboard.

◆ ***Note:***
Some formats might get lost.

Print..
Open the *Print* window. In it we can select the printer destination and specify the number of copies.

Buttons:

Print..
Open the *Print* window. In it we can select the printer destination and specify the number of copies.

Copy
Copy the data table to the clipboard.

Close
Close the window.

Examples

The following examples assume that the ionic product of water is $pk_w = 14.00$.

Example 1
Equilibrium of triprotic acid.

We have a solution of phosphoric acid (H_3PO_4) with a concentration of 0.2 mol/L.
The dissociation constants are $k_1 = 1.1{\cdot}10^{-2}$ $k_2 = 1.57{\cdot}10^{-7}$ $k_3 = 3.6{\cdot}10^{-13}$

a) Calculate the pH of this solution.

b) Make the graph of the distribution of molar fractions of species derived from the acid versus pH and its corresponding data table.

Resolution procedure

1) Select the tab *Single acid or base.*

2) Select the option *Weak triprotic acid.*

3) Enter values:

   C_a = 0.2 **k_1 = 1.1E-2** **k_2 = 1.57E-7** **k_3 = 3.6E-13**

4) Press *Calculate* button:

5) We get the value of pH:

   pH = 1,38

6) Press *Graphic* button to show the *Edit type of graphic* window.

7) In this window, select the option *Molar fractions α_i of acid derivatives versus pH.*

8) Then the *Graphic* window is shown. (see Fig. 8).
Recall that in this case, the molar fractions are:

$\alpha_0 = [H_3PO_4] / C_a$ $\alpha_1 = [H_2PO_4^-] / C_a$ $\alpha_2 = [HPO_4^{2-}] / C_a$ $\alpha_3 = [PO_4^{3-}] / C_a$

9) Press *Data table* button to show the *Data table* window. (see Fig. 9).

Example 2
Titration of weak acid

We have titrated 30 mL of a solution of acetic acid (weak acid) with 42 mL of 0.095 mol/L of sodium hydroxide solution (NaOH, strong base).

The dissociation constant of acetic acid is: $k_a = 1.8 \cdot 10^{-5}$

a) Calculate the concentration of acetic acid.
b) Find the pH at the equivalence point.
c) Make the graph of the pH versus volume of added strong base.

Resolution procedure

1) Select the tab *Titration.*

2) Select the option *Weak acid with strong base.*

3) Enter values:

V_a = 30 **k_a = 1.8E-5** **C_{SB} = 0.095** **V_{eq} = 42**

4) Press *Calculate* button:

5) We get the value of concentration of acetic acid and pH at the equivalence point:

C_a = 0.133 mol/L **pH_{eq} = 8.744**

6) Press *Graphic* button to show the *Edit type of graphic* window.

7) In this window, select the option *pH versus volume of added strong base.*

8) Then the *Graphic* window is opened showing the titration curve. (see Fig. 10).

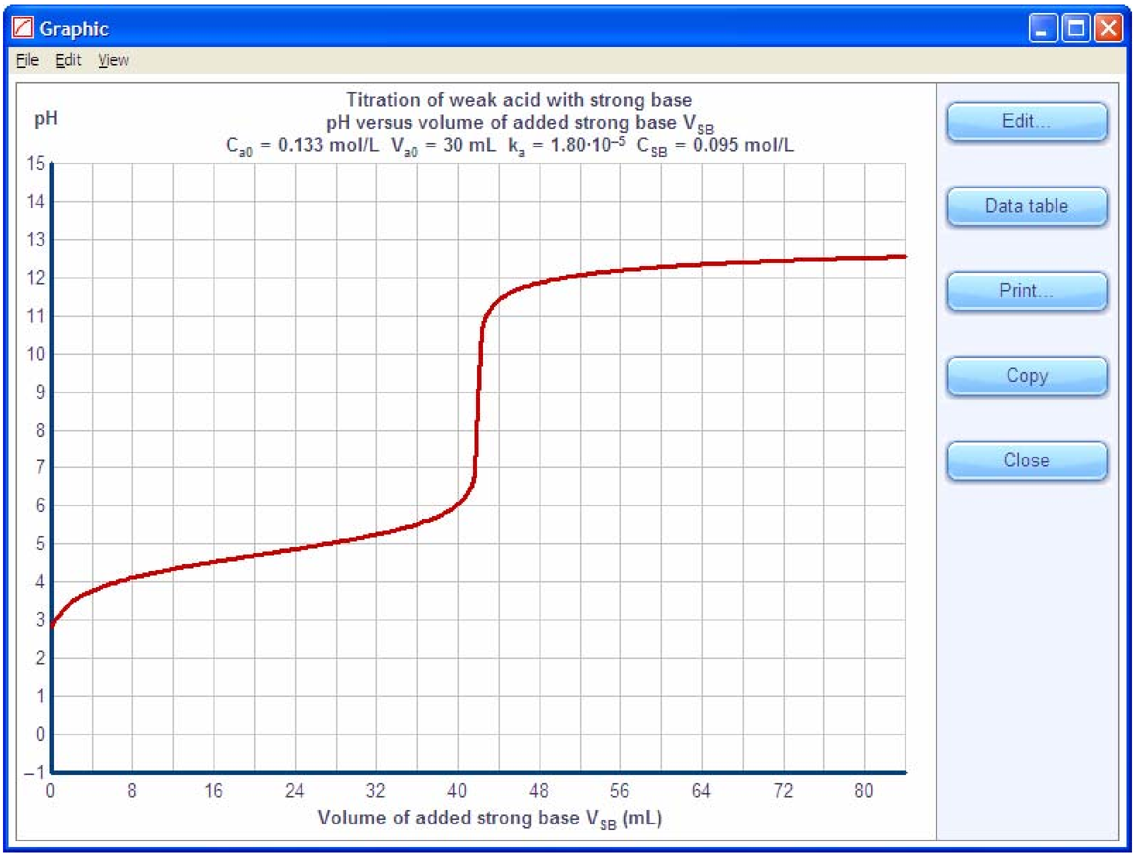


Fig. 10
Titration curve of acetic acid with sodium hydroxide.

Formulas of acid-base equilibriums

Single acid or base solution equilibrium

Strong acid	$HA \rightarrow H^+ + A^-$ $k_w = [H^+]\cdot[OH^-]$ $[HA] = 0$ Mass balance: $C_a = [A^-]$ Charge balance: $[H^+] = [OH^-] + [A^-]$
Strong base	$BOH \rightarrow B^+ + OH^-$ $k_w = [H^+]\cdot[OH^-]$ $[BOH] = 0$ Mass balance: $C_b = [B^+]$ Charge balance: $[H^+] + [B^+] = [OH^-]$
Weak base	$BOH \leftrightarrow B^+ + OH^-$ $\quad k_b = \frac{[B^+]\cdot[OH^-]}{[BOH]}$ $k_w = [H^+]\cdot[OH^-]$ $\quad \alpha = \frac{[B^+]}{C_b}$ Mass balance: $C_b = [BOH] + [B^+]$ Charge balance: $[H^+] + [B^+] = [OH^-]$
Weak monoprotic acid	$HA \leftrightarrow H^+ + A^-$ $\quad k_a = \frac{[H^+]\cdot[A^-]}{[HA]}$ $k_w = [H^+]\cdot[OH^-]$ $\quad \alpha = \frac{[A^-]}{C_a}$ Mass balance: $C_a = [HA] + [A^-]$ Charge balance: $[H^+] = [OH^-] + [A^-]$

Weak diprotic acid	$H_2A \leftrightarrow H^+ + HA^-$ $\quad k_1 = \frac{[H^+]\cdot[HA^-]}{[H_2A]}$ $HA^- \leftrightarrow H^+ + A^{2-}$ $\quad k_2 = \frac{[H^+]\cdot[A^{2-}]}{[HA^-]}$ $k_w = [H^+]\cdot[OH^-]$ Mass balance: $C_a = [H_2A] + [HA^-] + [A^{2-}]$ Charge balance: $[H^+] = [OH^-] + [HA^-] + 2[A^{2-}]$
Weak diprotic acid **First dissociation is complete:** $\boldsymbol{k_1 = \infty}$	$H_2A \rightarrow H^+ + HA^-$ $\quad k_1 = \infty$ $HA^- \leftrightarrow H^+ + A^{2-}$ $\quad k_2 = \frac{[H^+]\cdot[A^{2-}]}{[HA^-]}$ $k_w = [H^+]\cdot[OH^-]$ $[H_2A] = 0$ Mass balance: $C_a = [HA^-] + [A^{2-}]$ Charge balance: $[H^+] = [OH^-] + [HA^-] + 2[A^{2-}]$
Weak triprotic acid	$H_3A \leftrightarrow H^+ + H_2A^-$ $\quad k_1 = \frac{[H^+]\cdot[H_2A^-]}{[H_3A]}$ $H_2A^- \leftrightarrow H^+ + HA^{2-}$ $\quad k_2 = \frac{[H^+]\cdot[HA^{2-}]}{[H_2A^-]}$ $HA^{2-} \leftrightarrow H^+ + A^{3-}$ $\quad k_3 = \frac{[H^+]\cdot[A^{3-}]}{[HA^{2-}]}$ $k_w = [H^+]\cdot[OH^-]$ Mass balance: $C_a = [H_3A] + [H_2A^-] + [HA^{2-}] + [A^{3-}]$ Charge balance: $[H^+] = [OH^-] + [H_2A^-] + 2[HA^{2-}] + 3[A^{3-}]$

Weak triprotic acid **First dissociation is complete:** ***k*₁ = ∞**	$H_3A \rightarrow H^+ + H_2A^- \quad k_1 = \infty$ $H_2A^- \leftrightarrow H^+ + HA^{2-} \quad k_2 = \frac{[H^+]\cdot[HA^{2-}]}{[H_2A^-]}$ $HA^{2-} \leftrightarrow H^+ + A^{3-} \quad k_3 = \frac{[H^+]\cdot[A^{3-}]}{[HA^{2-}]}$ $k_w = [H^+]\cdot[OH^-]$ $[H_3A] = 0$ Mass balance: $C_a = [H_2A^-] + [HA^{2-}] + [A^{3-}]$ Charge balance: $[H^+] = [OH^-] + [H_2A^-] + 2[HA^{2-}] + 3[A^{3-}]$

Salt hydrolysis equilibrium

Salt: **Anion from strong acid** **Cation from strong base**	$BA \rightarrow B^+ + A^-$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0$ Mass balance: $C_S = [B^+] = [A^-]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$
Salt: **Anion from strong acid** **Cation from weak base**	$BA \rightarrow B^+ + A^-$ $BOH \leftrightarrow B^+ + OH^- \quad k_b = \frac{[B^+]\cdot[OH^-]}{[BOH]}$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0$ Mass balance: $C_S = [B^+] + [BOH] = [A^-]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$

Salt: **Anion from weak acid** **Cation from strong base**	$BA \rightarrow B^+ + A^-$ $HA \leftrightarrow H^+ + A^- \qquad k_a = \frac{[H^+]\cdot[A^-]}{[HA]}$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0$ Mass balance: $C_S = [B^+] = [HA] + [A^-]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$
Salt: **Anion from weak acid** **Cation from weak base**	$BA \rightarrow B^+ + A^-$ $BOH \leftrightarrow B^+ + OH^- \qquad k_b = \frac{[B^+]\cdot[OH^-]}{[BOH]}$ $HA \leftrightarrow H^+ + A^- \qquad k_a = \frac{[H^+]\cdot[A^-]}{[HA]}$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0$ Mass balance: $C_S = [B^+] + [BOH] = [HA] + [A^-]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$

Mixture of acid + base equilibrium

Strong acid + strong base	$HA \rightarrow H^+ + A^-$ $BOH \rightarrow B^+ + OH^-$ $k_w = [H^+]\cdot[OH^-]$ $[HA] = 0$ $[BOH] = 0$ Mass balance: $C_a = [A^-], \qquad C_b = [B^+]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$

Strong acid + weak base	$HA \rightarrow H^+ + A^-$ $BOH \leftrightarrow B^+ + OH^- \qquad k_b = \frac{[B^+]\cdot[OH^-]}{[BOH]}$ $k_w = [H^+]\cdot[OH^-]$ $[HA] = 0$ Mass balance: $C_a = [A^-], \quad C_b = [BOH] + [B^+]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$
Weak acid + strong base	$HA \leftrightarrow H^+ + A^- \qquad k_a = \frac{[H^+]\cdot[A^-]}{[HA]}$ $BOH \rightarrow B^+ + OH^-$ $k_w = [H^+]\cdot[OH^-]$ $[BOH] = 0$ Mass balance: $C_a = [HA^-] + [A^-], \quad C_b = [B^+]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$
Weak acid + weak base	$HA \leftrightarrow H^+ + A^- \qquad k_a = \frac{[H^+]\cdot[A^-]}{[HA]}$ $BOH \leftrightarrow B^+ + OH^- \qquad k_b = \frac{[B^+]\cdot[OH^-]}{[BOH]}$ $k_w = [H^+]\cdot[OH^-]$ Mass balance: $C_a = [HA^-] + [A^-]$ $C_b = [BOH] + [B^+]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$

<table>
<tr><td>Weak diprotic acid + strong base</td><td>

$H_2A \leftrightarrow H^+ + HA^- \quad k_1 = \frac{[H^+]\cdot[HA^-]}{[H_2A]}$

$HA^- \leftrightarrow H^+ + A^{2-} \quad k_2 = \frac{[H^+]\cdot[A^{2-}]}{[HA^-]}$

$BOH \rightarrow B^+ + OH^-$

$k_w = [H^+]\cdot[OH^-]$

$[BOH] = 0$

Mass balance:
$C_a = [H_2A] + [HA^-] + [A^{2-}]$
$C_b = [B^+]$

Charge balance:
$[H^+] + [B^+] = [OH^-] + [HA^-] + 2[A^{2-}]$

</td></tr>
<tr><td>Weak diprotic acid + strong base

First dissociation is complete:
$k_1 = \infty$</td><td>

$H_2A \rightarrow H^+ + HA^- \quad k_1 = \infty$

$HA^- \leftrightarrow H^+ + A^{2-} \quad k_2 = \frac{[H^+]\cdot[A^{2-}]}{[HA^-]}$

$BOH \rightarrow B^+ + OH^-$

$k_w = [H^+]\cdot[OH^-]$

$[H_2A] = 0$

$[BOH] = 0$

Mass balance:
$C_a = [HA^-] + [A^{2-}], \quad C_b = [B^+]$

Charge balance:
$[H^+] + [B^+] = [OH^-] + [HA^-] + 2[A^{2-}]$

</td></tr>
</table>

Weak triprotic acid + strong base	$H_3A \leftrightarrow H^+ + H_2A^- \quad k_1 = \frac{[H^+]\cdot[H_2A^-]}{[H_3A]}$ $H_2A^- \leftrightarrow H^+ + HA^{2-} \quad k_2 = \frac{[H^+]\cdot[HA^{2-}]}{[H_2A^-]}$ $HA^{2-} \leftrightarrow H^+ + A^{3-} \quad k_3 = \frac{[H^+]\cdot[A^{3-}]}{[HA^{2-}]}$ $BOH \rightarrow B^+ + OH^-$ $k_w = [H^+]\cdot[OH^-]$ $[BOH] = 0$ Mass balance: $C_a = [H_3A] + [H_2A^-] + [HA^{2-}] + [A^{3-}]$ $C_b = [B^+]$ Charge balance: $[H^+]+[B^+]=[OH^-]+[H_2A^-]+2[HA^{2-}]+3[A^{3-}]$
Weak triprotic acid + strong base **First dissociation is complete:** $\boldsymbol{k_1 = \infty}$	$H_3A \rightarrow H^+ + H_2A^- \quad k_1 = \infty$ $H_2A^- \leftrightarrow H^+ + HA^{2-} \quad k_2 = \frac{[H^+]\cdot[HA^{2-}]}{[H_2A^-]}$ $HA^{2-} \leftrightarrow H^+ + A^{3-} \quad k_3 = \frac{[H^+]\cdot[A^{3-}]}{[HA^{2-}]}$ $BOH \rightarrow B^+ + OH^-$ $k_w = [H^+]\cdot[OH^-]$ $[H_3A] = 0$ $[BOH] = 0$ Mass balance: $C_a = [H_2A^-] + [HA^{2-}] + [A^{3-}], \quad C_b = [B^+]$ Charge balance: $[H^+]+[B^+]=[OH^-]+[H_2A^-]+2[HA^{2-}]+3[A^{3-}]$

Buffer solution equilibrium

Buffer of weak acid and its salt	$BA \rightarrow B^+ + A^-$ $HA \leftrightarrow H^+ + A^- \qquad k_a = \dfrac{[H^+]\cdot[A^-]}{[HA]}$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0$ Mass balance: $C_a + C_S = [HA] + [A^-]$ $C_S = [B^+]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$
Buffer of weak base and its salt	$BA \rightarrow B^+ + A^-$ $BOH \leftrightarrow B^+ + OH^- \qquad k_b = \dfrac{[B^+]\cdot[OH^-]}{[BOH]}$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0$ Mass balance: $C_b + C_S = [BOH] + [B^+]$ $C_S = [A^-]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-]$
Buffer of weak acid and its salt (strong acid is added)	$BA \rightarrow B^+ + A^-$ $HA \leftrightarrow H^+ + A^- \qquad k_a = \dfrac{[H^+]\cdot[A^-]}{[HA]}$ $HX \rightarrow H^+ + X^-$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0, \quad [HX] = 0$ Mass balance: $C_a + C_S = [HA] + [A^-]$ $C_S = [B^+], \quad C_{SA} = [X^-]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-] + [X^-]$

Buffer of weak base and its salt (strong acid is added)	$BA \rightarrow B^+ + A^-$ $BOH \leftrightarrow B^+ + OH^- \qquad k_b = \frac{[B^+]\cdot[OH^-]}{[BOH]}$ $HX \rightarrow H^+ + X^-$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0, \quad [HX] = 0$ Mass balance: $C_b + C_S = [BOH] + [B^+]$ $C_S = [A^-], \quad C_{SA} = [X^-]$ Charge balance: $[H^+] + [B^+] = [OH^-] + [A^-] + [X^-]$
Buffer of weak acid and its salt (strong base is added)	$BA \rightarrow B^+ + A^-$ $HA \leftrightarrow H^+ + A^- \qquad k_a = \frac{[H^+]\cdot[A^-]}{[HA]}$ $ZOH \rightarrow Z^+ + OH^-$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0, \quad [ZOH] = 0$ Mass balance: $C_a + C_S = [HA] + [A^-]$ $C_S = [B^+], \quad C_{SB} = [Z^+]$ Charge balance: $[H^+] + [B^+] + [Z^+] = [OH^-] + [A^-]$
Buffer of weak base and its salt (strong base is added)	$BA \rightarrow B^+ + A^-$ $BOH \leftrightarrow B^+ + OH^- \qquad k_b = \frac{[B^+]\cdot[OH^-]}{[BOH]}$ $ZOH \rightarrow Z^+ + OH^-$ $k_w = [H^+]\cdot[OH^-]$ $[BA] = 0, \quad [ZOH] = 0$ Mass balance: $C_b + C_S = [BOH] + [B^+]$ $C_S = [A^-], \quad C_{SB} = [Z^+]$ Charge balance: $[H^+] + [B^+] + [Z^+] = [OH^-] + [A^-]$

Acid-base titration equilibrium

Titration of monoprotic base with strong acid	$\mathrm{BOH + HA \rightarrow BA + H_2O}$ $V_{eq} = \frac{C_b V_b}{C_{SA}}$
Titration of monoprotic acid with strong base	$\mathrm{HA + BOH \rightarrow BA + H_2O}$ $V_{eq} = \frac{C_a V_a}{C_{SB}}$
Titration of diprotic acid with strong base	$\mathrm{H_2A + 2BOH \rightarrow B_2A + 2H_2O}$ $V_{eq} = \frac{2 C_a V_a}{C_{SB}}, \quad V_{eq1} = \frac{V_{eq}}{2}$
Titration of triprotic acid with strong base	$\mathrm{H_3A + 3BOH \rightarrow B_3A + 3H_2O}$ $V_{eq} = \frac{3 C_a V_a}{C_{SB}}, \quad V_{eq1} = \frac{V_{eq}}{3}, \quad V_{eq2} = \frac{2 V_{eq}}{3}$

Types of graphics

pH vs. C_a	pH versus acid concentration C_a
pH vs. pC_a	pH versus acid concentration. $pC_a = -\log_{10}C_a$
pH vs. C_b	pH versus base concentration C_b
pH vs. pC_b	pH versus base concentration. $pC_b = -\log_{10}C_b$
pH vs. C_S	pH versus salt concentration C_S
pH vs. pC_S	pH versus salt concentration. $pC_S = -\log_{10}C_S$
pH vs. k_a	pH versus acidity constant k_a
pH vs. pk_a	pH versus acidity constant. $pk_a = -\log_{10}k_a$
pH vs. k_b	pH versus base dissociation constant k_b
pH vs. pk_b	pH versus base dissociation constant. $pk_b = -\log_{10}k_b$
α vs. C_a	Degree of dissociation α versus acid concentration C_a
α vs. pCa	Degree of dissociation α versus acid concentration. $pC_a = -\log_{10}C_a$
α vs. Cb	Degree of dissociation α versus base concentration C_b
α vs. pCb	Degree of dissociation α versus base concentration. $pC_b = -\log_{10}C_b$
α_0, α_1 vs. pH	Molar fractions α_i of acid derivatives versus pH
α_0, α_1 vs. pH	Molar fractions α_i of base derivatives versus pH
α_0, α_1, α_2 vs. pH	Molar fractions α_i of acid derivatives versus pH
α_0, α_1, α_2, α_3 vs. pH	Molar fractions α_i of acid derivatives versus pH
pH vs. C_{SA}	pH versus added strong acid concentration C_{SA}
pH vs. pC_{SA}	pH versus added strong acid concentration. $pC_{SA} = -\log_{10}C_{SA}$
pH vs. C_{SB}	pH versus added strong base concentration C_{SB}
pH vs. pC_{SB}	pH versus added strong base concentration. $pC_{SB} = -\log_{10}C_{SB}$
pH vs. V_{SA}	pH versus volume of added strong acid V_{SA}
pH vs. V_{SB}	pH versus volume of added strong base V_{SB}
$\Delta pH/\Delta pV$ vs. V_{SA}	Rate of change of pH with change of volume versus volume of added strong acid V_{SA}
$\Delta pH/\Delta pV$ vs. V_{SB}	Rate of change of pH with change of volume versus volume of added strong base V_{SB}

Shortcut keys

Main window

Ctrl + F4	Exit
Alt + F4	Exit
F1	Help: Show User's Manual (PDF document...)

Graphic window

Ctrl + E	Open the *Edit type of graphic* window
Ctrl + S	Save graphic as Bitmap file
Ctrl + P	Print graphic
Ctrl + C	Copy graphic to the clipboard
Ctrl + T	Open the *Data table* window
Ctrl + F4	Close window
Alt + F4	Close window

Data table window

Ctrl + S	Save data table as text file
Ctrl + P	Print data table
Ctrl + C	Copy data table to the clipboard as text
Ctrl + F4	Close window
Alt + F4	Close window

Specifications

Description	***ABEW*** is a Windows application to solve acid-base chemical equilibrium.
License	Shareware
Precision	Output: between 4 and 12 significant digits.
Decimal separator for input values	Point or comma.
Decimal separator for output values	The same separator that used in the last value entered or the last one selected in the setup menu.
Ionic product of water K_W	**2 values:** pK_W = 14.00 at 25 °C, pK_W = 13.59 at 37 °C
Types of graphics	**26 types** (see the *Types of graphics* table)
Main types of calculations:	**5 main types:** - Single acid-base - Salt hydrolysis - Mixture: acid and base - Buffer solution - Titration
Types of calculations (total):	**34 types:** - Single acid-base (8 types) - Salt hydrolysis (4 types) - Mixture: acid and base (8 types) - Buffer solution (6 types) - Titration (8 types)
Range of pH, pC_i and pK_i in graphics	**Minimum:** -1 **Maximum:** 15

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