

Buffers Plus

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Abstract

In 1989 *JCE Software* published *The Acid–Base Package: A Collection of Useful Programs for Proton Transfer Systems (1)*. This DOS program has been fully upgraded by the same author to the world of Windows 95. *Buffers Plus* takes advantage of a modern user interface and offers many new options not possible in the original version. The opening window (Figure 1) offers seven options that cover a wide variety of needs for students learning about theory, practical pH calculations, titration curves, buffer preparation, buffer capacity, ionic strength effects on equilibria, alpha curves, etc. A particularly useful feature is the use of scroll bars for dynamic views of how key parameters influence titration curves, buffer capacity, and alpha plots.

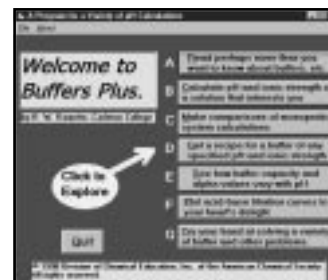


Figure 1. *Buffers Plus* presents seven options for the study of acid–base equilibria.

The seven *Buffers Plus* options are:

- A. A tutorial on the subjects of buffer algebra, alpha plots, ionic strength, activity coefficients, reference buffers, titration curves, buffer types, and buffer capacity.
- B. Calculates the equilibrium pH values from a specified initial composition chosen from a wide variety of acid–base mixtures.
- C. Demonstrates the effects of typical approximations of water ionization and acid dissociation, as well as ionic strength, on calculated pH and composition values.
- D. Calculates how a specific buffer could be prepared in the laboratory, given the desired values of buffer pH and ionic strength, as well as pK_a values.
- E. Explores graphically how the buffer capacity of mono-, di-, and triprotic systems, and also the related alpha values, vary with solution pH.
- F. Plots titration curves for acid–base and base–acid titrations, with options for showing the effects of ionic strength, alpha values, buffer capacity, and more. The pertinent pK value(s) are controlled by scroll bars, and the plotted curves change dynamically to show the pK dependence (Figure 2). A zoom feature applies to the endpoint regions.
- G. Presents typical problems to solve using *Buffers Plus* in areas of pH calculations, buffer recipes, titration curves, buffer capacity, and alpha values. Users may easily jump to and from any of the options, in any order.

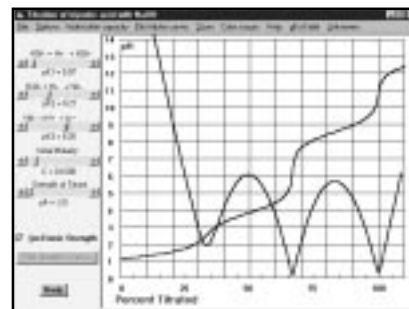


Figure 2. Titration curve of triprotic acid with buffer capacity. The plots are updated automatically as parameters are adjusted using the sliders.

Buffers Plus is intended for individual exploration by students, as a basis for assignments by the instructor, and for projecting illustrations in the classroom.

Instructor Notes

Buffers Plus is intended for individual exploration by students, as a basis for assignments by the instructor, and for projecting illustrations in the classroom.

Customizing Buffers Plus

These four files:

```
buffcap.txt
buffprep.txt
phcalc.txt
ticurve.txt
```

are short collections of problems to be solved using the Buffers Plus program (Option \ominus). Instructors may change or add problems to these files simply by separating successive problems with an asterisk (*). For example, from buffcap.txt:

```
*
Use the plots of BC and Alpha to convince yourself that the maximum buffer
capacity corresponds to equal concentrations of conjugate acid and con-
jugate base, assuming a fixed total concentration of both.
*
How close must the two pK values for a diprotic acid be to eliminate the
minimum in BC?
*
As the pH of a malonic acid solution is varied, at what pH does the HMal-
species reach a maximum?
*
```

The edited file **MUST** be saved in plain text (.TXT) format.

Rich text format files (RTF) are used for instruction by Buffers Plus. Instructors may modify them if desired, but should keep the originals backed up in case something goes wrong. Be sure to save them in .RTF format.

The first group is used in Option C, Make comparisons of monoprotic system calculations. FULL refers to exact calculations, INTER to calculations without ionic strength, and SIMPLE to the most approximate procedures. WA = weak acid, WB = weak base, BU = buffer

```
wafull.rtf      bufull.rtf      wbsimple.rtf   neutral.rtf
wainter.rtf    wbinter.rtf    wbfull.rtf
wasimple.rtf   buinter.rtf    busimple.rtf
```

This group of RTF files is used in Option A, a series of tutorials on buffers and related topics.

```
tabintro.rtf   Introduction tab
tabAlpha.rtf   Alpha Plots tab
tabIS.rtf      Ionic Strength tab
tabActCo.rtf   Activity Coefficients tab
tabrefbuff.rtf Reference Buffers tab
ticurves.rtf   Titration Curves tab
tabtypes.rtf   Buffer Types tab
tabbuffcap.rtf Buffer Capacity tab
```

Citations

1. Ramette, R. W. *J. Chem. Educ. Software* **1989**, 2B No. 2.