

Method validation of quantitative FTIR as rapid and green analytical technique for dyes

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Abstract

Analysis and detection of dyes, whether in solutions or on substrates, are of the requirements in textile and coloration fields related to dyeing, printing, and coating, in addition to non-destructive testing. This research aimed to study the most effective chemical groups in dispersed dye red (C.I. 11338) structure. Different concentrations were prepared gravimetrically by calibrated and traceable weighing and volumetric tools. An accurate fixed volume of 25 micrograms of the studied solubilized dye was added quantitatively to the KBr disk as a fast technique in FTIR instead of using a liquid sample compartment. Linearity of the concentration with the peak intensity was used to validate FTIR spectrophotometer as a quantitative analysis method. Firstly, we detect the dye's most detectable function chemical groups and find the best linear correlation between the concentration and transmission intensities. The results revealed that the distinct chemical groups that can be used are: strong C=C bending at 748.28 cm⁻¹, medium C=C bending at 808.07 cm⁻¹, and O-H bending at 1411.71 cm⁻¹ which give linear correlations of 0.9927, 0.9906 and 0.9998 respectively for concentration ranged from 0.001 to 0.05 ppm (w/v), LOD also studied and reached to a very low concentration less than 0.0005 ppm; the uncertainty of concentration at 1411.71 cm⁻¹ was 0.02% with coverage factor 2 to give 95% confidence level. The result revealed the applicability of this technique in the quantitative analysis of dyes.

Keywords: Quantitative analysis, FTIR, Disperse Dye, Green analytical technique, Method validation.

1 Introduction

Infrared spectroscopy (IRS) as green and rapid chemical analytical tool is popularly used in qualitative chemical analysis to figure out the type of chemical bonds with a dipole moment. Infrared systems have recently developed and combined with other analytical techniques, such as gas (GC) and liquid (LC) chromatography and thermal analysis (TGA) devices (referred to as hyphenated techniques), to produce highly sensitive, precise tools when compared to using each technique individually [1-4]. The main issue in quantitative method is the validity range

of the Beer-Lambert approximation, which refers to the promotion of substance concentration to absorption or transmission percentage. Only over the linear range of this correlation can quantitative analysis be used, allowing the concentration of a solution to be calculated by measuring its absorbance or transmission [5]. The analyst should determine the optimal IR absorption of the molecule and its bonds, choose a wavelength/wavenumber range that is fairly free of inter and intera-molecular interference, use a linear optical bath, quantify peak size as a factor of concentration, and finally test the repeatability, reproducibility, ruggedness, and uncertainty [6].

Quantitative analysis is the process of measuring and calculating the value of a quantity. It is the basis of chemical analysis and an essential chemistry tool. Quantitative analysis is used to determine the structure of a substance, recognize chemicals and their interactions, and characterize materials at the molecular level. Chemists use various analytical techniques to perform quantitative analyses in the lab or the field. The molecular weight, melting point, boiling point, solubility, density, acidity, reactivity, toxicity, color, and other physical properties of compounds can be calculated using various quantitative analyses. The structures, functions, and interactions of the molecules that make up a compound can also be revealed by quantitative analysis. By studying the physical and chemical properties of materials, chemists can better understand their behavior patterns and the chemical processes that occur within them. Quantitative analyses can help answer questions such as "What is the composition of a material" "How does one substance influence another?" "What chemicals are risky?" "How well does it work.

Fourier transforms infrared (FTIR) spectroscopy is a type of analysis that detects and interpreting infrared radiation. The FTIR spectrum is a series of spectral lines characteristic of specific molecules or ions. These spectra are then analyzed using peak fitting, multivariate analysis, and chemometrics mathematical algorithms to extract information about the tested sample. Much effort has been expended in recent years to use mid-infrared spectroscopy for the analytical control of various matrices. The IR main zones are divided into three regions: Far IR (10-400 cm⁻¹), Mid-IR (400-4000 cm⁻¹), and Near-IR (400-4000 cm⁻¹) (4000-14000 cm⁻¹) [7-9].

Ju et al. 2023 [10] used attenuated total refraction infrared (ATR-IR) spectroscopy and nearinfrared (NIR) spectroscopy in conjunction with chemometrics as a rapid detection technique to evaluate the quality and consistency of drugs in order to ensure therapeutic effect and drug safety. Many Authors [11-14] showed the effective use of IR as quantitively and highly sensitive robust, non-destructive, and efficient method to investigate chemical and structural changes.

In quantitative analysis, there are two steps: calibration and prediction, which tests the calibration validity. In general, at least (2n + 2) standards are required for calibration when analyzing n components in the mid-IR [15]. The LOD is the lowest concentration of an analyte that the analytical process can reliably detect, whereas the LOQ is the smallest concentration or mass that a given procedure can quantitatively analyse with reasonable reliability [16]. The LOD and LOQ were determined using both instrumental and statistical methods. LOD is the lowest amount to detect in the instrumental method, and LOQ is the lowest amount to quantify by the detector. LOD and LOQ for statistical methods are determined by a statistical formula:

LOD= 3.3 σ /Slope, LOQ= 10 σ /Slope, where σ is the standard deviation.

For each certified band wavelength and wavenumber, the expanded uncertainty, U, is provided. It is calculated as the sum of the coverage factor (k = 4) and the combined standard uncertainty. The root sum of squares of all the uncertainty components yields the combined standard uncertainty. [17-19].

This work is part of the validation of FTIR method and aims to detect the most efficient characteristic chemical group(s) in disperse dye 167 (C.I. 11338) that can be tracked with direct proportionality with low Limit of detection (LOD) rather than the use area under each individual peak. To be recommended as a green, quick and accurate quantitative chemical analysis technique for quality control in the textile, food, environmental, health and Non-destructive (ND) sectors.

2 Research Methodology

2.1 Materials

Dye used in this research was C.I. Disperse Red 167, C.I. 11338, CAS 61968-52-3/26850-12-4, Molecular formula (C23H26ClN5O7), Molecular weight (519.93), The dye also known as Disperse Rubine 2GFL,Disperse Rubine H-2GFL,Disperse Rubine S-2GFL,Disperse Rubine S-2GFLR, and Disperse Rubine S-5BL. Dye was manufactured by chemical reaction coupling of 2-Chloro-4-nitrobenzenamine diazo and 3-Propanoylamino-N,N-bis(2-acetoxyethyl) benzenamine [20]. The dye concentration was prepared gravimetrically (weight/volume) in deionized water. The concentrations ranged from 0.0001 to 0.01 ppm.

2.2 Testing and analysis

Fourier Transform Infrared (FTIR) spectroscopic analysis The IR spectra of the KBr disk loaded with fixed quantitative volume of the dye solution (ranged from 0.001 to 0.05 ppm) were measured by using Nicolet 380 (FTIR) Spectrometer, USA, in the wavelength range 4000-500 cm-1. The changes in the contents of some chemical groups for each sample were monitored with absorbed IR selected bands [20, 21]. Metrological traceability [22]was achieved by the calibration of the spectrophotometer by using standard polystyrene film traceable to NIST-USA (RM 1921b by NIST). All measurements in this study are the average of three measurements taken in exactly the same conditions [23].

3 Results and Discussion

Figure 1 show the transmission spectra of the studied disperse dye (C.I. 11338) with different concentration ranged from 0.0005 ppm to 0.05 ppm (w/v). In this chart different transmission peaks were observed. The behaviour of the transmission intensities for each concentration differs from one chemical group to other. The assignments of each peak were detected. In figure 1 the LOD was determined for the aqueous concentration of the disperse -reactive dye to the minimum achievable concentration 0.0005 ppm. The transmission spectra for all detected peaks[16].



Figure 1: FTIR spectrum for different aqueous concentration of Disperse dye (C.I. 11338).

Table 1 show the transmission peaks for the studied dye and the characteristic peaks appeared were at 620.99 cm⁻¹ for C-Br stretching, 748.282 cm⁻¹ for C=C bending, 808.07 for secondary C=C bending, 887.14 for C=C in alkene, 1041 cm⁻¹ for ether O-C, 1124.35 for C-O stretch in secondary alcohol, 1172.57 cm⁻¹ for aliphatic alcohol, 1226.57 for C-O stretch in vinyl ether, 1234.28 for C-N stretch in amine, 1332.64 C-N stretch in aromatic amine, 1371.21 cm⁻¹ for O-H in phenol, 1411cm⁻¹ for O-H bending in carboxylic acid, 1463.78 v for C-H bending in alkene,1521.64 cm⁻¹ and 1581.42 cm⁻¹ for N-O stretch in nitro compound, 621.92 cm⁻¹ for C=C stretch in α , β -unsaturated ketone, 1685.56 cm⁻¹ for N-H stretch in primary amine. Table 2 and Figures (2-4) show the linearity of each characteristic group in the dye structure expressed as the regression factor R2 and the equation of correlation. The highest linearity was found for C=C bending and O-H bending. This may be attributed to the out of plane position of the carboxylic groups to the main structure of the dye. This enable the carboxylic group to be detected easily by IR spectroscopy [16, 24].

By drawing a relationship between the dye concentration and T%, a chemical group within the dye synthesis obtained correlations showing proportionality, pacing behavior and the intersection point of the T% axis or concentration. Table 2 shows that the active group is P2, which has a more linear relationship, which indicates its consent to Lambert-Beer law and follows it in this linear relationship are P2 and P3, allowing for the use of secondary evidence in the case of a P2 group under the influence of hydrogen bonds or the influence of other partial active groups in high concentrations.

Peak Number	Peak detected (cm ⁻¹)	Absorption (cm ⁻¹) from reference	Appearance	Group	Compound Class	Comments
P1	620.99	690-515	strong	C-Br stretching	halo compound	
P2	748.282	730-665	strong	C=C bending	alkene	disubstituted (cis)
Р3	808.0674	840-790	medium	C=C bending	alkene	trisubstituted
P4	887.1385	895-885	strong	C=C bending	alkene	vinylidene
P5	1041.42	1050-1040	St. broad,	O-C stretching	anhydride	
P6	1124.35	1124-1087	strong	C-O stretching	secondary alcohol	
P7	1172.57	1150-1085	strong	C-O stretching	aliphatic ether	
P8	1226.57	1225-1200	strong	C-O stretching	vinyl ether	
P9	1234.28	1250-1020	medium	C-N stretching	amine	
P10	1332.64	1342-1266	strong	C-N stretching	aromatic amine	
P11	1371.21	1390-1310	medium	O-H bending	phenol	
P12	1411.71	1440-1395	medium	O-H bending	carboxylic acid	
P13	1463.78	1450	medium	C-H bending	alkane	CH ₃ - group
P14	1484.99	1465	medium	C-H bending	alkane	-CH ₂ - group
P15	1521.64	1550-1500	strong	N-O stretching	nitro compound	
P16	1581.42	1550-1500	strong	N-O stretching	nitro compound	
P17	1621.92	1620-1610	strong	C=C stretching	α,β-unsat. ketone	
P18	1685.56	1685-1666	strong	C=O stretching	conjugated ketone	
P19	1739.56	1740-1720	strong	C=O stretching	aldehyde	
P20	3430.91	3500	medium	N-H stretching	primary amine	

Table 1: Characteristic group and their wavenumbers for Disperse dye (C.I. 11338)[24]

P2 is considered effective in quantitative analysis than P2 and P3 due to it is location in the $(4000-1200 \text{ cm}^{-1})$ region, which is called the functional group region. while P2 and P3 located in region from 1200 to 400 cm⁻¹ which is called the fingerprint region. Fingerprint region is characterizing the compound as a whole. [25]. P2 and P3 T% intensity is lower than that of P12 due to the fact of vibration frequency decreased with increasing the conjugation in the double bond. Chemical groups containing C=O due the presence of Inductive and resonance effect, Nitrogen easily donates electron or ion pair of nitrogen undergoes delocalization with a C=O bond. Due to this delocalization double bond of a C=O change into a partial double bond, therefore force constant decreases, which decreases the C=O stretching frequency. P12 can be used because Intramolecular hydrogen bonding does not change its frequency even in a very dilute solution because upon dilution structure of the compound does not change[26, 27].

Peak Number	ber Chemical Bond Wavenumber Correlation Equation		Linearity	
		(cm ⁻¹)	conc. (x) vs. intensity (v)	Regression
				(R ²)
P1	C-Br stretching	620.99	y = 567.96x - 1.9593	0.9590
P2	C=C bending	748.28	y = 662.19x - 0.6646	0.9927
P3	C=C bending	808.07	y = 677.15x - 0.8466	0.9906
P4	C=C bending	887.14	y = 678.5x - 1.3515	0.9828
P5	O-C stretching	1041.42	y = 447.38x - 2.287	0.8822
P6	C-O stretching	1124.35	y = 492.43x - 2.3719	0.8996
P7	C-O stretching	1172.57	y = 387.29x - 2.2446	0.8291
P8	C-O stretching	1226.57	y = 388.33x - 2.2195	0.8334
P9	C-N stretching	1234.28	y = 7.3136x - 11.211	0.7626
P10	C-N stretching	1332.64	y = 436.55x - 2.3594	0.8631
P11	O-H bending	1371.21	y = 604.06x - 1.6862	0.9758
P12	O-H bending	1411.71	y = 670.34x + 0.5333	0.9998
P13	C-H bending	1463.78	y = 10.965x - 14.233	0.9137
P14	C-H bending	1484.99	y = 10.988x - 14.437	0.9104
P15	N-O stretching	1521.64	y = 8.9436x - 13.089	0.8388
P16	N-O stretching	1581.42	y = 9.649x - 13.358	0.8844
P17	C=C stretching	1621.92	y = 8.1933x - 11.742	0.8571
P18	C=O stretching	1685.56	y = 10.256x - 13.161	0.9170
P19	C=O stretching	1739.56	y = 8.968x - 12.993	0.8552
P20	N-H stretching	3430.91	y = 3.3381x - 4.3553	0.8917

Table 2: correlation between the dye concentration and peak intensities for the chemical bonds in the dye structure.

Figure 2 depicts the relationship between T% intensity and concentrations of the strong C=C bending groups present in the dye (P2) at wavenumber (748.28 cm⁻¹) in the concentration range 0.001 to 0.05 ppm, and the relationship was found linear with factor ($R^2 = 0.9927$), slope on the concentration axis equals to 662.19 and intersect the T% intensity axis at the point (-0.6646). Figure 3 depicts the relationship between T% intensity and concentrations of medium C=C bending groups present in dye (P3) at wavenumber (808.07cm⁻¹) (in the range of 0.001 to 0.05 ppm), and the relationship is linear to the ($R^2 = 0.9906$) factor with a tilt on the focal point equal to 677.15 intersect the T% intensity axis at point (-0.8466). Finally, figure 4 depicts the relationship between T% intensity and concentrations (P12) at wavenumber (1411.71cm⁻¹) in the concentration range of 0.001 to 0.05 ppm, which is linear (R = 0.9998) with slope on the concentration axis equal to 670.34, intersect the T% intensity axis at point (0.5333).



Figure 2: Correlation between the concentration and peak intensities for P2 chemical group in disperse dye (C.I. 11338).



Figure 3: Correlation between the concentration and peak intensities for P3 chemical group in disperse dye (C.I. 11338).



Figure 4: Correlation between the concentration and peak intensities for P12 chemical group in disperse dye (C.I. 11338).

3.1 Uncertainty of the measurement was estimated as follow

Uncertainty of repeatability, calculates as the standard repeatability (average of three individual measurements for each concentration) at wavenumber 1411.77 cm⁻¹ (for O-H bending that gave the highest linear correlation with the dye concentration).

Type A uncertainty:

Repeatability = standard deviation \sqrt{n} where n=3 ; = 0.12/1.732=0.0692 cm⁻¹

Type B Uncertainty:

It includes the uncertainties of type A, Balance Calibration (0.0005 g), Volume glassware (100 ml flask is 0.01 ml), standard polystyrene film (at 1411.77 cm⁻¹ = 0.09 cm⁻¹),

Parameter	Value	Relative	divisor	Sensitivity	result
		value		coefficient	
		(%)			
Туре А	0.0692 cm ⁻¹	0.0049	1	1	0.0049
Balance calib	0.0005 g	0.0500	2	1	0.0025
Volume calib	0.01 ml	0.0100	2	1	0.0050
Thermometer Calib.	0.01 °C	0.0400	2	1	0.0200
Polystyrene (RM)	0.09 cm-1	0.0063	4	1	0.0016

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Combined uncertainty = $\sqrt{UA^2 + U Balance^2 + U Volume^2 + U Therm^2 + U Polystyrene^2}$ = $\sqrt{0.0049^2 + 0.0025^2 + 0.005^2 + 0.02^2 + 0.0016^2} = 0.02\%$

Expanded Uncertainty (with coverage factor =2 for confidence level 95%)=0.02*2=0.04%. According to the values of linearity, and uncertainty we can validate this technique as a green, rapid, precise analytical tool.

4 Conclusions

The use of infrared analysis of Disperse red dye 167 (C.I. 11338) as a quantitative analysis method in the range from 400 to 4000 wavenumbers for concentrations ranging from 0.001 to 0.05 ppm has proven to be reliable as an accurate and effective method with respect to linear correlation between the peak intensities and the values of the studied concentrations. C=C bending and O-H bending in the dye structure showed the acceptable linearity with value ranged from 0.9927 to 0.9998 respectively. Uncertainty of measurement was found 0.04% at wavenumber 1411.77. Moreover, the LOD reached 0.0005 parts per million which is very sensitive and can be used in trace analysis of similar structures in environmental, medicinal, nutrition nanotechnological fields.

5 Declarations

5.1 Acknowledgements

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5.2 Competing Interests

Declare any potential conflict of interest exist in this publication.

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