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Determination of Acid Dissociation Constant of Bromocresol Green, Phenolphtalein and Methyl Orange by a Novel Program in MATLAB Software and Changing Color of pH Paper

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Abstract
In this study, the acid dissociation constants (pKa) of three indicators, bromocresol green, phenolphthalein and methyl orange, were determined by scanning the solution of indicators and deposited pH paper in these solutions (in each step of color-changing solution) and then chemometrics method. These methods are simple, fast, and inexpensive. For this reason, first, the vessels containing the indicator solution and pH paper (in each step of color-changing solution) were scanned by the scanner, and then the images of sample solutions and pH papers were transferred to a computer using Microsoft Photo Editor (Microsoft XP). RGB values were measured, in each pixel, with the image processing tool box of MATLAB. In MATLAB (2013) software, a novel program was written based on RGB values, for calculating pKa indicators. The agreement between obtained pKa by this method and values reported in the literature demonstrates the utility of the method here used.

Keywords
Acid Dissociation Constant; Solution Scanometric Method; Chemometric Method; MATLAB Software.

1. INTRODUCTION

The extent of ionization of molecules in solution at different pH values, are indicated by dissociation constants. The acidity constants of organic reagents are important factors in many analytical procedures such as acid–base titration, solvent extraction, complex formation, and ion transport [1]. The knowledge of ionization constants is important in the understanding of certain chemical phenomena. Dissociation in chemistry and biochemistry is a general process in which ionic compounds [complexes, or salts] separate or split into smaller particles, ions, or radical, usually in a reversible manner [2].

Dissociation constant is most important parameter to understand chemical phenomenon such as biological activity, absorption and extent of ionization of compound in different pH, so is the key parameter in drug development and optimization [3-12]. The pK_a of a compound is the pH at which the compound is 50 % protonated [13].

The pK_a is the pH at which concentrations of ionized and un-ionized forms are equal. When the pH is lower than the pK_a, the un-ionized form of a weak acid predominates [14, 15]. In many experimental methods to determine pK_a values, a certain parameter is measured as a function of pH. This results in a characteristic sigmoid curve from which the pK_a may be determined by locating the inflection point [16]. It is customary to express the dissociation constant of both acidic and basic media by pK_a values. The lower the pK_a of an acidic media, stronger the acid [17]. Ionization constant [pK_a] is one of the important physicochemical properties. Dissociation constant is also helpful in screening salts, developing pre-clinical and clinical formulation. The pK_a is the negative logarithm of the equilibrium constant of the acid-base reaction of the compound of interest [18].

Different methods are available to determine the pK_a of drugs, such as potentiometry, spectrophotometry and solubility methods. The potentiometric titration and spectrometric method are commonly used and widely accepted techniques [19]. Poor solubility of the compounds hampers traditional potentiometric methods [20].This method can be applied only forcompounds having solubility greater than 100 µM. Spectrophotometric methods can be appliedto the compounds having solubility even 1.0µM. However, this method is limited to molecule shaving chromophores at ionization center, which shows spectral dissimilarity at protonated anddeprotonated form [20]. Also methods such as Fourier transform IR (FT-IR) spectrometry, fluorescence spectrophotometry, H NMR, chromatographic, capillary electrophoresis, calorimetric and conductometry methods for the determination of acidity constants are available [21-23]. Recently, Shokrollahi et al [24] developed

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solution scanometric method [25-31], and they determined the stability constants of indicators.
Solution scanometry method has advantages and disadvantages. Advantages of this method include simplicity, high scanning speed, inexpensive, portable systems and easy immobilizing of reactants, no need to find the λ_{max}, intensive archive of experiences, short response time, limiting the interferences, capability of various simultaneous tests and using non-transparent solution and investigation of the reflective properties of the surface. But, its disadvantages such as the lack of uniformity in the membrane cause serious effects on the relative standard deviation percent and precision of analysis.
Bromocresol green (BCG) (3', 3", 5', 5"-tetrabromo-mcresolsulfonphthalein)(Fig. 1a) is a sulfonphthalein dye, with a transition range of pH 3.8 to 5.4. In the acidic form, it appears yellow, and in the basic form, it is blue. It is used as a pH indicator and as a tracking dye for DNA agarose gel electrophoresis. It can be used in its free acid form (light brown solid), or as a sodium salt (dark green solid). In aqueous solution, BCG will ionize to give the mono anionic form (yellow), that further deprotonates at higher pH to give the dianionic form (blue), which is stabilized by resonance. It is widely used in Sol-gel matrix [32], fuel cells [33], and sensors [34]. Also, it is suitable for visualizing the compounds with functional groups whose pKa is below 5.0 (carboxylic acids, sulfonic acids, etc.). These appear as yellow spots on a light or dark blue background; no heating is necessary [35].
Methyl orange (MO) (Fig. 1b) is a pH indicator frequently used in titrations because of its clear and distinct colour change. Its transition range of pH is 3.8 to 5.4. Because it changes colour at the pH of a mid-strength acid, it is usually used in titrations for acids. Unlike a universal indicator, methyl orange does not have a full spectrum of colour change, but has a sharper end point. Methyl orange shows red colour in acidic medium and yellow colour in basic medium.
Methyl orange was first used in 1946 by Klotz et al [36].to investigate the interaction of small ions with proteins. Klotz et al. and later Takagishi et al. [37] focused on the interactions of MO with synthetic polymers, i.e. poly cations. In later studies similar spectral information was used to determine the binding stoichiometry and the influence of binding competition effects of salts, surfactants and poly anions [38]. These were generally interpreted – especially in the case of added ions - as arising from a generic effect of ionic strength.
Phenolphtalein(Fig. 1c) is often used as an indicator in acid–base titrations. For this application, it turns colorless in acidic solutions and pink in basic solutions. Its pH range is 8.3-10. Phenolphthalein is slightly soluble in water and usually is dissolved in alcohols for use in experiments. The phenolphthalein molecule is colorless, and the phenolphthalein ion is pink. Phenolphthalein has been used for over a century as a laxative, but is now being removed from over-the-counter laxatives [39] because of concerns over carcinogenicity [40, 41]. Thymolphethale in is a related laxative made from thymol. Despite concerns regarding its carcinogenicity, the use of phenolphthalein as a laxative is unlikely to cause ovarian cancer [42]. Phenolphthalein has been found to inhibit human cellular calcium influx via store-operated calcium entry (SOCE, see Calcium release activated channel & Structure). This is effected by its inhibiting thrombin and thapsigargin, two activators of SOCE that increase intracellular free calcium [43].

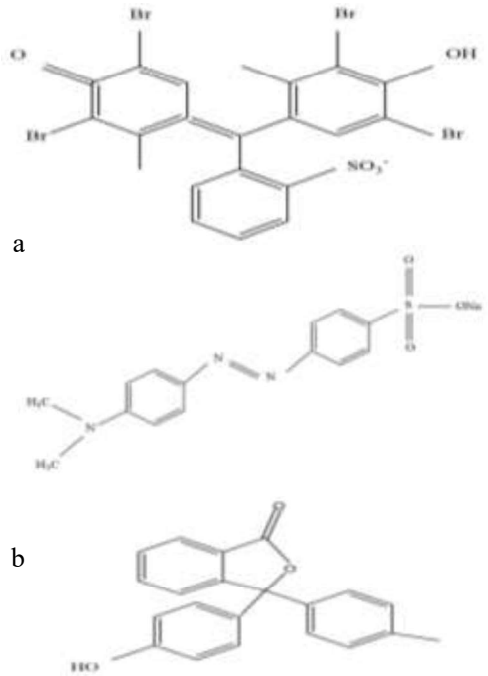

Fig. 1 Chemical structure of bromocresol green (a) methyl orange (b), and phenol phetalein(c)

In this work, the analytical feasibility of the basic colors and their representativeness by using chemometrics were studied. It represents a fundamental work in order to demonstrate the applicability of basic RGB color measurements in analytical determinations. Finally, a method for rapid and quantitative determination of pK_a, which relies on color development with a selective reagent and then chemometrics, (a novel program was written based on RGB values), for calculating

pK_a indicators, was developed. Results have been applied as a simplified and fast method that could be applied to different samples. Its use as a field method has also been probed.

2. EXPERIMENTAL

2.1. Apparatus

Cylindrical vessel (capsule) with 1000 µL volume. A scanner with resolution 600, a computer, for reading colorimetric data (RGB), and computing pK_a by chemomerics, were used.A pipette(100 to 1000 µL) and micro syringe were used to inject samples into the vessel (capsule) and titration indicator solution, respectively.

2.2.Software

The MATLAB (2013) software was used to convert the recorded pictures of color of vessel and pH paper to RGB data. Also, a novel program was written in MATLAB (2013), for analysis of RGB data and calculating pK_a of three indicators on the basis RGB data.

2.3. Principles of Color System RGB (Red, Green and Blue)

The RGB color model is an additive color model in which red, green, and blue lights are added together in various ways to reproduce a broad array of colors. In computing, the color values are often stored as integer numbers in the range of 0 to 255, the range that a single 8 bit byte can offer (by encoding 256 distinct values).In the RGB system, any color is represented in the form of (R, G, B), in which the (0, 0, 0) and (255, 255, 255) refer to black and white, respectively. Therefore, by increasing the intensity of colors, the color values decrease. In this system16777216 colors can be made. Any color can be described by the parameter V (Value) with the following formula:

Eq. (A.1) $V= R + 256G + (256)^2B$

Where, R, G and B are red, green and blue values of the main color. For black and white, V is equal to 0 and 16777216, respectively. In fact, V is the basis of RGB system and is defined this way to identify a specific number for each color.

2.4. Reagents

All reagents were of analytical grade and deionized water from a Milli Q water purification system was always used. NaOH solution (3.0M) was prepared by dissolving 3.0 g NaOH in deionized water and dilution (with deionized water) to the volume of 25 mL in calibrated flasks. Diluted solutions (NaOH 0.02M) were prepared from the previous concentrated NaOH solution by convenient dilution with deionized water in calibrated flasks. Therefore, for the preparation of 0.02M NaOH solution, 0.17 mL of NaOH solution (3.0M) was diluted by deionized water to the volume of 25 mL in calibrated flask. Indicators solutions (bromocresol green, phenolphetalein, methylorange) were prepared by dissolving 0.02 g of indicator in 1.45 mL NaOH (0.02 M) and dilution with deionized water to the volume of 50 mL, in calibrated flasks, and then 25mL from this solution (indicator) was diluted (4 times) by deionized water to the volume of 100 mL, in calibrated flasks.

2.5. Procedure

In this study, two procedures including solution scanometric and chemometrics methods were employed to obtain the acidity constants of the three indicators (BCG, MO, and PP). For this reason, in a vessel (capsule), 1.0 mL of indicator solution was acidified by HCl and vessel was scanned (resolution 600). Then this solution was titrated by NaOH (3.0M). In each step of color changing, solution was placed on pH paper and then pH paper and indicator solution were scanned (Fig.2-Fig.4).Images of sample solutions and pH paper were transferred to a computer and any color changes in each vessel and pH paper were analyzed by using a novel program written in MATLAB 2013.In this program, the color of each cellis analyzed based on the RGB system into R, G and B values. In different steps of changing colour, images of pH paper was compared with pH paper and then pH value was obtained in various steps of titration.

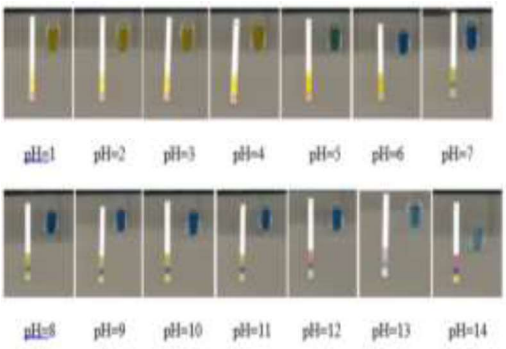

Fig. 2 Schematic of the solutions in cells and pH paper in different steps of titration, for indicator Bromo cresol.

Fig. 3 Schematic of the solutions in cells and pH paper in different steps of titration, for indicator Methyl orange.

Fig. 4. Schematic of the solutions in cells and pH paper in different steps of titration, for indicator Phenol phtalein.

3. RESULT AND DISCUSSION

Acid–base indicators are compounds that are simply weak acids (or bases) that exhibit different colors depending on whether they are present in a solution in their acidic form (HIn) or in their basic form (In^-). As the pH of a solution is changing (indicated by the color change of the indicator), the equilibrium Eq. (b.1) is driven either toward reactants (HIn) or products (In^-), therefore the color change of solution depends on the concentration of each of the forms present. At intermediate pH values, depending on the relative amounts of HIn and In^- present, the color of solution will be a mix of the color of HIn and In^-.

$$HIN_{(aq)} \rightleftharpoons H^+ + In^-_{(aq)} \qquad (b.1)$$

The acid dissociation constant, *K*a, is defined as:

$$Ka = \frac{[H^+][In^-]}{[HIn]} \qquad (b.2)$$

Converting Eq. (b.2) into the form of the Henderson–Hassel bach equation:

$$pKa = pH - \frac{[In^-]}{[HIn]} \qquad (b.3)$$

The acid dissociation constant may be calculated from measurements of the ratio $\frac{[In^-]}{[HIn]}$at known pH values. When pH is less than pKa, the indicator is mainly in the acidic form (HIn), and in pH values greater than pKa, the indicator is mainly in the basic form (In^-).At half-way through the color change, the concentrations of the acid and its ion are equal. In that case, they are canceled out of the K_{ind} expression and following equation is obtained:

$$pKa = pH \qquad (b.4)$$

The new pKa determination method described here is simple, fast and inexpensive. In this method, RGB of four parts of pH papers for surveyed indicators (bromocresol green, phenol phetalein, methyl orange) were calculated. Then graphs of RGB in terms of pH (1-14) were drawn (Fig.5-Fig. 7) and acid dissociation constants were calculated by a novel program written in MATLAB software which was called pKa Deilamy (pKa (D)) (Given in Supplementary Information**).**

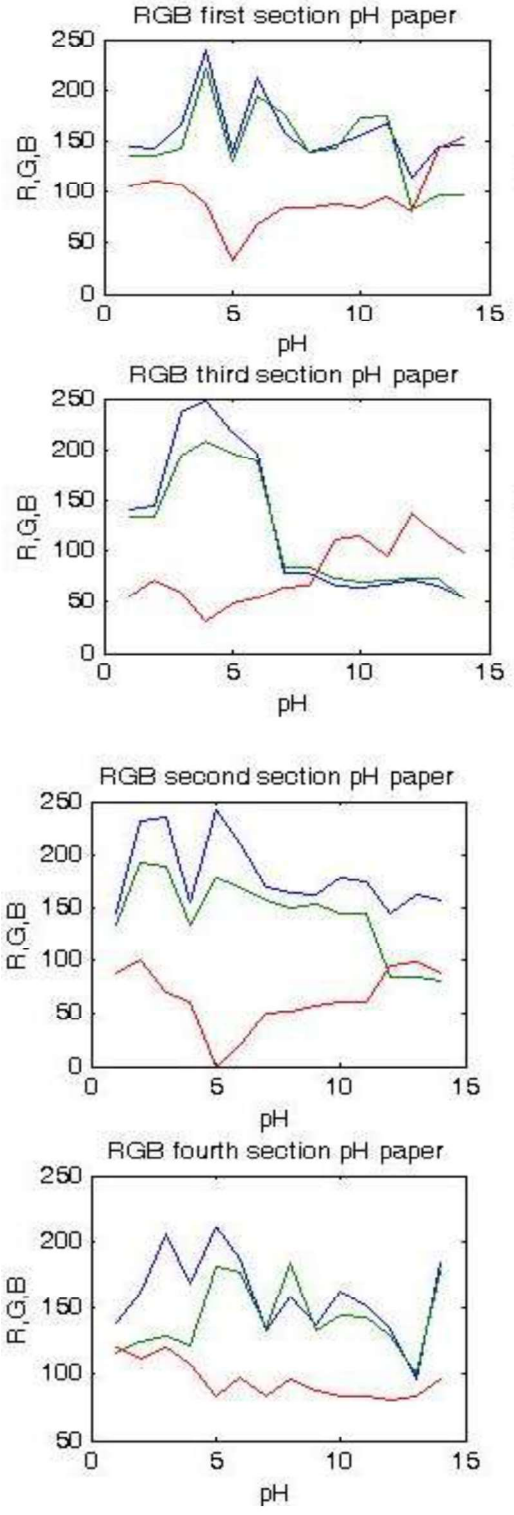

Fig. 5 Obtained RGB for indicator Bromocresol green

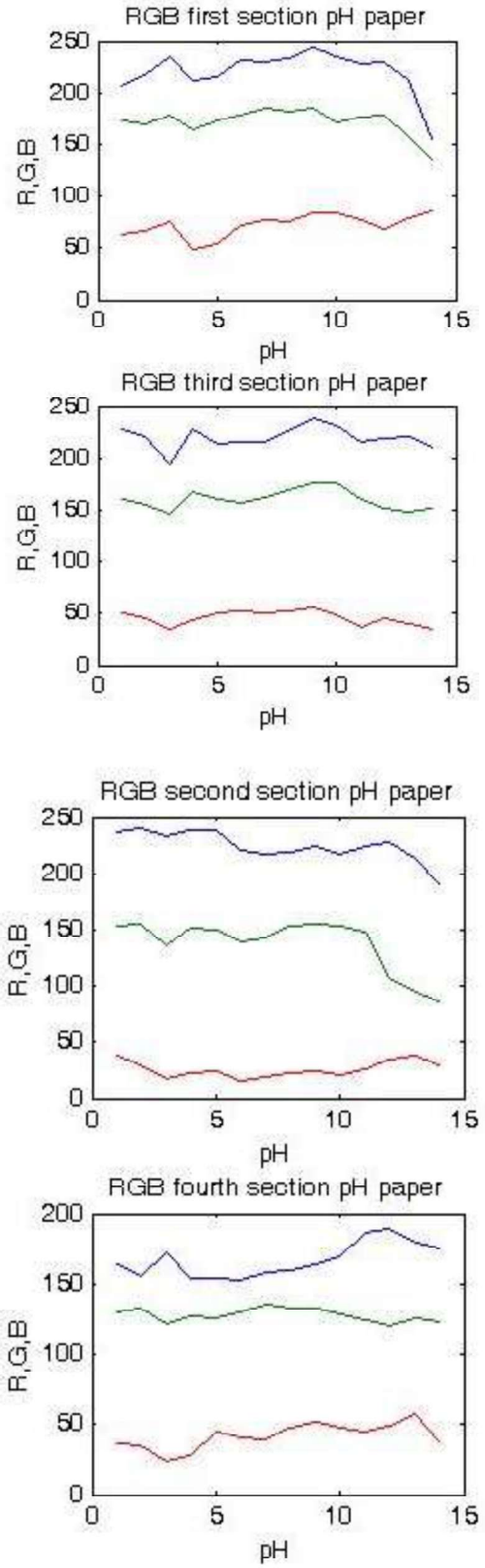

Fig. 6 Obtained RGB for indicator Methyl orange

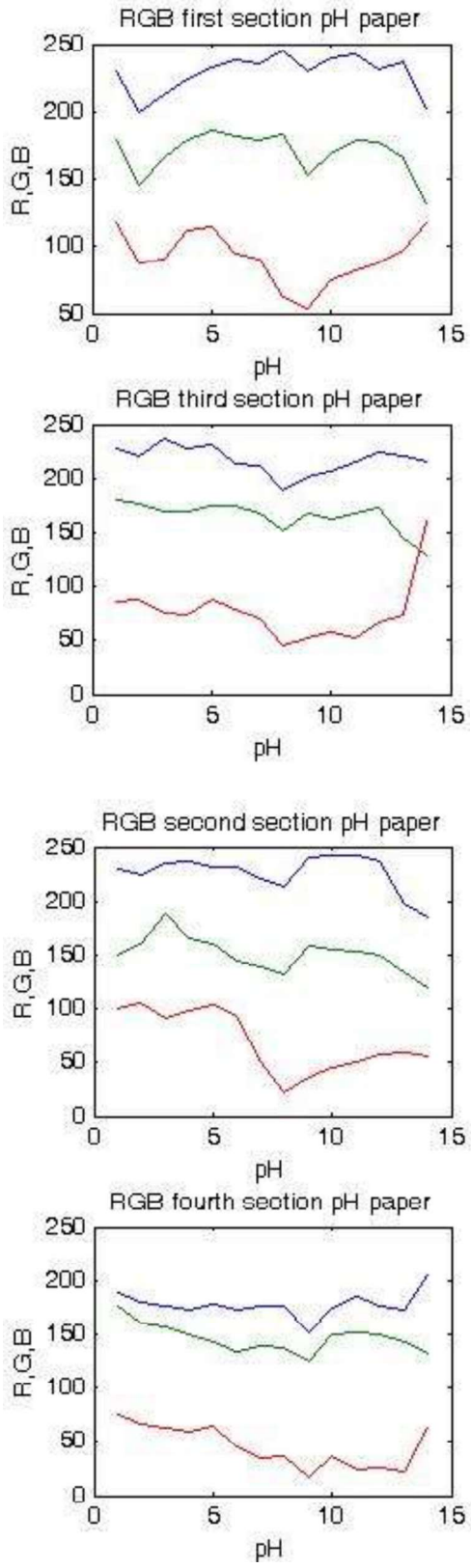

Fig.7 Obtained RGB for indicator Phenolphetalein

For each of indicators, four graphs of RGB in terms of pH were drawn which correspond to four parts of pH paper, and the highest difference between values of R, G and B were calculated by this new program (line 43 to line 55), because the highest difference is equal to the highest sensitivity. It should be noted which these commands are repeated for other indicators. Then this difference is plotted against pH (1-14). In this graph, the pH of the maximum point is equal to pKa (Fig. 8-Fig.10).

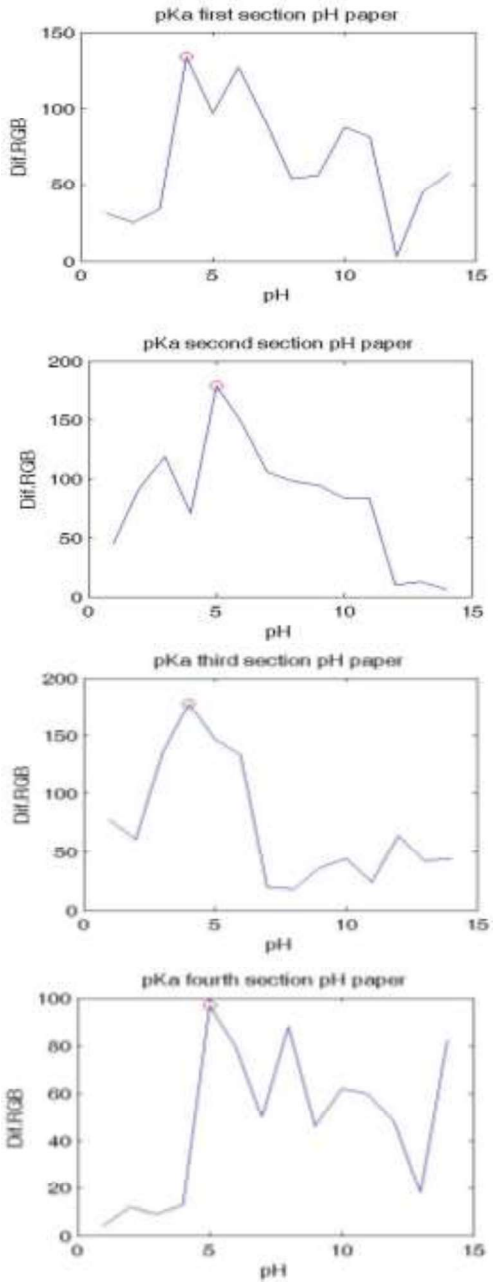

Fig. 8 Obtained pKa for indicator Bromocresol green

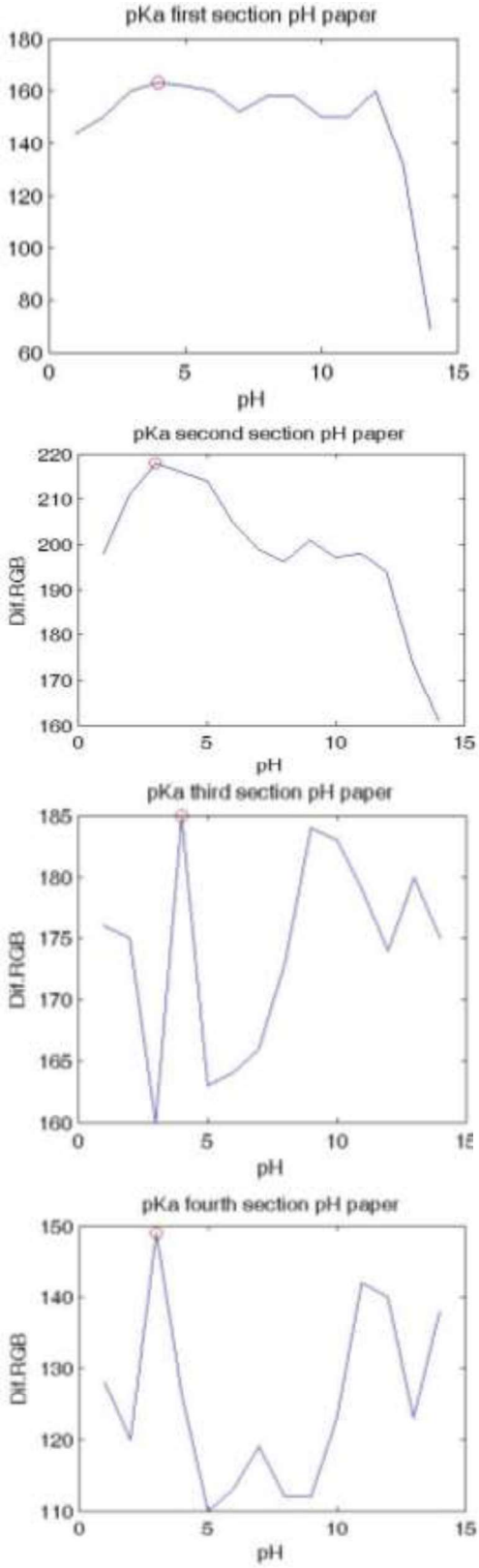

Fig. 9 Obtained pKa for indicator Methyl orange

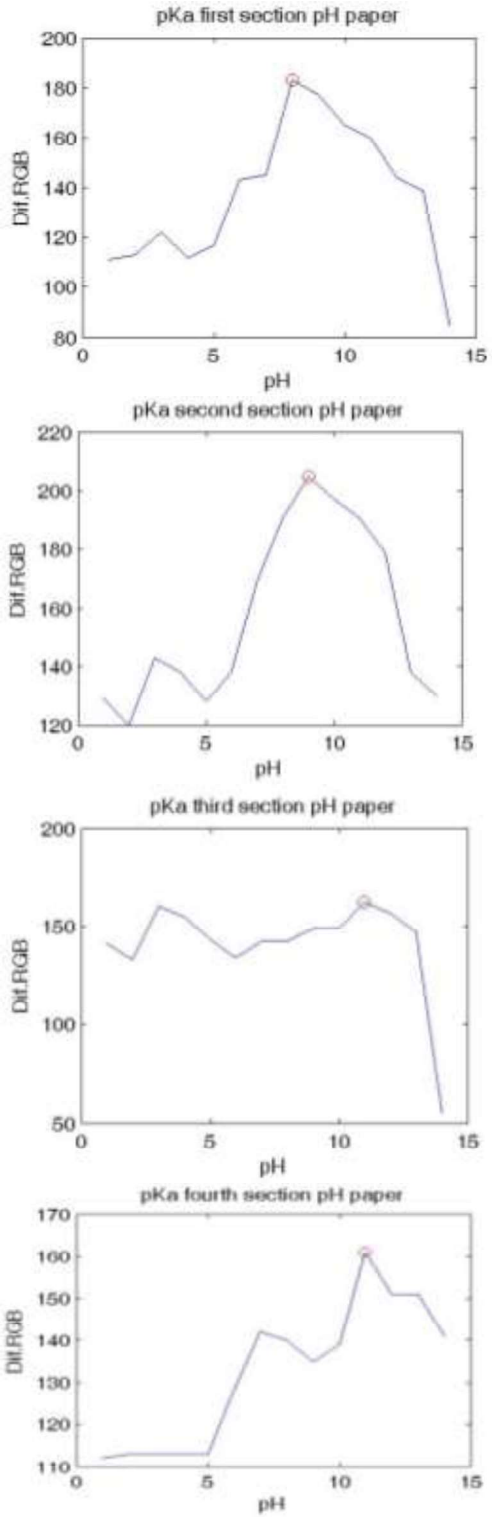

Fig. 10 Obtained pKa for indicator Phenolphetalein

Since these indicators (Bromocresol green, Phenol phetalein, Methyl orange) are weak acids, at the concentration of 0.2 M, the pH of the solution did not maintain well below the pKa of indicators and hence the derived pKa was different from the reported value. In order to eliminate this mentioned problem and make pKa determination more accurate, titrating solutions containing the indicators were pre acidified with 1.0M HCl to keep the initial pH value around 2 units below the pKa [44]. The 1.0 M HCl solution was added just before titration and titration was initiated once stable pH reading was attained.

The pKa values of indicators obtained after acidification were in close agreement with the values reported by literatures (Table 1).Since, in different references of chemometrics, the values of accepted error are less than 8% [45], in this study, obtained results were satisfactory. For different indicators, the values of pKa are shown in graphs of RGB (Fig. 8-Fig.10).

Table 1. Obtained error values for calculated pK_a

Indicator	Real pK_a	Calculated pK_a	Error (%)
Bromocresolgreen	4.7	4.5	-4.2
Phenolphetalein	9.4	9.7	3.2
Methylorange	4.2	4.5	7.1

4. CONCLUSION

This paper is centered on digital image based methods with two main objectives: first, evaluation of the representativeness of the individual basic RGB colors and second, the application of this current technology to implement fast and reliable analytical methods.

In addition, this protocol allows to determine the pKa value in a short time and without using the potentiometric method. This strategy for the determination of the pKa can also be used to discuss the case of other chemical species in which the non-ionized form has color [46].

Basic studies of the digital image colorimetry demonstrated the meaning of RGB data for analytical quantitative determinations. The procedure could be implemented to provide acid dissociation constant (pK_a) as a fast method based on capturing digital images with a scanner and only measuring the RGB color. It demonstrated a great potential for high throughput analysis and could be applied as a field method with a capacity to determination pK_a at low cost. This study is based on the analytical application of digital image colorimetry and other analytes are currently being considered.

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تعیین ثابت تفکیک اسیدی بروموکرزول سبز، فنل فتالئین و متیل اورانژ به وسیله ی یک برنامه ی جدید در نرم افزار MATLAB و تغییر رنگ کاغذ pH

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چکیده

در این مطالعه، ثابت تفکیک اسیدی سه شناساگر بروموکرزول سبز، فنل فتالئین و متیل اورانژ به وسیله اسکن محلول این شناساگرها، قرار دادن کاغذ pH در محلول‌ها (در هر مرحله از تغییر رنگ محلول) و سپس با استفاده از روش کمومتریکس تعیین گردید. این روش‌ها ساده، سریع و کم هزینه هستند. برای این منظور، ابتدا ظروف حاوی محلول شناساگر و کاغذ pH (در هر مرحله از تغییر رنگ محلول) اسکن شدند و سپس تصاویر محلول‌های نمونه و کاغذهای pH به یک کامپیوتر مجهز به Microsoft Photo Editor (Microsoft XP) منتقل گردیدند. مقادیر RGB در هر پیکسل با استفاده از جعبه ابزار پردازش نرم افزار MATLAB اندازه گیری شد. در نرم افزار MATLAB (۲۰۱۳) یک برنامه ی جدید بر اساس مقادیر RGB، برای محاسبه ی ثابت تفکیک اسیدی شناساگرها نوشته شد. تطابق ثابت تفکیک اسیدی به دست آمده با این روش و مقادیر گزارش شده در متون، کارایی روش به کار برده شده در اینجا را نشان می دهد.

واژه‌های کلیدی

ثابت تفکیک اسیدی، روش اندازه گیری پیمایشی محلول، روش کمومتریک، نرم افزار MATLAB.