

phtitration

Package Manual

Numerical pH–Metric Titration Curves with TikZ and PGFPlots

XeLaTeX Edition

Eight acid–base titration systems
Monoprotic, diprotic and triprotic models
Numerical charge-balance solution

Khaldi Mohammed Elhadi

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This manual describes the interface and numerical model of **phtitration** v1.0.0.

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1 Introduction

`phtitration` is a LaTeX package for generating educational pH-metric acid–base titration curves directly in a $\text{\LaTeX}$ document. It is built on `TikZ` and `PGFPlots` and is intended to be compiled with **XeLaTeX**.

The package provides one main command:

```
\phtitration[ ... ]
```

The chemical system is selected by a single key, `type`. The remaining keys specify concentrations, initial volume, acid/base dissociation constants and the visible titration range.

Important design principle: `phtitration` does not create a separate plot when used in its main form. The command is intended to be placed **inside an existing `PGFPlots axis` environment**. This makes it possible to use the package together with a personal graph style or another `TikZ`-based coordinate-system package.

2 Installation

2.1 Local installation

The simplest method is to place

```
phtitration.sty
```

in the same directory as the `.tex` document.

Then load it in the preamble:

```
\usepackage{phtitration}
```

The package loads the internal dependencies `TikZ`, `PGFPlots`, and `etoolbox` itself.

2.2 TeXstudio

For a local project, keeping `phtitration.sty` beside the main `.tex` file is recommended.

If a future version provides a TeXstudio completion file (`phtitration.cwl`), it can be installed separately to obtain command/key completion.

2.3 Compiler

Use:

XeLaTeX

The package itself does not load `fontspec`, `polyglossia` or `bidi`. This is intentional: the package remains independent of the language and typography of the user's document.

3 Minimal Working Example

The smallest practical example is:

```

\documentclass{article}
\usepackage{tikz}
\usepackage{pgfplots}
\pgfplotsset{compat=1.18}
\usepackage{phtitration}

\begin{document}

    \begin{tikzpicture}
        \begin{axis}[
            width=14cm,
            height=8cm,
            xmin=0, xmax=40,
            ymin=0, ymax=14,
            axis lines=left,
            grid=both,
            xlabel={Titrant volume (mL)},
            ylabel={pH}
        ]
            \phtitration[
                type=weak-acid,
                Ca=0.100,
                Va=20,
                Cb=0.100,
                pKa=4.76
            ]
        \end{axis}
    \end{tikzpicture}

\end{document}

```

The important point is the nesting:

```

\begin{tikzpicture}
    \begin{axis}[...]
        \phtitration[...]
    \end{axis}
\end{tikzpicture}

```

4 Supported Titration Systems

The package supports eight systems.

Type	Titration system	Equivalence points
strong-acid	Strong acid + strong base	1
weak-acid	Monoprotic weak acid + strong base	1
diprotic-acid	Diprotic acid + strong base	2
triprotic-acid	Triprotic acid + strong base	3
strong-base	Strong base + strong acid	1
weak-base	Monoprotic weak base + strong acid	1
dibase	Dibase + strong acid	2

Type	Titration system	Equivalence points
tribase	Tribase + strong acid	3

Thus the complete list is:

```
strong-acid
weak-acid
diprotic-acid
triprotic-acid

strong-base
weak-base
dibase
tribase
```

5 Command Syntax

The main command has the form

```
\phtitration[
type=...,
...
]
```

The key `type` selects the chemical model.

5.1 Acid titration group

```
\phtitration[
type=strong-acid,
Ca=...,
Va=...,
Cb=...
]
```

```
\phtitration[
type=weak-acid,
Ca=...,
Va=...,
Cb=...,
pKa=...
]
```

```
\phtitration[
type=diprotic-acid,
Ca=...,
Va=...,
Cb=...,
pKa1=...,
pKa2=...
]
```

```
\phtitration[
type=triprotic-acid,
Ca=...,
Va=...,
Cb=...,
pKa1=...,
pKa2=...,
pKa3=...
]
```

5.2 Base titration group

```
\phtitration[
type=strong-base,
Cb=...,
Vb=...,
Ca=...
]
```

```
\phtitration[
type=weak-base,
Cb=...,
Vb=...,
Ca=...,
pKb=...
]
```

```
\phtitration[
type=dibase,
Cb=...,
Vb=...,
Ca=...,
pKb1=...,
pKb2=...
]
```

```
\phtitration[
type=tribase,
Cb=...,
Vb=...,
Ca=...,
pKb1=...,
pKb2=...,
pKb3=...
]
```

6 Parameter Reference

6.1 Chemical parameters

Key	Meaning	Unit / use
type	Chemical system	One of the eight supported types
Ca	Initial acid concentration	mol L ⁻¹
Va	Initial acid volume	mL
Cb	Titrant/base concentration	mol L ⁻¹
Vb	Initial base volume	mL
pKa	Monoprotic acid pK_a	dimensionless
pKa1	First acid pK_a	dimensionless
pKa2	Second acid pK_a	dimensionless
pKa3	Third acid pK_a	dimensionless
pKb	Monoprotic base pK_b	dimensionless
pKb1	First base pK_b	dimensionless
pKb2	Second base pK_b	dimensionless
pKb3	Third base pK_b	dimensionless

6.2 Plotting parameters

Key	Meaning	Default
xmin	Minimum titrant volume used for curve generation	0
xmax	Maximum titrant volume used for curve generation	40
samples	Number of calculated curve intervals	41
mark size	Size of equivalence/half-equivalence markers	2pt
show-equivalence	Enables equivalence-point markers	false
show-half-equivalence	Enables half-equivalence markers	false

PGFPlots options are not package keys. Options such as `width`, `height`, `ymin`, `ymax`, `grid`, `xlabel`, `ylabel`, `axis lines`, `colours`, `line width`, `ticks`, and `fonts` belong to the surrounding `axis` environment.

This separation is deliberate and allows the user to keep a personal PGFPlots style.

7 Equivalence Volumes

For a monoprotic acid titrated by a strong base,

$$V_{\text{eq},1} = \frac{C_a V_a}{C_b}.$$

For a diprotic acid,

$$V_{\text{eq},1} = \frac{C_a V_a}{C_b}, \quad V_{\text{eq},2} = 2 \frac{C_a V_a}{C_b}.$$

For a triprotic acid,

$$V_{\text{eq},n} = n \frac{C_a V_a}{C_b}, \quad n = 1, 2, 3.$$

For bases titrated with a strong acid, the analogous expressions are

$$V_{\text{eq},1} = \frac{C_b V_b}{C_a},$$

with successive equivalence volumes equal to integer multiples for dibases and tribases.

7.1 Why the plotting range matters

For polyprotic systems, the final equivalence point may be far from the origin. Therefore, choose `xmax` large enough to display the whole titration.

For example:

```
type=triprotic-acid,
Ca=0.100,
Va=20,
Cb=0.100,
pKa1=2.10,
pKa2=6.30,
pKa3=10.30,
xmax=75
```

8 Equivalence and Half-Equivalence Markers

8.1 Equivalence markers

Use:

```
show-equivalence
```

or explicitly:

```
show-equivalence=true
```

To suppress them:

```
show-equivalence=false
```

For example:

```
\phtitration[
type=weak-acid,
Ca=0.100,
Va=20,
Cb=0.100,
pKa=4.76,
show-equivalence=true
]
```

8.2 Half-equivalence markers

Use:

```
show-half-equivalence=true
```

For a monoprotic weak acid,

$$\text{pH} = \text{p}K_a$$

at half-equivalence.

For a polyprotic acid, the successive half-equivalence regions correspond to the successive $\text{p}K_a$ values.

For a weak base,

$$\text{pH} = 14 - \text{p}K_b$$

at half-equivalence under the usual 25°C relation $\text{p}K_w = 14$ used by the model.

9 The Numerical Model

Version 1.0.0 uses a numerical charge-balance approach for weak and polyprotic systems.

For a monoprotic acid, the charge-balance residual is constructed from the hydrogen-ion concentration, hydroxide concentration, titrant concentration, and the analytical concentration of the acid family.

For diprotic and triprotic acids, the package computes the fractional distribution of the protonation states from the supplied $\text{p}K_a$ values and evaluates the corresponding average charge.

The pH is then found by a **bisection search** over the interval

$$0 \leq \text{pH} \leq 14.$$

The same strategy is used for weak bases, dibases and tribases after converting the supplied $\text{p}K_b$ values through the standard relation

$$\text{p}K_a = 14 - \text{p}K_b.$$

The package therefore avoids the old approach in which every region of a polyprotic curve was simply stitched together with independent Henderson–Hasselbalch expressions.

9.1 Numerical precision

The solver in v1.0.0 performs a fixed number of bisection iterations. Consequently, the result is a numerical approximation rather than a symbolic exact solution.

Increasing **samples** increases the number of volume positions at which the chemistry is evaluated; it does **not** increase the internal bisection iterations.

10 Why samples Matters

The key

```
samples=...
```

controls how many volume positions are evaluated along the curve.

For a normal curve:

```
samples=101
```

is usually sufficient.

For a very steep transition or a publication-quality graph, a larger value may be preferable:

```
samples=301
```

or

```
samples=501
```

However, a larger value also increases compilation time.

11 Using a Personal PGFPlots Style

This is one of the main advantages of the current interface.

Suppose your document already defines:

```
\pgfplotsset{
  myaxis/.style={
    width=12cm,
    height=8cm,
    xmin=0,
    xmax=40,
    ymin=0,
    ymax=14,
    axis lines=middle,
    grid=both,
    ticklabel style={font=\tiny}
  }
}
```

You can then simply write:

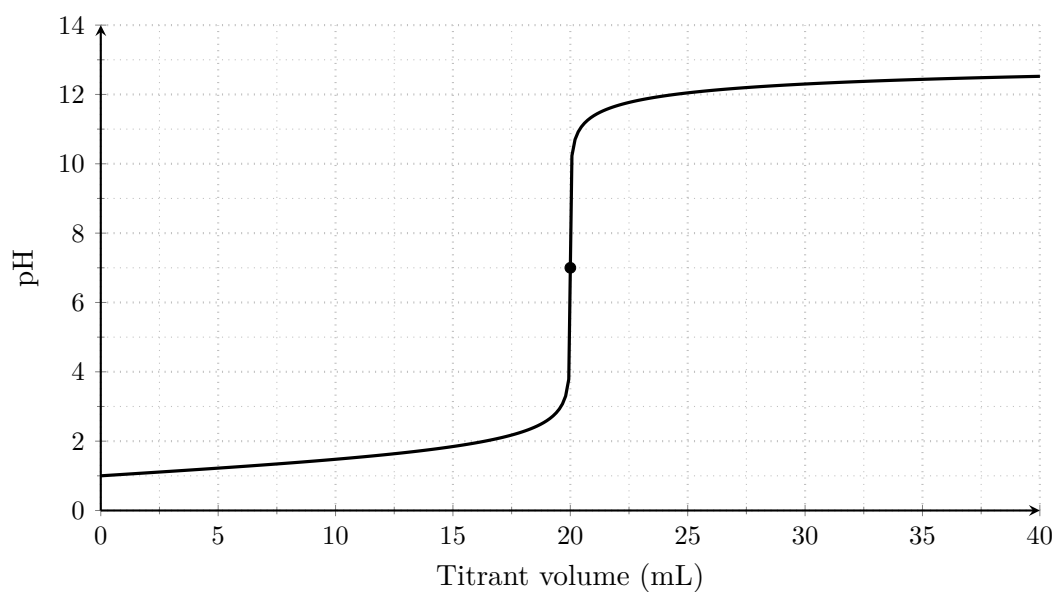
```
\begin{tikzpicture}
  \begin{axis}[myaxis]
    \phtitration[
      type=weak-acid,
      Ca=0.100,
      Va=20,
      Cb=0.100,
      pKa=4.76
    ]
  \end{axis}
\end{tikzpicture}
```

The chemistry remains controlled by `phtitration`, while the appearance remains controlled by your own PGFPlots style.

12 Complete Examples

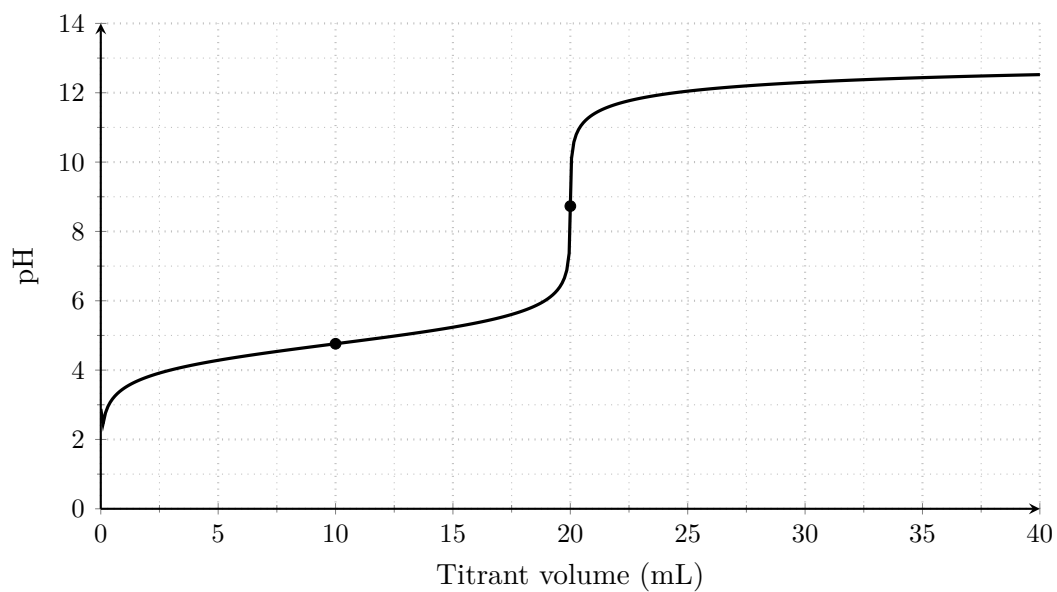
12.1 1. Strong Acid + Strong Base

```
\begin{tikzpicture}
  \begin{axis}[phtmanualaxis,xmax=40]
    \phtitration[
      type=strong-acid,
      Ca=0.100,
      Va=20,
      Cb=0.100,
      show-equivalence=true
    ]
  \end{axis}
\end{tikzpicture}
```



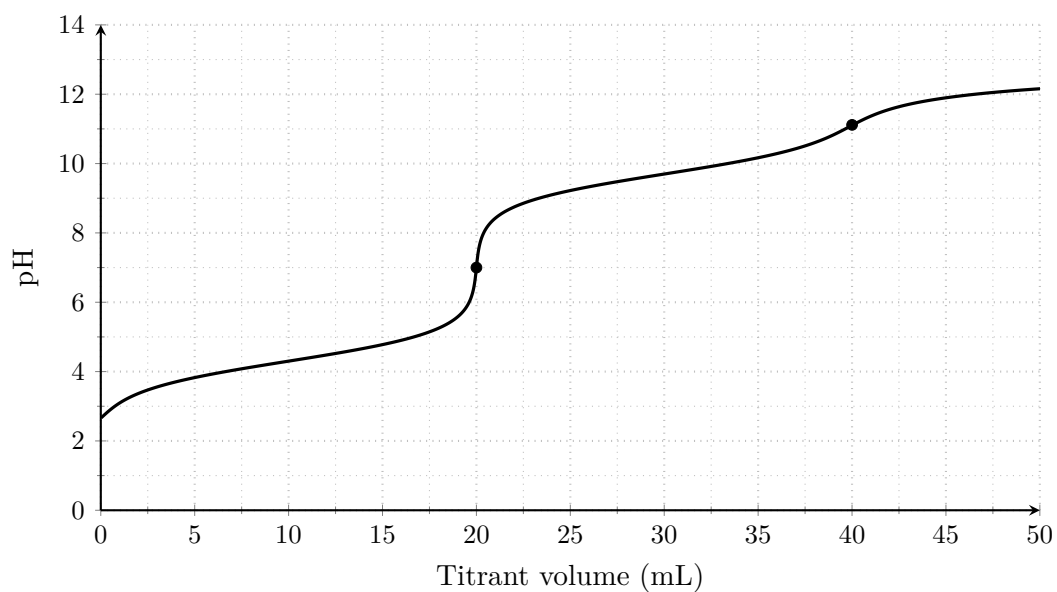
12.2 2. Monoprotic Weak Acid + Strong Base

```
\begin{tikzpicture}
  \begin{axis}[phtmanualaxis,xmax=40]
    \phtitration[
      type=weak-acid,
      Ca=0.100,
      Va=20,
      Cb=0.100,
      pKa=4.76,
      show-equivalence=true,
      show-half-equivalence=true
    ]
  \end{axis}
\end{tikzpicture}
```



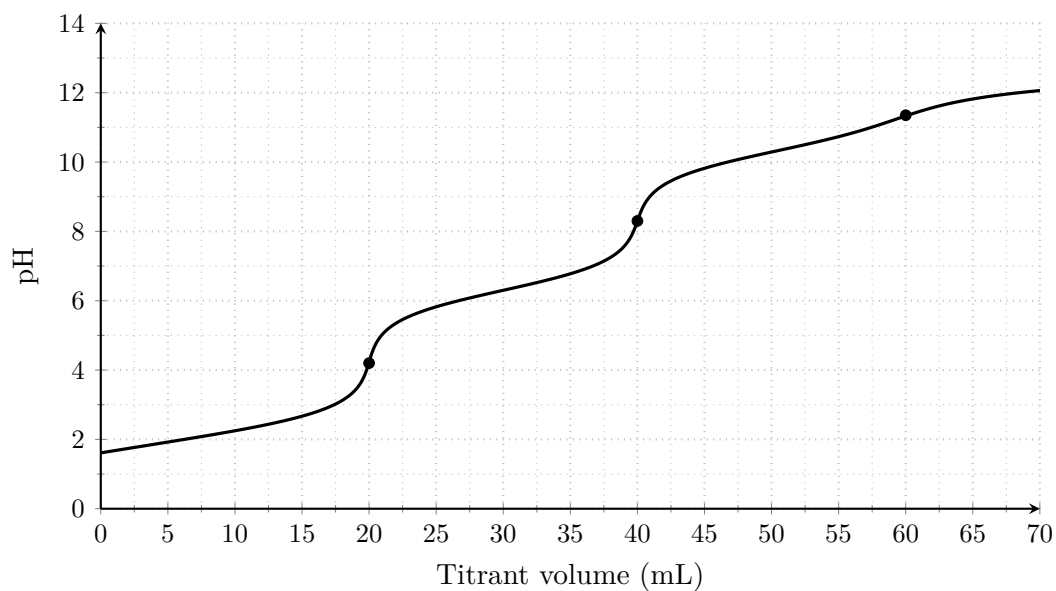
12.3 3. Diprotic Acid + Strong Base

```
\begin{tikzpicture}
  \begin{axis}[phtmanualaxis,xmax=50]
    \phtitration[
      type=diprotic-acid,
      Ca=0.100,
      Va=20,
      Cb=0.100,
      pKa1=4.30,
      pKa2=9.70,
      show-equivalence=true,
      show-half-equivalence=true
    ]
  \end{axis}
\end{tikzpicture}
```



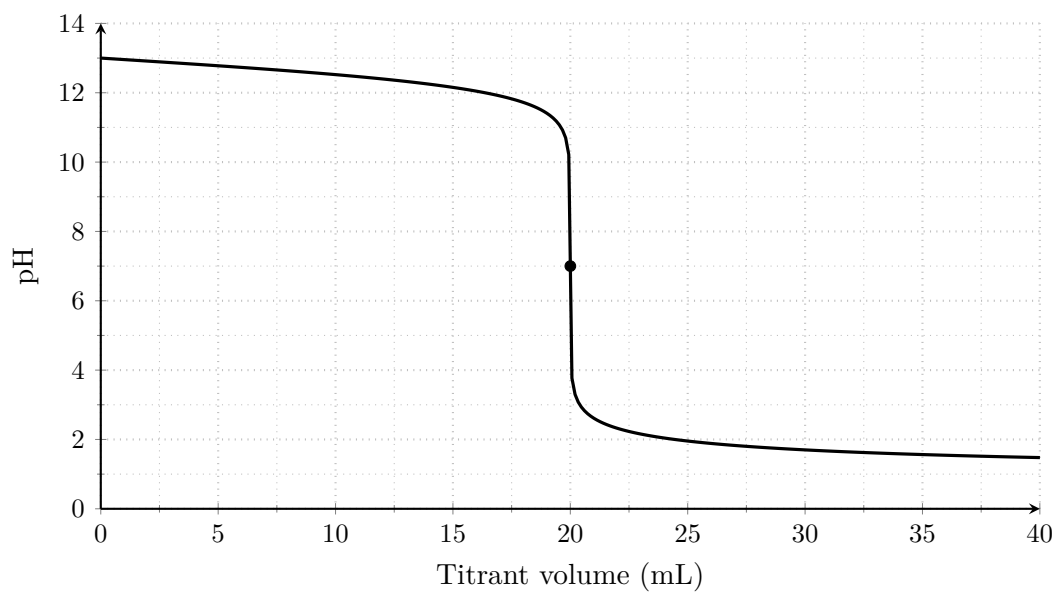
12.4 4. Triprotic Acid + Strong Base

```
\begin{tikzpicture}
  \begin{axis}[phtmanualaxis,xmax=70]
    \phtitration[
      type=triprotic-acid,
      Ca=0.100,
      Va=20,
      Cb=0.100,
      pKa1=2.10,
      pKa2=6.30,
      pKa3=10.30,
      show-equivalence=true,
      show-half-equivalence=true
    ]
  \end{axis}
\end{tikzpicture}
```



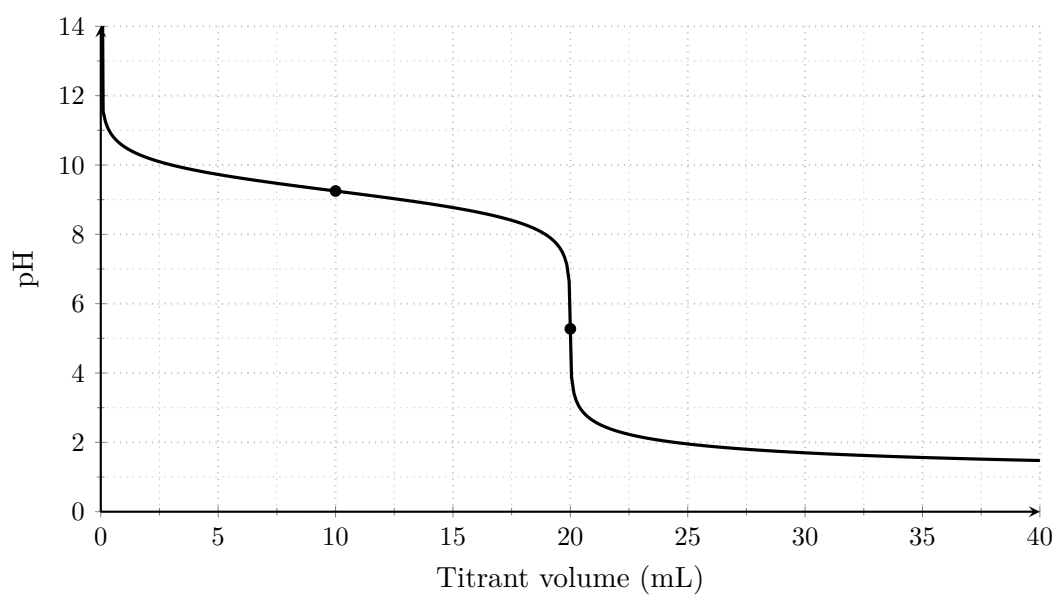
12.5 5. Strong Base + Strong Acid

```
\begin{tikzpicture}
  \begin{axis}[phtmanualaxis,xmax=40]
    \phtitration[
      type=strong-base,
      Cb=0.100,
      Vb=20,
      Ca=0.100,
      show-equivalence=true
    ]
  \end{axis}
\end{tikzpicture}
```



12.6 6. Monoprotic Weak Base + Strong Acid

```
\begin{tikzpicture}
  \begin{axis}[phtmanualaxis,xmax=40]
    \phtitration[
      type=weak-base,
      Cb=0.100,
      Vb=20,
      Ca=0.100,
      pKb=4.75,
      show-equivalence=true,
      show-half-equivalence=true
    ]
  \end{axis}
\end{tikzpicture}
```

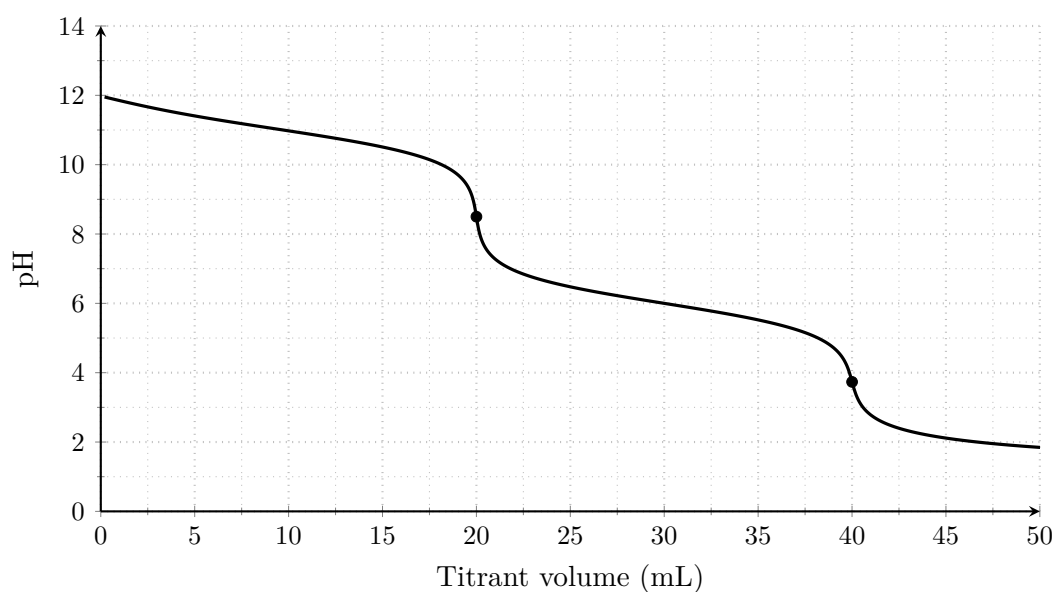


12.7 7. Dibase + Strong Acid

```

\begin{tikzpicture}
  \begin{axis}[phtmanualaxis,xmax=50]
    \phtitration[
      type=dibase,
      Cb=0.100,
      Vb=20,
      Ca=0.100,
      pKb1=3.00,
      pKb2=8.00,
      show-equivalence=true,
      show-half-equivalence=true
    ]
  \end{axis}
\end{tikzpicture}

```

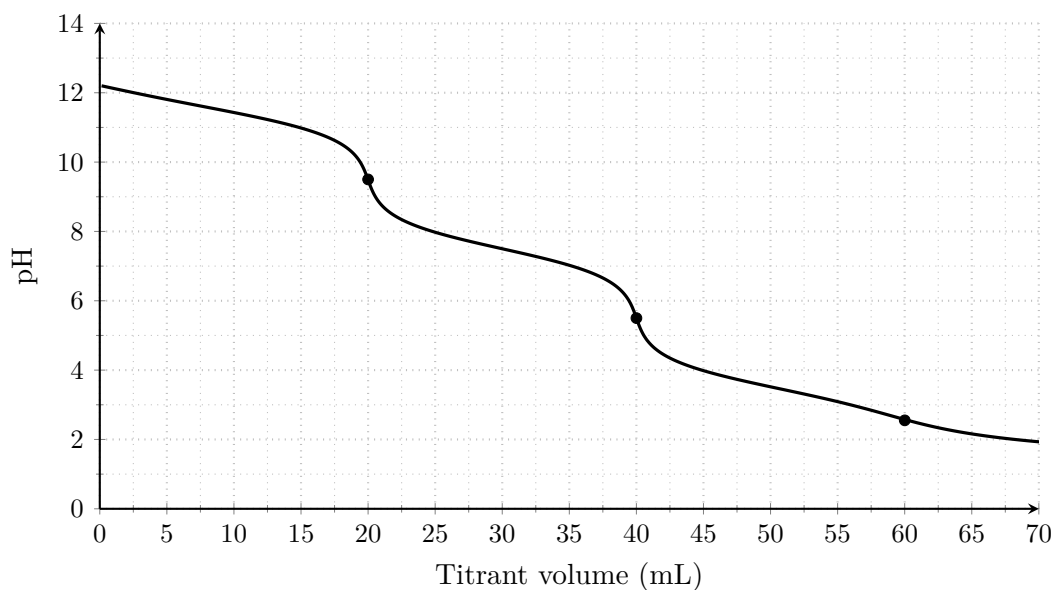


12.8 8. Tribase + Strong Acid

```

\begin{tikzpicture}
  \begin{axis}[phtmanualaxis,xmax=70]
    \phtitration[
      type=tribase,
      Cb=0.100,
      Vb=20,
      Ca=0.100,
      pKb1=2.50,
      pKb2=6.50,
      pKb3=10.50,
      show-equivalence=true,
      show-half-equivalence=true
    ]
  \end{axis}
\end{tikzpicture}

```



13 Changing the Plot Appearance

Because `phtitration` adds a PGFPlots curve, ordinary PGFPlots commands can be used around it.

For example:

```
\begin{axis}[
  width=13cm,
  height=8cm,
  xmin=0, xmax=40,
  ymin=0, ymax=14,
  axis lines=middle,
  grid=both,
  major grid style={dotted},
  minor x tick num=1,
  minor y tick num=1,
  xlabel={\mathit{V}_{\mathrm{NaOH}} (mL)},
  ylabel={pH},
  ticklabel style={font=\small}
]
  \phtitration[
    type=weak-acid,
    Ca=0.100,
    Va=20,
    Cb=0.100,
    pKa=4.76
  ]
\end{axis}
```

The curve itself is inserted by an `\addplot` operation, so it inherits the surrounding PGFPlots environment.

14 Integration with a TikZ-Only Physics Package

If your main document already contains a personal TikZ-only package for physics diagrams or coordinate systems, there is no requirement to replace it with PGFPlots.

A typical preamble can be:

```
\usepackage{yourphysics}
\usepackage{phtitration}
```

Your physics package can continue to define colours, TikZ styles, coordinates and graphical constructions. `phtitration` is responsible only for generating the pH titration data/curve inside the PGFPlots axis.

This separation is useful when a larger educational package already has its own visual identity.

15 Arabic Documents with XeLaTeX

The manual is written in English, but `phtitration` can be used in Arabic XeLaTeX documents.

For example:

```
\documentclass{article}

\usepackage{fontspec}
\usepackage{polyglossia}
\setdefaultlanguage{arabic}
\newfontfamily\arabicfont[Script=Arabic]{Amiri}

\usepackage{tikz}
\usepackage{pgfplots}
\pgfplotsset{compat=1.18}
\usepackage{phtitration}

\begin{document}

    \begin{tikzpicture}
        \begin{axis}[
            xmin=0, xmax=40,
            ymin=0, ymax=14,
            xlabel={Volum (mL)},
            ylabel={pH},
            grid=both
        ]
            \phtitration[
                type=weak-acid,
                Ca=0.100,
                Va=20,
                Cb=0.100,
                pKa=4.76
            ]
        \end{axis}
    \end{tikzpicture}

\end{document}
```

The important rule is that `fontspec`, `polyglossia` and other language-related packages belong to the document. They are not loaded automatically by `phtitration`.

16 Troubleshooting

16.1 The command is undefined

Make sure the package is loaded:

```
\usepackage{phtitration}
```

Also verify that `phtitration.sty` is in the same directory as the main `.tex` file.

16.2 PGFPlots or TikZ errors appear

Make sure PGFPlots is available and use:

```
\pgfplotsset{compat=1.18}
```

The package itself loads TikZ and PGFPlots.

16.3 The curve stops before the final equivalence point

Increase `xmax`. For example:

```
xmax=70
```

This is especially important for triprotic and tribasic systems.

16.4 The curve is visually too coarse

Increase:

```
samples=101
```

or:

```
samples=301
```

16.5 The graph looks strange near a steep transition

Avoid excessively low values of `samples`. Also avoid using a plotting range that is much larger than necessary when the transition region is the main feature of interest.

The chemical calculation and the visual interpolation are separate issues: `samples` controls the number of chemical evaluations, while PGFPlots controls the visual rendering.

16.6 A key is reported as unknown

Only the keys documented in Section 5 are package keys in v1.0.0.

For example, `width`, `height`, `grid`, `ymin`, `ymax`, `colours` and `line styles` should be placed in the surrounding `axis` environment, not inside `\phtitration`.

17 Scientific Scope and Limitations

`phtitration` is designed primarily for **educational and graphical purposes**.

The numerical model assumes ideal-solution behaviour and uses the standard $pK_w = 14$ convention for the pH range considered here. Activity coefficients, ionic-strength corrections and detailed thermodynamic effects are not modelled.

The numerical solver is a fixed-iteration bisection method. Therefore, the package should not be presented as a general-purpose research-grade chemical-equilibrium solver.

For advanced equilibrium calculations involving, for example,

- significant activity effects,
- very dilute solutions,
- coupled equilibria,
- metal–ligand complexation,
- precipitation,
- redox equilibria,
- temperature-dependent K_w ,

a dedicated chemical-equilibrium program or a more advanced numerical model should be used.

18 Recommended Workflow

A practical workflow for creating a graph is:

1. Choose the chemical system through `type`.
2. Enter the initial analytical concentrations and volume.
3. Enter the relevant pK_a or pK_b values.
4. Set `xmax` beyond the last equivalence point.
5. Choose the surrounding PGFPlots dimensions and axis limits.
6. Enable `show-equivalence` when equivalence markers are useful.
7. Enable `show-half-equivalence` when teaching buffer regions.
8. Increase `samples` only when the curve requires finer volume resolution.

19 Quick Reference

```
% Acid group
type=strong-acid
type=weak-acid
type=diprotic-acid
type=triprotic-acid
```

```
% Base group
type=strong-base
type=weak-base
type=dibase
type=tribase
```

Monoprotic weak acid

```
\phtitration[
type=weak-acid,
Ca=0.100,
Va=20,
Cb=0.100,
pKa=4.76,
xmax=40,
show-equivalence=true,
show-half-equivalence=true
]
```

Diprotic acid

```
\phtitration[
type=diprotic-acid,
Ca=0.100,
Va=20,
Cb=0.100,
pKa1=4.30,
pKa2=9.70,
xmax=50,
show-equivalence=true
]
```

Triprotic acid

```
\phtitration[
type=triprotic-acid,
Ca=0.100,
Va=20,
Cb=0.100,
pKa1=2.10,
pKa2=6.30,
pKa3=10.30,
xmax=70,
show-equivalence=true
]
```