

DETERMINATION OF pK_a USING

UV-VIS SPECTROSCOPY

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ABSTRACT

In this lab, the pK_a of the indicator phenol red was determined using UV-Vis spectroscopy. A mixture of acidic and basic forms of phenol red, produced using a sodium biphosphate/dihydrogen phosphate buffer, was analyzed in order to determine the concentration of each species in the buffered solution. These concentrations were then used to calculate the pK_a from the pH of the solution and the Henderson-Hasselbach equation. The pK_a of the indicator was calculated to be 5.881, differing significantly from the predicted range of 6.4 – 8.0. This discrepancy most likely indicates an experimental error, as the pK_a of phenol red should lie inside its transition range.

RESULTS

Phenol red indicator stock solution at 0.3949 mg/mL was used to prepare strongly acidic, basic, and buffered solutions, which were analyzed using UV-Vis spectroscopy. Using a molecular weight of phenol red of 345.38 g/mol, the molar concentration of this stock solution was calculated to be 1.143×10^{-3} M. Acidic, basic, and buffered phenol red solutions at diluted concentrations of 2.287×10^{-5} M were analyzed via UV-Vis spectroscopy. The buffered solution was produced using a sodium biphosphate/dihydrogen phosphate buffer at a pH 7.199. In order to determine the molar extinction coefficients for each pure substance, absorbances of the strongly acidic and basic solutions of phenol red were measured at 340 nm and 505 nm. The data obtained is shown in Table 1.

Table 1 – Absorbances of Acidic and Basic Indicators at Specified Wavelengths

	<i>340nm</i>	<i>505nm</i>
Acid Phenol Red	0.10221	0.49123
Base Phenol Red	0.43375	0.27050

Using the known concentration of each solution, the molar extinction coefficient values for the solutions at each wavelength were calculated. These values are shown in Table 2.

Table 2 – Molar Extinction Coefficients ($M^{-1}cm^{-1}$) of Acidic and Basic Indicators

	<i>340nm</i>	<i>505nm</i>
Acid Phenol Red	4470.	21480
Base Phenol Red	18970	11830

The buffered phenol red solution produced a relatively flat UV-Vis spectrum compared to the purely acidic and basic phenol red spectra (Appendix). An isosbestic point was observed at approximately 370 nm. The absorbance of the buffered solution was found

to be 0.18636 at 340 nm and 0.12495 at 505 nm, leading to a system of Beer's Law equations (Figure 2).

Figure 2 – Beer's Law: System of Equations

340 nm	$A_1 = bc_a e_a^{l_1} + bc_b e_b^{l_1}$ $0.18636 = (1cm)c_a (4470M^{-1}cm^{-1}) + (1cm)c_b (18970M^{-1}cm^{-1})$
505 nm	$A_2 = bc_a e_a^{l_2} + bc_b e_b^{l_2}$ $0.12495 = (1cm)c_a (21480M^{-1}cm^{-1}) + (1cm)c_b (11830M^{-1}cm^{-1})$

Using Microsoft Excel matrix algebra techniques to solve these equations, it was determined that the concentration of acidic phenol red in the buffered solution sample was 4.670×10^{-7} M and the concentration of basic phenol red was 9.715×10^{-6} M. Using the Henderson-Hasselbach equation and a buffered pH of 7.199, the pK_a of phenol red was calculated to be 5.881 with a corresponding K_a of 1.316×10^{-6} .

CONCLUSIONS

In conclusion, the concentrations of acidic and basic phenol red in a buffered solution were successfully determined using UV-Vis spectroscopy. These concentrations were used to calculate a pK_a of 5.881 for the phenol red indicator. However, the reported transition range of phenol red, a range which should include the compound's pK_a , is 6.4-8.0.¹ This discrepancy was unexpected, since the pH of the biphosphate/dihydrogen phosphate buffer was chosen based on its proximity to phenol red's transition range.

One possible source of error was in the UV-Vis analysis of the buffered solution. The spectrum produced was not very defined, although an isosbestic point was present on the graph. The lack of definition, including the reduced absorbance values, could have

resulted in a pK_a below the accepted value. Also, the pH of the buffered solution was not remeasured upon analysis, an especially important point since almost one month passed between the creation of the buffer and its use in the experiment. Although a buffer would be expected to be stable, it is possible an error could have been made in its creation, leading to false initial readings of pH or chemical instability.

REFERENCE

¹Harris, D.C., Quantitative Chemical Analysis. W.H. Freeman and Company, 2003.

pg. 243.