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Color Measurements by Agilent UV-Vis and UV-Vis-NIR Spectrophotometers

Using the Agilent Cary WinUV Color application to fully characterize color based on calculations of spectral data

Introduction

Light can be reflected, scattered, transmitted, or absorbed from matter, or cause photochemical reactions. Ultraviolet visible (UV-Vis) spectrophotometers use a light source to illuminate a sample with light across the UV to visible wavelength range, typically 190 to 1,100 nm. The instruments then measure the light that is absorbed, transmitted, or reflected by the sample at each wavelength.

Humans perceive color when light interacts with objects by the use of photoreceptors in the eye, primarily through the processes of transmission or reflection. Color measurements using UV-Vis spectrophotometers use the same principle as the human eye. However, UV-Vis spectrophotometers can objectively obtain a value that describes the color by offsetting the color of light used to illuminate the sample.

This white paper describes the options for color measurements that are available from Agilent, including an overview of the Cary WinUV Color application that translates spectral data according to various geometrical coordinates and illumination systems. The best choice of instrument for a particular application will depend on sample type and analysis requirements.

Color testing using UV-Vis

Color measurements are an important part of quality control processes in many industries, ensuring color consistency of products for branding, aesthetic, or clarity purposes. UV-Vis can also be used in industrial processes to measure a change of color in a solution. It is often used to assess if a reaction has occurred or is proceeding without the need for visual inspection by an operator. As a fast, non-destructive analytical technique, UV-Vis has also been used in art restoration and conservation projects to help match paint colors.[1] Example applications of UV-Vis color testing can be found in sectors such as foods and beverages, pharmaceuticals, textiles, automotive, plastics, paints, electronics, personal care products, cosmetics, plus many more.

Agilent Cary UV-Vis and UV-Vis-NIR spectrophotometers

Agilent offers a range of instruments for color measurements that cover liquid and solid sample types. The Agilent Cary 60 UV-Vis and Cary 5000 UV-Vis-NIR spectrophotometers are shown in Figure 1 and a full list of instruments is provided in Table 1. These Cary instruments, which are controlled by Agilent Cary WinUV software for UV-Vis or UV-Vis-NIR, address a variety of analytical needs, e.g., high throughput, ease of use, and sample accessibility.

Figure 1. Agilent UV-Vis spectrophotometers used for color measurements include the Agilent Cary 60 UV-Vis spectrophotometer (top) and Agilent Cary 5000 UV-Vis-NIR spectrophotometer with an external diffuse reflectance accessory (DRA) (bottom).

Table 1. Agilent UV-Vis and UV-Vis-NIR spectrophotometers that are widely used for color measurements.

System	Sample Types	Accessory Options	Analysis Requirements	Application Examples
Cary 60	Liquids and solids	− Cuvette − Fiber optic probe and coupler for liquids − Remote fiber optic diffuse reflectance accessory for solids[1]	− High-throughput with the 18-cell changer or fiber optic dip probe − Ease of use − Sample accessibility − Remote measurements	− Food and beverages − Water analysis − Pharmaceuticals − Petrochemicals − Fine/specialty chemicals
Cary 4000 Cary 5000 Cary 6000i Cary 7000 UMS	Liquids and solids	− Cuvette − Solid sample holder − Integrating sphere/diffuse reflectance accessory − Fiber-optic probe and coupler − Universal Measurement Accessory (0/45°)	− Color research − Small or very large samples − Extended wavelength into NIR − Measurement flexibility	− Textiles and fabrics − Plastics and paints − Haze/gloss measurements

Dedicated software for color measurements

Cary WinUV Color application is an optional software package that expands the Cary WinUV software and allows users to perform color calculations on data collected by Cary spectrophotometers. Users can select from multiple calculation options within the Color application, as described in Table 2, including the first standardized color system coordinates that were defined by Commission Internationale pour l'Eclairage (CIE) in 1931. Once selected, any calculations are performed automatically.

Table 2. Options within the Agilent Cary WinUV Color application.

System	Parameters Calculated
Color Coordinates	
Tristimulus	X, Y, Z
Chromaticity	x, y, z
CIE	L*a*b* L*, a*, b*
CIE	L*u*v* L*, u*, v*
Hunter	Lab L, a, b
Metric	L*, C*, h
Whiteness Index	WI
Yellowness ASTM E313-00	$YI_{E313\text{-}00}$
Tint Index	$T_{E313\text{-}00}$
Gardner ASTM D6166	G_{TM}
Haze Calculations	According to ASTM Method D1003 (requires an integrating sphere)
Color Difference Measurements	
CIE	ΔE^*_{ab}, ΔL^*, Δa^*, Δb^*, h_{ab}, C^*_{ab}, ΔH^*_{ab}
FMC-2	$\Delta E_{FMC\text{-}2}$, $\Delta L_{FMC\text{-}2}$, ΔC_1, ΔC_3
CMC (l:c)	$\Delta E(CMC)$
BFD (l:c)	$\Delta E(BFD)$
Hunter Lab	ΔE_H, ΔL_H, Δa_H, Δb_H
Other Options	
Illuminants	– CIE A, B, C, D_{65}, D_{55}, D_{50}, and D_{75} – F1 to F12
Observer Angles	– CIE 2° (1931) – CIE 10° (1964) – Photopic observer – Scotopic observer – Two user defined observers
Calculation Intervals	1, 5, or 10 nm
Graphics	– 1931 x,y and 1976 u',v' chromaticity diagrams for both 2° (1931) and 10° (1964) observers – CIE L*a*b* color space – Hunter Lab color space – %Transmission or %Reflectance versus wavelength

Other features of the Cary WinUV Color application include:

– Selection of up to 50 samples at one time for calculations.

– Calculations are performed over one of three selectable wavelength ranges (360 to 830, 380 to 780, or 400 to 700 nm) at one of three data intervals (1, 5, or 10 nm).

– Thickness correction is also provided when comparing the color of samples of varying thicknesses.

– The Match feature highlights the difference between the L*a*b* of a sample and a standard.

An analysis of the color of a sample can be achieved by simply setting up data collection parameters and baseline correction in the Cary WinUV Color application. The user then selects the illuminant (or illuminants) and observers, followed by the color coordinates needed for the calculations. Once the data have been collected, the color calculations will be performed automatically by the software, and graphs will be generated. A final report can then be produced based on user requirements.

Data collected from the Agilent Cary 3500 UV-Vis spectrophotometer series (Multicell, Compact, and Flexible modules) using the Cary UV Workstation software can also be imported into the Cary WinUV Color application and color analysis can be performed accordingly.

Application example

Figure 2 shows an application example for the color measurement of a green food dye using a Cary 60 spectrophotometer with illuminant CIE C. A section of the transmission spectrum and color data obtained using different coordinate systems (tristimulus, chromaticity, and CIELAB) are shown.
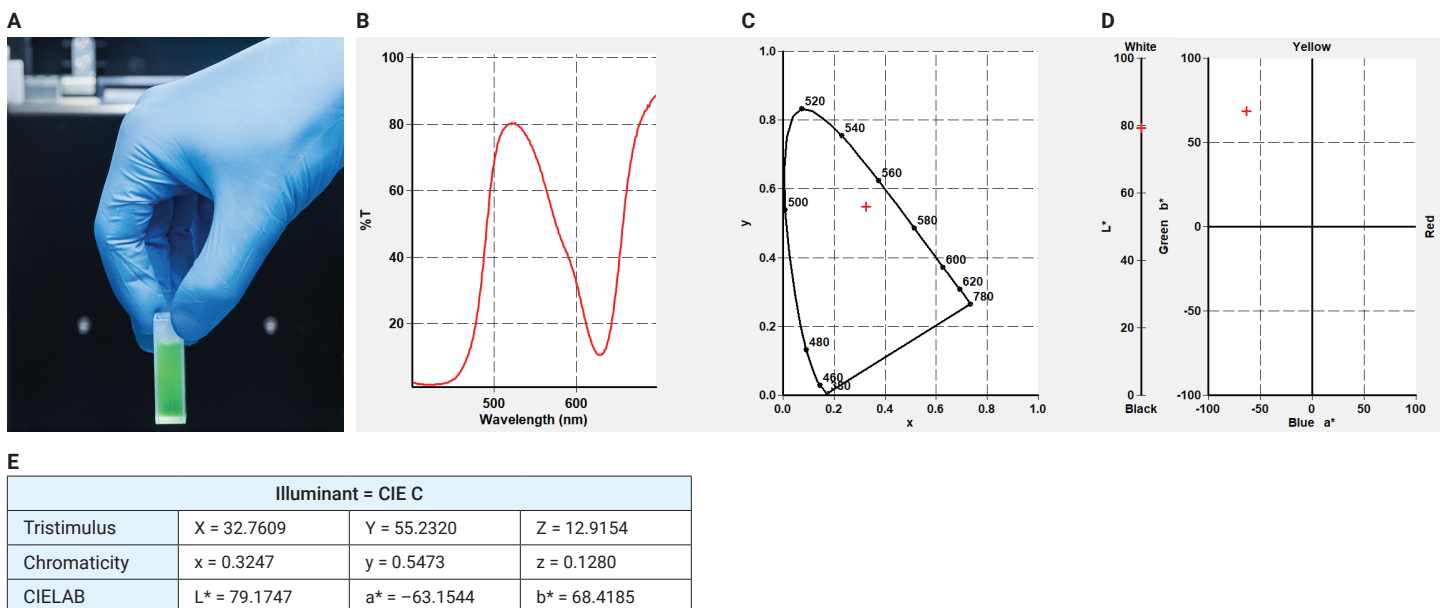
Figure 2. (A) Green food dye color measured using the Agilent Cary 60 spectrophotometer with illuminant CIE C; (B) %Transmission spectrum of dye; (C) chromaticity data; (D) CIELAB data; (E) summary of the tristimulus, chromaticity, and CIELAB calculations for the food dye.

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Illuminant = CIE C			
Tristimulus	X = 32.7609	Y = 55.2320	Z = 12.9154
Chromaticity	x = 0.3247	y = 0.5473	z = 0.1280
CIELAB	L* = 79.1747	a* = −63.1544	b* = 68.4185

Conclusion

The combination of an Agilent Cary UV-Vis spectrophotometer with Cary WinUV Color application provides an ideal tool for color testing of samples. The software quickly compares and verifies spectral information obtained by the instrument and generates color measurement data using a wide selection of color coordinate systems.

Agilent color measurement workflows can be used with liquid and solid samples in many industries such as electronics, materials, food and beverages, as well as art restoration and conservation projects.

Reference

1. Teragni, P.; Scardina, P. Measuring the Color of a Paint on Canvas via the Agilent Cary 60 UV-Vis Spectrophotometer with the Remote Fiber Optic Diffuse Reflectance Accessory. *Agilent Technologies application note*, 5991-3783EN, **2021**.

Further information

– Agilent Cary 60 UV-Vis Spectrophotometer
– Agilent High-Performance UV-Vis, Cary 5000 UV-Vis-NIR spectrophotometer
– Cary WinUV Software for UV-Vis Applications
– Agilent Cary WinUV Software for UV-Vis-NIR Applications
– UV-Vis Spectroscopy and Spectrophotometer FAQs
– UV-Vis Spectrophotometer Uses and Applications

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