

**pH CALCULATION OF A PARTICULAR
METHANOL-AQUEOUS BUFFER MOBILE PHASE**
Xavier Subirats - Version 1.0 - 2007

INTRODUCTION

The present spreadsheet allows the calculation of the pH of a particular mobile phase containing methanol as organic modifier up to 80% in volume, at 25°C.

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 methanol) 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 methanol in the mobile phase; this value must be in the range of 0-80% (e.g. 60)

MeOH fraction in hydroorganic mixture (% v/v)	60	(0-80%)
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3. Introduce the pH of the aqueous buffering system, before adding the methanol (e.g. 4.00).

$w_w \text{pH}$	4.00	(0-14)
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4. Introduce the concentration of the aqueous buffer, before adding the methanol; 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: $s_w \text{pH}$ and $s_s \text{pH}$

$s_w \text{pH}$	5.17
$s_s \text{pH}$	4.99

REFERENCE

Retention of ionisable compounds on high-performance liquid chromatography XVII. Estimation of the pH variation of aqueous buffers with the change of the methanol fraction of the mobile phase.

Xavier Subirats, Elisabeth Bosch, Martí Rosés

Journal of Chromatography A, 1138 (2007) 203–215

(doi:10.1016/j.chroma.2006.10.087)