



A green chemical analysis of iron (III) in water sample using a smart phone



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ARTICLE INFO

Method name:
Green analysis

Keywords:
Digital image
Iron (III)
Water
Smartphone

ABSTRACT

In this study, a smartphone was used as the photometer for determination of iron (III) by forming a complex with thiocyanate. After color formation at concentrations of, image capture with mobile phone, signal analysis of each sample was performed by the application and converted to the absorption number. The calibration curve was completely linear in the range of 10 to 80 mg L⁻¹ used and the linear coefficient was better than 0.9833. The limits of detection (LOD) and quantification (LOQ) were 0.1 and 0.3 mg L⁻¹, respectively. Finally, this method was successfully used to measure iron in real samples.

- A smartphone was used for the determination of iron (III), showcasing its potential in color compound analysis.
- The method demonstrated superior performance in terms of calibration curve range and measurement speed compared to traditional atomic absorption devices.
- The technique was successfully applied in the measurement of iron in real samples, indicating its practical applicability.

Specifications table

Subject area:	Environmental Science
More specific subject area:	Analysis
Name of your method:	Green analysis
Name and reference of original method:	EPA
Resource availability:	No

Method details

Iron, an essential mineral, plays a crucial role in the human body as it contributes to the formation of oxygen-transporting proteins, namely hemoglobin and myoglobin. A deficiency of iron can result in symptoms such as fatigue and lethargy, and may eventually lead to anemia. Iron is present in trace amounts in various foods that form part of our daily diet. To quantify the iron content, several techniques are employed, including Atomic Absorption Spectrophotometry (AAS) and High-Performance Liquid Chromatography (HPLC). However, the accessibility of these tools is often restricted due to their high cost. Furthermore, the application of the atomic absorption method demands a high level of expertise and precision. An alternative method for iron measurement involves the use of

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<https://doi.org/10.1016/j.mex.2024.102724>

Received 27 February 2024; Accepted 16 April 2024

Available online 17 April 2024

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Table 1
The relationship between the color and the transmitted wavelength.

Oerved Color	Transmitted Light Wavelength
Red	620 nm-750 nm
Green	500 nm-580 nm
Blue	440 nm-500 nm
Yellow	580 nm-600 nm
Orange	600 nm-620 nm

UV-visible spectrophotometry. In this method, iron reacts with thiocyanate in an acidic environment to form a red-orange Fe-SCN complex, which can be detected at wavelengths ranging from 450 to 530 nm [1,2]. A spectrophotometer is a versatile instrument with various applications, one of which is the generation of an absorbance spectrum. This spectrum represents the intensity of light absorption as a function of its wavelength. For instance, the absorbance spectrum of the FeSCN^{2+} ion exhibits a strong absorption region centered around 450 nm, while absorption is almost negligible above 650 nm. This absorption of blue light and transmission of red light gives the material a red appearance. The specific absorption of light at 450 nm makes it the optimal wavelength for measuring the concentration of FeSCN^{2+} . Light consists of energy units known as photons that propagate in a wave-like pattern. The distance between two consecutive peaks of this wave is defined as the wavelength, measured in nanometers (nm). The instruments typically used operate within a range of 200 nm (ultraviolet light) to 750 nm (infrared light). Interestingly, the energy of light is inversely related to its wavelength. The human eye is capable of detecting light emitted from sources like the sun or a tungsten filament, which is perceived as white due to the mixture of wavelengths. The color of a solution is determined by its ability to transmit light at specific wavelengths. For example, a solution will appear blue if it transmits light between wavelengths of 440 nm-500 nm, red if it transmits light between 620 nm-750 nm, and green if it transmits light between 500 nm-580 nm. The relationship between the observed color and the wavelength of the transmitted light is summarized in Table 1.

Despite the utility of spectrophotometers, their high cost can be prohibitive for many laboratories. In light of recent advancements in digital imaging technology, digital image-based colorimetry has emerged as a cost-effective alternative to traditional analytical methods. This technique leverages digital imaging to measure and analyze color, offering a more accessible solution for laboratories operating on a budget. [3–7]. These techniques utilize the red-green-blue (RGB) color space or its derivatives, such as hue and saturation. Digital image data can be sourced from various devices, including scanners, webcams, digital cameras, and mobile phones. Typically, the color and intensity of a digital image are represented as 24-bit data (8-bit red, 8-bit green, and 8-bit blue), forming an additive color space. Here, red, green, and blue (RGB) lights are combined in varying proportions to reproduce a broad spectrum of colors. By altering the values of R, G, and B, a multitude of colors can be generated. Each color intensity has 256 levels (ranging from 0 to 255). In this color scheme, a total of 16,777,216 colors (2563 or 224) can be achieved. The combination of $R = 0$, $G = 0$, and $B = 0$ corresponds to pure black, while $R = 255$, $G = 255$, and $B = 255$ signifies pure white. This system, with its unique combinations of R, G, and B values, allows for the creation of millions of distinct colors, saturations, and hues. This extensive color range serves as an excellent database for quantitative measurements. Consequently, digital image-based lenses can be employed as an alternative for quantitative measurements in analytical chemistry. Recently, smartphone-based colorimetry and fluorometry methods have become more important than traditional bulky devices due to their many features, including fast analysis, low-cost and simple production, portability, and ease of use. Smartphone-based methods show a very acceptable performance compared to traditional methods. With the popularization of digital cameras and their integration in smartphones, colorimetry detection using digital images for quantitative analysis and use in portable devices without the need for a laboratory has become possible [8–10,1,11]. In this field, the RGB color model is commonly used to represent the color spectrum. This method leverages digital images captured using smartphone cameras. The smartphone camera functions as a sensor, reader, and recorder for complex color intensities. Each pixel is then processed using digital imaging techniques via an application. The primary advantage of this digital imaging method is its efficiency in terms of material usage and its elimination of the need for expensive and complex equipment. In this study, a simple colorimetric method is proposed for iron content analysis in samples of tap water.

Materials and methods

Apparatus and software

A Vis-spectrophotometer from Unicam (USA), fitted with a one-centimeter glass cell (internal volume of 3 mL), and a Huawei P10 mobile phone equipped with a 12-megapixel color sensor were utilized in this study. The Spotxel® Reader 1.1 application was employed to process the digital images and extract data. Microsoft Excel was used for further processing of the digital image data

Materials

ferrous nitrate iron ($\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$), ammonium thiocyanate (NH_4SCN), and concentrated hydrochloric acid (HCl 37%) were procured from Merck, Germany. A stock solution of 1000 mg l-1 was prepared using $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ in 0.2% concentrated HCl. A 1000 mg l-1 thiocyanate solution was prepared from ammonium thiocyanate salt in freshly distilled deionized water.

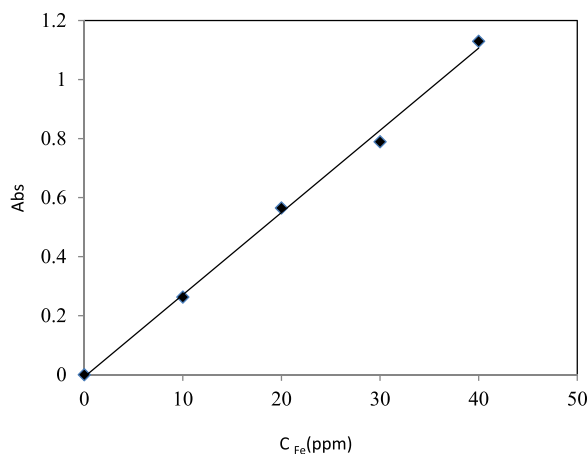


Fig. 1. Calibration curve obtained for iron using a photometer at 480 nm.

Table 2

Absorption obtained using mobile phones and repeatability of the obtained data for different modes.

C(ppm)	Average RGB absorbance		
	Microarray	Purple	Blue
0	167.1	51.1	50.8
10	132.3	31.3	31.2
20	107.7	13.1	12.7
30	94.2	7.7	7.5
40	85.5	6.8	6.7
50	70.5	4.4	4.2
60	55.7	1.6	1.7
70	47.3	1.1	1.0
80	41.8	0.5	0.5

Spectrophotometric measurement of iron (III)

Calibration standard solutions were prepared by diluting the stock solutions to various concentrations (0–10–20–30–40–50–60–70–80–90–100) containing 25% of 1000 mg L⁻¹ thiocyanate and 0.005% of concentrated hydrochloric acid. The absorption readings of the dye solutions were taken at 480 nm using a spectrophotometer, and an absorption calibration curve was plotted against the iron concentration.

Mobile phone-based measurement of iron (III)

Calibration standard solutions were prepared similarly as in section 2.3. Then 0.5 mL of each solution was dispensed into the wells of a 96-well microplate and photographed using a mobile phone. The color of the obtained image was analyzed to derive the signal corresponding to each concentration. In this method, the logarithm of the control solution signal exhibited a linear relationship with the standard solution signal, enabling the construction of a calibration curve.

Method validation

Beer-Lambert law, is one of the basic laws in photometric and optical spectroscopy. This law includes the relationship between the intensity of light absorbed by passing through a homogeneous material without scattering and the properties of the material. This law is generally expressed as follow

$$A = \text{Log}T = \log \frac{I_0}{I}$$

Where I_0 is the light intensity of the initial control solution, I is the light transmittance of the sample solution, and A is the amount of material absorption.

In this study, the absorption of iron-thiocyanate complex at a wavelength of 480 nm was obtained as follows. As can be seen, the linear range of the calibration curve is between 0.3–40 mg L⁻¹ (ppm) and its detection limit is 0.09 mg L⁻¹ and the linear range of the curve is 0.3–40 mg L⁻¹ (Fig. 1 and Table 2)

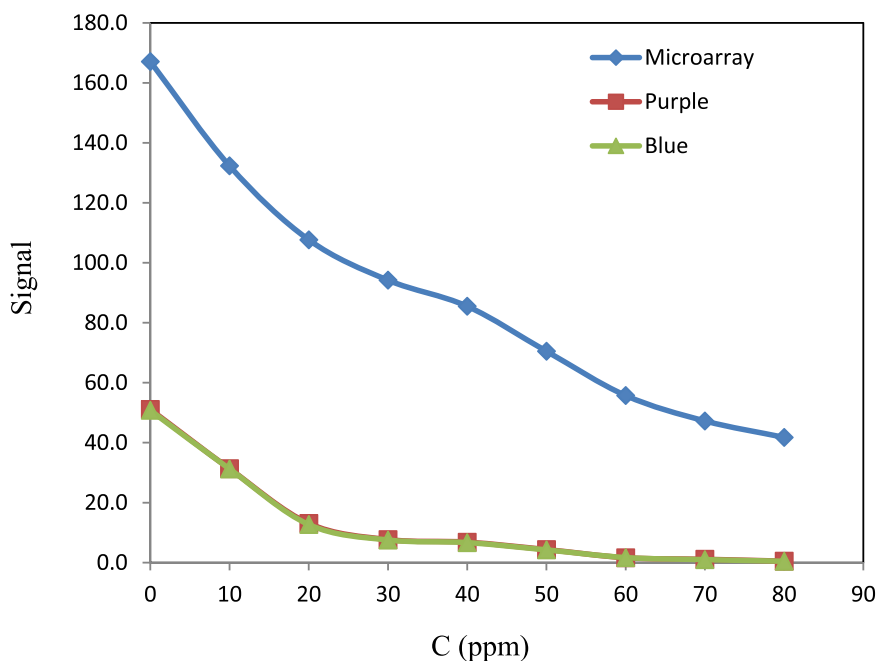


Fig. 2. Signal obtained for purple, blue and raw signal colors using a mobile phone.

Table 3
Figures of merit obtained for measurement with a photometer and smartphone.

Analyte	Equation	R2	LOD (ppm)	LOQ (ppm)	RSD%	DLR (ppm)
Photometer	Abs= 0.0276C _{Fe} -0.012	0.9988	0.09	0.27	0.1–0.5	0.3–40
Microarray	Abs= 0.0074C _{Fe} + 0.0185	0.9932	0.33	1.1	0.1–0.4	1–80
Blue	Abs= 0.0244C _{Fe} + 0.0036	0.9833	0.1	0.33	0.2–0.8	0.3–80
Purple	Abs= 0.0241C _{Fe} + 0.0081	0.9833	0.1	0.33	0.2–0.8	0.3–80

Table 4
Analysis of real samples.

sample	RGB absorbance	added	Found	Error%
1	116.7	20.0	19.90	-0.5
2	70.5	50.0	49.50	-1

Alternatively, using a smartphone and the Spotxel® Reader 1.1 app, the signal value was measured in three modes: blue, purple, and microarray mode. By plotting the values obtained from the color analysis of the iron-thiocyanate complex by the smartphone relative to the concentration produces a hyperbolic trend curves (Fig. 2).

To convert these values to the absorption number, the Beer-Lambert relationship was used (logarithm values were obtained) and then these values were used to plot the calibration curve. The results show that the blue, purple modes and the microarray mode the calibration curve is acceptable. The initial RGB color values were converted to log ratios following the Lambert-Beer law derivation formula as follow:

$$A = \text{Log}T = \log \frac{S_0}{S}$$

S₀, and S are the color values of blank and sample, respectively (Fig. 3).

The figures of merit obtained for the modes used are given in Table 3. As shown in Table 3, there is no significant difference between the calibration equations obtained by the photometer and the mobile phone. The limits of detection (LOD) and quantification (LOQ) were respectively calculated as 0.1 and 0.3 mg L⁻¹ comparable for photometric method for iron determination (Table 3). Iron concentration in analyzed water samples was lower than LOQ. Relative standard deviation for photometric and mobile phone-based measurement method was in the range of 0.1–0.5% and 0.10–0.8%, respectively.

In order to evaluate the efficiency of the system used by the mobile phone, two samples with concentrations of 20 and 50 mg L⁻¹ in tap water were prepared and evaluated using the mentioned method. As can be seen in Table 4, the data error obtained is very

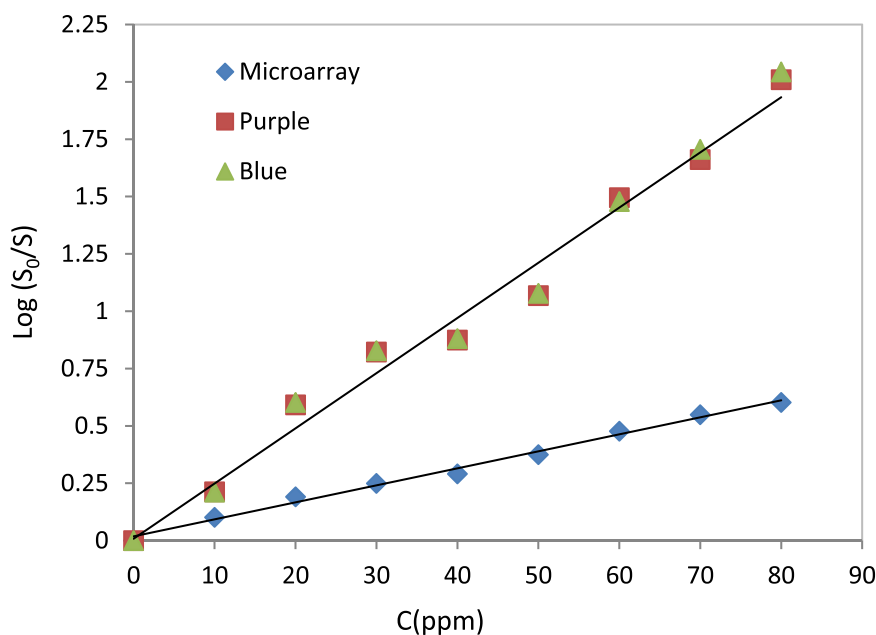


Fig. 3. Calibration curve obtained for iron using a smart phone in three different modes.

close to the actual error values Recovery testing using a tap water sample with iron solution at concentrations of 20 and 50 mg/L resulted in recoveries ($n = 3$) in the range of 99–99.5% (less than one percent), indicating acceptable accuracy.

Conclusion

Determination of Fe (III) by the wells of a 96-well microplate and photographed using a mobile phone was carried with good accuracy and precision. This method is fast, inexpensive, without need for toxic solvent, green, simple and portable. This proposed method has advantages such as reducing the consumption of chemicals and using inexpensive devices, especially in centers that have a limited budget.

Ethics statement

This study, titled “A green chemical analysis of iron (III) in water sample using a smart phone” was conducted in strict accordance with the ethical guidelines of the MethodsX Journal.

CRediT author statement

Jalal Hassan: Methodology—Analysis **Safdar Mehdizadeh shermeh:** Data acquisition—Writing **Mohammad Kazem Koohi:** Methodology **Ali Pourshaban-Shahrestani:** Writing—review and editing —Data acquisition

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgments

We would like to express our deepest appreciation to all those who provided us the possibility to complete this work.

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