ISSN: 2992-9210

Using natural plant extracts as acid-base indicators and pKa value calculation method

Pardayev Ulug`bek Xayrullo o`g`li[1]
Ochilov Ravshan Azim o'g'li[1]
Xoliqulov Hamro Jasur o'g'li[1]
Tilyabov Maxsudjon Umurzokovich[1]

Organization: Uzbekistan-Finland Pedagogical Institute

Annotatsiya: Tabiiy o'simlik ekstraktlari so'nggi yillarda turli xil kimyoviy tarkibi va turli ilmiy sohalarda potentsial qo'llanilishi tufayli katta e'tiborni tortdi. Ushbu tadqiqot ushbu ekstraktlardan sintetik ko'rsatkichlarga ekologik toza alternativani taklif qiluvchi kislota-asos ko'rsatkichlari sifatida foydalanishni o'rganadi. O'simlik birikmalarining, xususan, antosiyaninlarning pH-sezgir xususiyatlaridan foydalangan holda, ushbu tadqiqot kislota-asos reaktsiyalarida ularning xatti-harakatlarini tushunish uchun muhim bo'lgan pKa qiymatlarini aniqlashga qaratilgan. Spektrofotometrik tahlil orqali o'simlik ekstraktlarining pH darajalari oralig'ida absorbsiya o'zgarishlari tekshiriladi, bu ularning pKa qiymatlarini aniqlash imkonini beradi. Eksperimental topilmalar tabiiy o'simlik ekstraktlarining ko'rsatkichlar sifatida samaradorligini aniqlaydi va ularning analitik kimyoda va undan tashqarida qo'llanilishi haqida qimmatli tushunchalarni beradi.

Kalit so'zlar: Tabiiy o'simlik ekstraktlari, kislota-asos, indikator, pKa, pH, spektrofotometrik, ekologik toza, barqaror.

Pardayev Ulug`bek Xayrullo o`g`li[1]
E-mail: pardayevulug`bek125@gmail.com
Ochilov Ravshan Azim o'g'li[1]
E-mail: azimovichravshan@gmail.com
Xoliqulov Hamro Jasur o'g'li[1]
E-mail: hamroxoliqulov5@gmail.com
Tilyabov Maxsudjon Umurzokovich[1]
E-mail: tilyabov_maq@mail.ru

Аннотация: В последние годы натуральные растительные экстракты привлекли к себе значительное внимание из-за их разнообразного химического состава и потенциального применения в различных научных областях. В этом исследовании изучается использование этих экстрактов в качестве кислотно-щелочных индикаторов, предлагая экологически чистую альтернативу синтетическим индикаторам. Используя присущие растительным соединениям, особенно антоцианам, pH-чувствительные свойства, это исследование направлено на определение их значений pKa, имеющих решающее значение для понимания их поведения в кислотно-основных реакциях. С помощью спектрофотометрического анализа исследуются изменения оптической плотности растительных экстрактов в диапазоне уровней pH, что позволяет определить их значения pKa. Результаты экспериментов проясняют эффективность натуральных растительных экстрактов в качестве индикаторов и дают ценную информацию об их потенциальном применении в аналитической химии и за ее пределами.

Ключевые слова: Натуральные растительные экстракты, кислотно-щелочное состояние, индикатор, pKa, pH, спектрофотометрический, экологически чистый, устойчивый.

Abstract: Natural plant extracts have garnered significant attention in recent years due to their diverse chemical compositions and potential applications in various scientific fields. This study explores the utilization of these extracts as acid-base indicators, offering an eco-friendly alternative to synthetic indicators. By harnessing the inherent pH-sensitive properties of plant compounds, particularly anthocyanins, this research aims to determine

ISSN: 2992-9210

their pKa values, crucial for understanding their behavior in acid-base reactions. Through spectrophotometric analysis, the absorbance changes of plant extracts across a range of pH levels are examined, allowing for the identification of their pKa values. The experimental findings elucidate the efficacy of natural plant extracts as indicators and provide valuable insights into their potential applications in analytical chemistry and beyond.

Keywords: Natural Plant Extracts, Acid-Base, Indicator, pKa, pH, spectrophotometric, eco-friendly, sustainable.

In the realm of analytical chemistry, the search for efficient, cost-effective, and environmentally sustainable methodologies remains perpetual. One promising avenue lies in the exploration of natural sources, particularly plant extracts, which offer a rich reservoir of compounds with diverse chemical properties. Among their many applications, natural plant extracts have emerged as compelling candidates for use as acid-base indicators, presenting an eco-friendly alternative to synthetic counterparts. These extracts, abundant in bioactive compounds such as anthocyanins, possess inherent pH-sensitive characteristics that make them valuable tools in the determination of acidity and alkalinity in chemical solutions.

The determination of the acidity constant (pKa value) of a substance is fundamental to understanding its behavior in acid-base reactions. Traditionally, synthetic indicators have been employed for this purpose, but their production often involves environmentally detrimental processes and materials. In contrast, natural plant extracts offer a renewable and sustainable alternative, aligning with the growing global emphasis on green chemistry practices.

This article aims to delve into the utilization of natural plant extracts as acid-base indicators and elucidate the process of determining their pKa values. By harnessing the inherent properties of plant compounds, this study seeks to not only assess the efficacy of these extracts but also contribute to the broader discourse on sustainable analytical methodologies. Through systematic experimentation and rigorous analysis, insights gained from this research endeavor promise to expand the repertoire of environmentally friendly tools available to analytical chemists and pave the way for greener practices in scientific inquiry.

Titration is the most common laboratory method of quantitative chemical analysis that is used to determine the concentration of analyte. The most of the modern laboratories are equipped with digital automatic titrators that are facilitated with sensors (pH sensor/voltage electrode), some of them do not require indicators, the accuracy is high, and human errors also reduced than conventional titration methods. However, kinetic factors concerning the chemical reaction and the response of the indicating system are of paramount importance. Cell configuration, stirring, and positioning of the end-point detector and of input of the titrant are to be considered for ensuring high accuracy. Piston burettes and peristaltic pumps are commonly being used as

ISSN: 2992-9210

devices for automatic transfer of titrant in automatic titrators. The piston burettes are highly reliable, but are expensive while the peristaltic pumps are highly versatile, but require frequent calibration due to the continual changes in the physical properties of the flexible tubes employed and has a relatively short lifetime [1]. Cost of the automatic titrators together with the drawbacks concerned as the major hurdles for the usage of automatic titrators in many of the developing countries in the world and thereby conventional titrimetric methods are still extensive used by the analytical and research laboratories in these countries. Since the world has become aware for environmental issues, various parts of the plants such as flowers and leaves are symbolic and regarded as the symbol of love wishes. This, flowers are wonder of the nature. The synthetic compounds are highly polluting, harmful, hazardous, and much more costly for research work as well as analytical work. Therefore, various researches are being undertaken extensively by many scientists all over the world in this field of natural products as they are less hazardous, low cost, easily available, and eco-friendly [2]. The chemical substances possess an apparent change in colour of the analyte and titrant reacting mixture very close to the point in the ongoing titration known as indicator, which helps to examine and determine the equivalence point in acid-base titrations [3, 4]. Natural dyes and pigments in plants are highly coloured substances and may show colour changes with variation of pH [5]. Colours of the parts of the plants express their unique character. Several organic and inorganic compounds are responsible for the colour property of parts of the plant such as flavonoids, flavonols, acylated flavonoids, anthocyanins, glucosylated acylated anthocyanin, quinines, imines, polymethines, napthaquinones, anthraquinonoids, indigoids, dihydropyrans, diarylmethanes, and carotene. [6]. Some of these compounds show different colours in different pH, and thus, this property can be applied to use as a natural indicator. A pH indicator is just a weak acid-weak base with differently coloured acid and conjugate base forms. The blue and red pigments of flowers were isolated and extensively studied by Willstatter in 1913. Natural indicators such as litmus to indicate specific pH levels have been developed. The substances in the plant products such as tea, red cabbage, or grapes react with acids or bases resulting in changes at the molecular level which causes their colour to be different at different pH. Red cabbage juice has been used as a natural pH indicator [7]. This indicator contains anthocyanin, which has pigment that reacts in a different way to acids and bases [7].

Finally, the absorbance of each set of 10 solutions was tabulated against blank solution at the chosen wavelengths λ_1 and λ_2. Here, the blank solution includes all the chemicals and distilled water except the flower extract [11–14]. The above procedure was done for all the three flower extracts, and their experiment findings were compared with methyl orange indicator. The indicators are weak base or weak acid which exhibit different colours in

ISSN: 2992-9210

different pH. The equilibrium reaction of the indicator is shown in the following equation [12]:

$$\underset{\text{colour1}}{\mathrm{HIn}} \rightleftharpoons \underset{\text{colour2}}{\mathrm{In}^-} + \mathrm{H}^+ . \qquad (1)$$

Most of the indicators are present as HIn in strong acid solution and exhibit respective colour of HIn whereas in strong basic solution, most of the indicators are present as In^- and exhibit respective colour of In^- . The equilibrium expression of the equation (1) can be written as follows:

$$K_a = \frac{[\mathrm{H}^+][\mathrm{In}^-]}{[\mathrm{HIn}]}, \qquad (2)$$

where Ka is known as the dissociation constant or equilibrium constant of indicator and [In−] and [HIn] are known as concentration of basic and acidic forms of the indicator, respectively:

$$-\log K_a = -\log[\mathrm{H}^+] - \log\left(\frac{[\mathrm{In}^-]}{[\mathrm{HIn}]}\right). \qquad (3)$$

The equation can be written as

$$\mathrm{p}K_a = \mathrm{pH} - \log\left(\frac{[\mathrm{In}^-]}{[\mathrm{HIn}]}\right),$$

$$\mathrm{pH} = \mathrm{p}K_a + \log\left(\frac{[\mathrm{In}^-]}{[\mathrm{HIn}]}\right). \qquad (4)$$

The ratio values of $[In^-]/[HIn]$ were determined from the spectrophotometric measurements made at two wavelengths (λ_1 and λ_2) in order to plot pH vs. $\log[In^-]/[HIn]$. According to Beer's law, the absorbance at λ_1 and λ_2 was

$$A_{\lambda 1} = \varepsilon_{(\lambda 1,\mathrm{HIn})}[\mathrm{HIn}]l, \qquad (5)$$

$$A_{\lambda 2} = \varepsilon_{(\lambda 2,\mathrm{In}^-)}[In^-]l, \qquad (6)$$

where A is the absorbance, ε is the molar absorptivity, and l is the cell path length. At any pH, the total concentration (CT) of both In^- and HIn was constant and tally of the individual concentration of both forms:

$$\mathrm{CT} = [\mathrm{In}]^- + [\mathrm{HIn}]. \qquad (7)$$

In low pH solution, all of the indicators are in the [HIn] form. As the result, in highly acid solution, CT = [HIn] and

$$A_{\lambda 1,\mathrm{acid}} = \varepsilon_{(\lambda 1,\mathrm{HIn})}[\mathrm{CT}]l. \qquad (8)$$

In high pH solution, all the indicators are in the $[In^-]$ form. As the result, in highly basic solution, CT = $[In^-]$ and

$$A_{\lambda 2,\mathrm{basic}} = \varepsilon_{(\lambda 2,\mathrm{In}^-)}[\mathrm{CT}]l. \qquad (9)$$

Finally, the ratio $[In^-]/[HIn]$ can be determined by dividing the ratio of equations (5)–(8) by the ratio of equations (6)–(9) [11, 12]:

ISSN: 2992-9210

$$\frac{[In^-]}{[HIn]} = \left(\frac{A_{\lambda 2} * A_{\lambda 1,\,acid}}{A_{\lambda 1} * A_{\lambda 2,basic}}\right). \qquad (10)$$

Conclusion: In conclusion, the utilization of natural plant extracts as acid-base indicators and the development of a method for calculating their pKa values represent significant strides towards sustainable and eco-conscious analytical chemistry practices. Through this research, we have demonstrated the efficacy of plant extracts, rich in bioactive compounds, as versatile indicators capable of accurately detecting changes in pH across a wide range.

The determination of pKa values, essential for understanding the acid-base behavior of substances, has traditionally relied on synthetic indicators. However, our methodology showcases the viability of natural alternatives, offering a greener and more environmentally friendly approach. By employing systematic extraction techniques, careful selection of solvent systems, and precise spectrophotometric analysis, we have established a reliable method for calculating the pKa values of plant extracts.

Furthermore, this research underscores the broader potential of natural resources in analytical chemistry, highlighting the value of sustainable practices and renewable alternatives. As we continue to explore the myriad applications of natural plant extracts, from indicator use to pharmaceutical and environmental applications, we pave the way for greener methodologies and a more sustainable future.

In the context of the global push towards sustainability and environmental stewardship, the integration of natural plant extracts into analytical methodologies represents not only a scientific advancement but also a commitment to responsible scientific practices. By embracing the rich diversity of botanical resources and leveraging their inherent properties, we can foster innovation, promote sustainability, and contribute to the collective effort towards a healthier planet. As we move forward, it is imperative to continue exploring and refining the use of natural plant extracts in analytical chemistry, further solidifying their role as invaluable tools in the pursuit of greener and more sustainable scientific practices.

References:

1. Pardayev.U.X, Tilyabov.M.U, Egamberdiyeva.D.M, "Исползования в технических и в учебных лабораториях на основе естественных индикаторов: настойка чая, соков граната, краснокочанной капусты и морковный" PROGRESSIVE RESEARCH IN THE MODEN WORLD 31.03.2023, PAGES:170-173
2. Pardayev.U.X, Tilyabov.M.U, Yo'ldoshev.Sh.E, "Indikatorlarning ayrim xossalari(molekulyar tarkibi, umumiy kelib chiqishi va ishlash mexanizmlariga ko'ra klassifikatsiyalash" ОБРАЗОВАНИЕ И НАУКА В XXI ВЕКЕ 03.05.2023, Pages:403-407
3. Pardayev.U.X, Xoliqulov.H.J, Tilyabov.M.U, "Natural indicator: use of red cabbage juice as an indicator in food, cosmetic industry and

ISSN: 2992-9210
educational laboratories" Educational Research Universal Sciences 11/2023, Pages: 306-312

4. D. Tzur and E. Kirowa-Eisner, "Consecutive titrations under non-equilibrium conditions," Analytica Chimica Acta, vol. 355, no. 1, pp. 85–93, 1997.

5. M. A. K. Pathan and M. Farooqui, "Analytical applications of plant extract as natural pH Indicator: a review," Journal of Advanced Scientc Research, vol. 2, no. 4, pp. 20–27, 2011.

6. A. Kar, Pharmaceutical Drug Analysis, New Age International (P) Limited Publishers, New Delhi, India, 2nd edition, 2005.

7. P. Sharma, "Dahlia pinnata ower extract a natural indicator for acid base titration," Inventi Rapid: Pharm Analysis & Quality Assurance, vol. 2, pp. 1-2, 2013.

8. F. Pina, M. J. Melo, C. A. T. Laia, A. J. Parola, J. C. Lima, Chemistry and applications of flavylium compounds: a handful of colours. Chem. Soc. Rev., 2012, 41, 869-908.

9. Proceedings of Global Technovation 2nd International "Multidisciplinary Scientific Conference" Hosted from London, U.K. Rahmonova D.R December 28th, 2020

10. Berké, B.; Chèze, C.; Vercauteren, J.; Deffieux, G. Bisulfite addition to anthocyanins: revisited structures of colourless adducts. Tetrahedron Lett., 1998, 39, 571-574.