pH CALCULATION OF A PARTICULAR ACETONITRILE-AQUEOUS BUFFER MOBILE PHASE

Xavier Subirats - Versió 1.0 - 2007

INTRODUCTION

The present spreadsheet allows the calculation of the pH of a particular mobile phase containing acetonitrile as organic modifier up to 60% in volume, at 25ºC.

The studied buffering systems included in the present *Version 1.0* are:

- Acetic acid-acetate
- Ammonium-ammonia
- Citric acid-dihydrogencitrate-hydrogencitrate-citrate
- Phosphoric acid-dihydrogenphosphate-hydrogenphosphate

Concentrations of the aqueous buffer (before adding the acetonitrile) cover the range between 0.001 and 0.1 mol·L^{-1}.

INSTRUCTIONS

1. Choose the buffering system (*acetic*, *citric*, *phosphoric* or *ammonium*)
2. Introduce the % in volume of acetonitrile in the mobile phase; this value must be in the range of 0-60% (e.g. *60*)

MeCN fraction in hydroorganic mixture (% v/v)	60	(0-60%)

3. Introduce the pH of the aqueous buffering system, before adding the acetonitrile (e.g. *5.00*).

${}^{w}_{w}$pH	5.00	(0-14)

4. Introduce the concentration of the aqueous buffer, before adding the acetonitrile; this value must be in range of 0.001-0.1 mol·L^{-1} (e.g. 0.01)

Initial aqueous concentration - c_T (mol·L^{-1})	0.01	(0.001-0.1M)
log c_T	-2.00	

5. Result is obtained in two different pH scales: ${}^{s}_{w}$pH and ${}^{s}_{s}$pH

${}^{s}_{w}$pH	6.37
${}^{s}_{s}$pH	6.81

REFERENCE

Retention of ionisable compounds on high-performance liquid chromatography XV. Estimation of the pH variation of aqueous buffers with the change of the acetonitrile fraction of the mobile phase.
Xavier Subirats, Elisabeth Bosch, Martí Rosés
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