pH Adjustment for NMR Applications

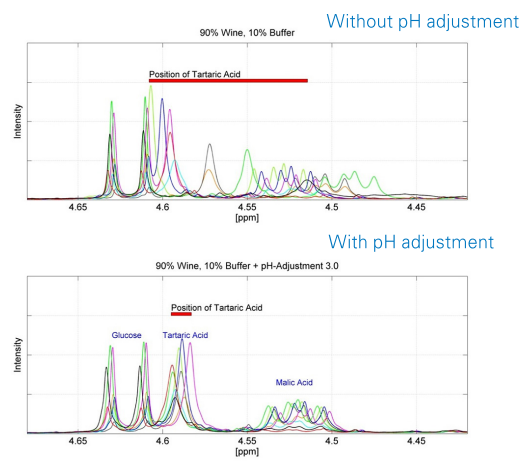
pH Titration Unit

Motivation

The adjustment of the pH value of the sample solution is crucial for the acquisition of NMR spectra. Slight pH variations of just 0.05 units can change the chemical shift of the NMR spectra substantially. For statistical evaluation of NMR spectra, the pH value should be adjusted to more than +/- 0.04 tolerance, but this necessitates careful pH adjustment. A problem arises from the fact that the totally available sample volumes are only in the order of 1-2ml. Currently, this adjustment is done manually, by adding reagents in the low µl range. pH adjustment under these conditions is relatively tedious, time consuming work and requires an experienced person.

Solution

Buffer solution, with an optional internal standard, is added to the sample and mixed. The pH is measured and, depending on the predefined pH value, small amounts of acid/base are automatically added and mixed. Additional cycles of pH measurement, acid/base addition and mixing are executed until the target pH is reached. Automating this procedure saves time and delivers higher reproducibility of results.



pH Titration Unit with high precision pumps, syringes with minimized void volume, vial shaker and touch panel for control

One-Step pH adjustment

The specialized pH-electrode with integrated capillaries for buffer, acid and base, enables treatment of small sample volumes down to 300 µl in a *One-Step* pH-endpoint titration.

The *One-Step* procedure requires the calibrated pH electrode to be placed into the sample just once. With predefined values for buffer volume, mixing frequency and final pH, the pH adjustment will run without the need for further manual interaction and lists the total volume added. This is needed for precise quantification.

Integration into complete automation is a further step to be realized in the future.

Special pH Electrode