Standard Practice for Computing the Colors of Fluorescent Objects from Bispectral Photometric Data¹

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INTRODUCTION

The fundamental procedure for evaluating the color of a fluorescent specimen is to obtain bispectral photometric data for specified irradiating and viewing geometries, and from these data to compute tristimulus values based on a CIE (International Commission on Illumination) standard observer and a CIE standard illuminant. Procedures for such computation are contained in this practice. This practice also contains procedures for computing illuminant-specific spectral radiance factor values from illuminant-independent bispectral photometric data.

1. Scope

1.1 This practice provides the values and practical computation procedures needed to obtain tristimulus values, designated X, Y, Z and X_{10} , Y_{10} , Z_{10} for the CIE 1931 and 1964 observers, respectively, from bispectral photometric data for the specimen. Procedures for obtaining such bispectral photometric data are contained in Practice E 2153.

1.2 Procedures for conversion of results to color spaces that are part of the CIE system, such as CIELAB and CIELUV are contained in Practice E 308.

1.3 This standard may involve hazardous materials, operations, and equipment. This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.

2. Referenced Documents

2.1 ASTM Standards:

- E 284 Terminology of Appearance²
- E 308 Practice for Computing the Colors of Objects by Using the CIE System²
- E 2153 Practice for Obtaining Bispectral Photometric Data for Evaluation of Fluorescent Color²

2.2 CIE Standards:

CIE Publication 15.2, Colorimetry³

2.3 ISO Standards:

ISO 11476 Paper and Board—Determination of CIE-Whiteness, C/2 Degrees⁴

3. Terminology

3.1 *Definitions*—The definitions contained in Terminology E 284 are applicable to this practice.

3.2 Definitions of Terms Specific to This Standard:

3.2.1 *bispectrometer*—an optical instrument equipped with a source of irradiation, two monochromators, and a detection system, such that a specimen can be measured at independently-controlled irradiation and viewing wavelengths. The bispectrometer is designed to allow for calibration to provide quantitative determination of the bispectral radiationtransfer properties of the specimen.(5)

NOTE 1—Typically, a reference detection system monitors the radiation incident on the specimen. This reference detection system serves to compensate for both temporal and spectral variations in the flux incident upon the specimen, by normalization of readings from the instrument's emission detection system.

3.2.2 *diagonal elements*—elements of a bispectral matrix for which irradiation and viewing wavelengths are equal.

3.2.3 *fluorescence*—this standard uses the term "fluorescence" as a general term, including both true fluorescence (with a luminescent decay time of less than 10^{-8} s) and phosphorescence with a delay time short enough to be indistinguishable from fluorescence for the purpose of colorimetry.

3.2.4 off-diagonal element-any element of a bispectral

¹ This practice is under the jurisdiction of ASTM Committee E12 on Color and Appearance and is the direct responsibility of Subcommittee E12.05 on Fluorescence.

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² Annual Book of ASTM Standards, Vol 06.01.

³ Available from the USNC/CIE Publications Office, TLA-Lighting Consultants, Inc., 7 Pond St., Salem, MA 01970–4819.

⁴ Available from American National Standards Institute, 11 W. 42nd St., 13th Floor, New York, NY 10036.

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matrix for which irradiation and viewing wavelengths are not equal.

4. Summary of Practice

4.1 *Procedures*—Procedures are given for computing from bispectral photometric measurements the CIE tristimulus values X, Y, Z for the CIE 1931 standard observer and the CIE 1964 supplementary standard observer. While recognizing the CIE recommendation of numerical integration at 1nm intervals (in Publication 15.2) as the basic definition, this practice is limited in scope to measurements and calculations using spectral intervals greater than or equal to 5 nm.

4.2 *Calculations*—CIE tristimulus values X, Y, Z or X_{10} , Y_{10} , Z_{10} are calculated by numerical summation of the products of weighting factors for selected illuminants and observers with the bispectral Donaldson radiance factor of the specimen. The tristimulus values so calculated may be converted to coordinates in a more nearly uniform color space such as CIELAB or CIELUV.

5. Significance and Use

5.1 The bispectral or two-monochromator method is the definitive method for the determination of the general radiation-transfer properties of fluorescent specimens (4). In this method, the measuring instrument is equipped with two separate monochromators. The first, the irradiation monochromator, irradiates the specimen with monochromatic light. The second, the viewing monochromator, analyzes the radiation leaving the specimen. A two-dimensional array of bispectral photometric values is obtained by setting the irradiation monochromator at a series of fixed wavelengths (μ) in the ultraviolet and visible range, and for each μ , using the viewing monochromator to record readings for each wavelength (λ) in the visible range. The resulting array, once properly corrected, is known as the Donaldson matrix, and the value of each element (μ, λ) of this array is here described as the Donaldson radiance factor $(D(\mu,\lambda))$. The Donaldson radiance factor is an instrument- and illuminant-independent photometric property of the specimen, and can be used to calculate its color for any desired illuminant and observer. The advantage of this method is that it provides a comprehensive characterization of the specimen's radiation-transfer properties, without the inaccuracies associated with source simulation and various methods of approximation.

6. Procedure

6.1 *Selecting Standard Observer*—Select standard observer according to the guidelines of Practice E 308.

6.2 Selecting Illuminants—Select illuminants that are similar to the light under which the objects will be viewed or for which their colors will be specified or evaluated. In general, follow the recommendations of Practice E 308. For fluorescent samples, however, special attention must be given to the relative UV content of the selected illuminants and the light under which the objects will be viewed.

6.2.1 When object will be viewed indoors, by daylight filtered through a glass window, use values for the extended version of Illuminant C defined in ISO 11476.

6.2.2 When object will be viewed outdoors, by unfiltered

daylight, use values for CIE Illuminant D65, or other daylight illuminants, as defined by the formulas developed by Judd, and presented in CIE 15.2.

6.2.3 When object will be viewed under well-defined special conditions of irradiation which are not similar to any standard illuminant, a provisional illuminant may be defined. Such a provisional illuminant must represent the relative spectral irradiance upon the object surface under these special conditions.

7. Calculation

7.1 *Calculation of Colorimetric Quantities*—Use the method of calculating tristimulus values at 5 nm intervals over the viewing wavelength range 380 to 780 nm, and irradiation wavelength range 300 to 780 nm.

7.2 Calculation of Tristimulus Values—The calculation procedures described below involve numerical summation of the products of the Donaldson radiance factor of the specimen and a bispectral factor derived from the tabulated standard illuminant and observer functions. After normalization, the sums are the CIE tristimulus values X, Y, Z. (3, 4, 5)

7.2.1 Application of Illuminant Weights—Select the desired CIE standard illuminant from Tables given in Practice E 308. Multiply each element $D(\mu,\lambda)$ of the specimen's Donaldson matrix by the tabulated value of the relative spectral power of the illuminant Φ at the element's irradiation wavelength (μ).

7.2.2 Calculation of Stimulus Function—Obtain the sum over μ of these products at 5 nm intervals over the wavelength range 300 to 780 nm. The sum obtained at each viewing wavelength λ is the value of the specimen's stimulus function (relative spectral radiance) $F(\lambda)$, under the specified conditions of irradiation. From these values, either tristimulus values or spectral radiance factor values may be derived.

$$F(\lambda) = \sum_{\mu=300}^{780} \Phi(\mu) D(\mu, \lambda) \tag{1}$$

7.2.3 Derivation of Tristimulus Values—Use the colormatching functions selected in 6.1. Multiply the specimen's stimulus function at each viewing wavelength (λ) by the corresponding tabulated values of the observer color-matching functions. Obtain the sum of these spectral products at 5 nm intervals over the wavelength range 380 to 780 nm:

$$X = k \sum_{\lambda = 380}^{780} \overline{x}(\lambda) F(\lambda)$$
(2)

$$Y = k \sum_{\lambda = 380}^{780} \overline{y}(\lambda) F(\lambda)$$
(2)

$$Z = k \sum_{\lambda = 380}^{780} \overline{z}(\lambda) F(\lambda)$$

where:

k = the normalization constant:

$$k = \frac{100}{\frac{780}{\lambda = 380} \Phi(\lambda)\overline{y}(\lambda)}$$
(3)

7.3 Derivation of Other Colorimetric Quantities—Other colorimetric values, such as chromaticity coordinates, CIELAB and CIELUV values, may be calculated from tristimulus values as described in Practice E 308.

NOTE 2—The validity of CIELAB and CIELUV values for describing the color of fluorescent materials is subject to question, for two reasons. First, because the appearance of a fluorescent material may be influenced by irradiation at wavelengths outside the visible range, the appropriate definition of the "white point" (incorporated in the CIELAB and CIELUV calculations) is not clear. Second, the perceptual uniformity of these color spaces has not been evaluated in regions where L* exceeds 100, as it may for fluorescent materials. It is the responsibility of the user to determine the appropriateness of such metrics for any particular specimen and application.

7.4 Derivation of Spectral Radiance Factors—Calculate the specimen's stimulus function (relative spectral radiance) $F(\lambda)$ for the selected illuminant as described in section 7.2.2. Divide *F* at each viewing wavelength (λ) by the corresponding tabulated value of the relative spectral power Φ_I of the selected illuminant. Note that for a fluorescent specimen, the spectral radiance factor (β_I (λ) is illuminant-specific. (3)

$$\beta_I(\lambda) = \frac{F_I(\lambda)}{\Phi_I(\lambda)} = \sum_{\mu=300}^{780} \frac{\Phi_I(\mu)}{\Phi_I(\lambda)} D(\mu, \lambda)$$
(4)

7.5 Separation of Fluorescence and Reflection Components—Fluorescence and reflection components of tristimulus and spectral radiance factor values can be calculated by substituting the fluorescent or reflection components of Donaldson radiance factor (D_F or D_R) for Donaldson radiance factor (D) in the calculations described in sections 7.2 and 7.3. This separation of components is valid for D, β , and tristimulus values; it may not be valid for other colorimetric values.

7.5.1 *Estimation of Components*—To a first approximation, the contribution of fluorescence and reflectance to the appearance of the specimen can be separated by treating diagonal values of the Donaldson matrix as representing reflectance only, and off-diagonal values as representing fluorescence.

7.5.2 *Calculation of Components*—While more rigorous and accurate methods for the separation of reflection and fluorescence components may be employed, description of such calculations lies outside the scope of this standard.

7.6 Abridged Calculation Procedures:

7.6.1 Wavelength Intervals of Greater than 5 nm—When data for $D(\mu,\lambda)$ are not available at 5 nm intervals, estimated values at 5 nm intervals should be derived by appropriate interpolation, as described in Annex A1.

7.6.2 Viewing Wavelength Range Less Than 380-780 nm— When data for $D(\mu,\lambda)$ are not available for the full viewing wavelength range, add the illuminant or observer weights, or both, at the wavelengths for which data are not available to the weights at the shortest and longest wavelength for which spectral data are available. Note that such use of spectrally-truncated data is not recommended when significant fluorescent emission occurs in the region of truncation.

7.6.3 Irradiation Wavelength Range Less Than 300-780 nm—When the bispectral region of fluorescence is known for a particular specimen, it is acceptable to limit the collection of fluorescence data (off-diagonal values) to this region. Complete the standard Donaldson matrix by setting off-diagonal values outside this region to zero.

8. Report

8.1 The report of the measurement of colorimetric for fluorescent samples data shall include the following:

8.2 Specimen Description—Including the following:

8.2.1 Type and identification,

8.2.2 Date of preparation or manufacture, if required,

8.2.3 Method of cleaning and date, if cleaned,

8.2.4 Orientation of the specimen during measurement, and

8.2.5 Any changes in the specimen during measurement.

8.3 *Source of Date*—Give instrument identification, irradiating and viewing geometry, spectral bandpass, and date of measurement.

8.4 *Observer*—Indicate whether the reported data were computed for the CIE 1931 standard observer (2°) or the 1964 supplementary standard observer (10°) .

8.5 Illuminants-Indicate which illuminants were used.

8.6 *Method of Calculation*—Indicate whether the procedure using a 5 nm wavelength interval, or a specified abridged procedure was used, and what wavelength range of spectral data was available.

8.7 *Colorimetric Data*—Report according to the guidelines of Practice E 308.

8.8 *Spectral Radiance Factor (Optional)*—When reporting spectral radiance factor values for fluorescent samples, indicate for which illuminant the reported spectral radiance factor is defined.

9. Keywords

9.1 bispectral; bispectrometer; color; colorimetry; Donaldson matrix; Donaldson radiance factor; fluorescence; luminescence; radiance factor; tristimulus

ANNEX

(Mandatory Information)

A1. BISPECTRAL INTERPOLATION PROCEDURE

A1.1 *Discussion*—This annex presents a procedure for bispectral Lagrange interpolation, appropriate for deriving the 5 nm interval data required in Section 7 from abridged bispectral data.

A1.1.1 *Alternate Methods*—Other methods of interpolation may be equally appropriate, and some may yield more accurate results than Lagrange interpolation, but consideration of these alternatives lies beyond the scope of this standard. If an alternate method of interpolation is selected, this should be reported along with calculation results.

A1.1.2 *Summary of Procedure*—The following interpolation procedure consists of three basic steps: First, an abridged Donaldson matrix is separated into its fluorescence and reflection components. Second, these components are interpolated separately to 5 nm interval data; the fluorescence component is interpolated bispectrally, while the reflection component is interpolated spectrally. Third, these components are recombined to obtain a 5 nm interval Donaldson matrix.

A1.2 *Separation of Components*—Separate the specimen's abridged Donaldson matrix into its fluorescence and reflection components, and reformat reflectance data as follows:

A1.2.1 *Estimate Fluorescence Component*—Derive fluorescence component of the specimen's Donaldson radiance factor by setting diagonal values of $D(\mu, \lambda)$ equal to zero. if

 $\mu = \lambda$

then else

$$D_F(\mu,\lambda) = 0$$

$D_F(\mu,\lambda) = D(\mu,\lambda)$

A1.2.2 *Extract Reflectance Factor Values*—Extract spectral reflectance factor values, $R(\lambda)$, from the Donaldson matrix, by setting $R(\lambda)$ equal to diagonal values at the corresponding emission wavelengths:

$$R(\lambda) = D(\lambda, \lambda) \tag{A1.2}$$

A1.3 *Interpolation*—Interpolate fluorescence component bispectrally, and reflection component spectrally, as described below.

A1.3.1 *Discussion*—The fluorescence properties of many materials can be described by a continuous bispectral function, but reflectance, when represented bispectrally, is essentially discontinuous (5). For this reason, bispectral interpolation is appropriate for the fluorescence component of Donaldson radiance factor, but inappropriate for the reflection component. Instead, the reflection component of the specimen's Donaldson radiance factor must be interpolated spectrally, as a function of a single spectral variable.

A1.3.2 Interpolate Fluorescence Component—Interpolate the values of D_F in two steps, to obtain 5 nm interval data D'_F : First, by 4-point Lagrange interpolation over emission wavelength for each excitation wavelength; second, by 4-point Lagrange interpolation over excitation wavelength for each emission wavelength.

A1.3.2.1 *Discussion*—The indicated order of operations is arbitrary; equivalent results will be obtained if interpolation is performed first over excitation wavelength, and then over emission wavelength.

A1.3.3 Interpolate Reflection Component—Interpolate the values of $R(\lambda)$ by 4-point Lagrange interpolation to obtain 5 nm interval data $R'(\lambda)$.

A1.4 *Interpolation Over Terminal Intervals*—For first and last intervals, where 4-point interpolation is impossible, use three-point Lagrange interpolation instead.

A1.5 *Recombination of Components*—Recombine interpolated reflection and fluorescence data to obtain a 5 nm interval Donaldson matrix, D'.

 $\mu = \lambda$

(A1.3)

then

else

if

(A1.1)

 $D'(\mu,\lambda) = R'(\lambda)$

$$D'(\mu,\lambda) = D'_F(\mu,\lambda)$$

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