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Standard Practice for Rectification of Spectrophotometric Bandpass Differences[1]

This standard is issued under the fixed designation E2729; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This standard outlines the methods that can be used to deconvolve, at least partially, the spectral bandpass differences of raw spectral data acquired by abridged spectrophotometry. Such differences are introduced because the spectral passband must be of significant bandwidth to allow sufficient energy to reach the detector. On the other hand, the spectral data that should be reported is that of a virtual 1-nm bandwidth spectrum in order to be useful in the CIE method of tristimulus integration which involves 1-nm summation.

1.2 The standard establishes practices for whether, when, and how a bandpass rectification should be made to any reflectance or transmittance spectrum acquired by abridged spectrophotometry.

1.3 It is applicable where the shape of the passband is triangular and the bandwidth is equal to the measurement interval between passbands. Information is provided in Section 7 for users when that condition is not satisfactorily met.

1.4 *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, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.5 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E284 Terminology of Appearance

E308 Practice for Computing the Colors of Objects by Using the CIE System

3. Terminology

3.1 *Definitions*—For definition of terms used in this practice, refer to Terminology E284.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *virtual 1-nm bandwidth spectrum, n*—spectral data that have been corrected by numerical methods so as to match as closely as possible a spectrum from the same source but with a putative bandwidth of 1 nm.

4. Summary of Practice

4.1 The practice assumes that the shape of the passband is triangular and that the bandwidth is equal to the measurement interval between passbands. This condition is thought to be met by a majority of commercial instruments in use in spectrophotometry and spectrocolorimetry. Under those conditions, the methods of Section 6 are to be utilized to rectify the raw reflectance or transmittance data for its bandpass differences immediately upon the return of the data to the host computer program from the acquiring instrument, or before presentation of the data to the user.

5. Significance and Use

5.1 Failure to make such a rectification introduces differences from the true value of the spectrum of about 0.02 to 0.4 ΔE^*_{ab} units. All users are required to make a rectification of such bandpass differences. It is especially incumbent upon writers of computer programs whose function it is to acquire such spectra from instruments to see that a competent rectification is implemented in the program before any additional processing of the spectrum, or calculations involving the spectrum are accomplished, or before the spectrum is made available to a user.

5.2 Legacy measuring systems are explicitly exempted from any requirements for retrofitting of hardware or software and may continue to utilize previously accepted methods of making the bandwidth rectification.

6. Methodology

6.1 *The First and Last Passbands*—In the first and last passband being rectified, no correction is called for. The

[1] This practice is under the jurisdiction of ASTM Committee E12 on Color and Appearance and is the direct responsibility of Subcommittee E12.04 on Color and Appearance Analysis.

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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

corrected spectral value $R_{s,\lambda}$ should be set equal to the measured spectral value $R_{m,\lambda}$.

$$R_{s,1} = R_{m,1} \quad (1)$$

$$R_{s,n} = R_{m,n}$$

where the subscripts 1 and n refer to the wavelength index of the first and last passbands being corrected.

6.2 *The Second and Next-to-last Passbands*—The second and next-to-last passbands being rectified are subject to the following correction:

$$R_{s,2} = -0.10R_{m,1} + 1.21R_{m,2} - 0.12R_{m,3} + 0.01R_{m,4} \quad (2)$$

$$R_{s,n-1} = -0.10R_{m,n} + 1.21R_{m,n-1} - 0.12R_{m,n-2} + 0.01R_{m,n-3}$$

where the second subscript refers to the wavelength index of the bandpass considered.

6.3 *The Remaining Interior Passbands*—The remaining interior passbands are subject to the following five-point rectification:

$$R_{s,i} = 0.01R_{m,i-2} - 0.12R_{m,i-1} + 1.22R_{m,i} - 0.12R_{m,i+1} + 0.01R_{m,i+2} \quad (3)$$

where the subscript i is the wavelength index of the passband being corrected and varies over the range of 3 to $n-2$.

7. Applicable Bandpass Shapes

7.1 The coefficients of the foregoing rectification equations have been calculated under the assumption that the passbands are spaced at equal intervals. The interval is assumed to be equal to the full-width half-height of the passbands. Further, assumption is made that the passbands are triangular in shape and that the reflectance, or transmittance, functions may be characterized by a quadratic function in the range of any passband. These assumptions are believed to be true for most instruments, materials, and measurements known to the Subcommittee with jurisdiction for this practice. Accordingly, the above correction is among the best practices for making a rectification of bandpass differences.

7.2 While the underlying theory leading to the rectification equations is based on triangular passbands, some related bandpass shapes may be adequately rectified by the methods of this practice. This is true of Gaussian and Lorentzian function band shapes, and may be true of instruments with concave diffraction gratings imaged on diode arrays with more pixels than wavelengths being reported. Those passbands are trapezoidal in shape.

7.3 If the user has specific knowledge as to departures from the above assumptions with respect to his particular measurement conditions, he may calculate a set of correction coefficients fitting his own case from principles laid down in the published literature. Most helpful in this regard will be articles by Stearns (**1**,**2**),[3] Fairman (**3**), Oleari (**4**), Venable (**5**), Gardner (**6**), and Ohno (**7**). Corrections using such coefficients are deemed to meet the requirements of this practice.

8. Precision and Bias

8.1 The rectification has no impact on the precision of any test method.

8.2 In the absence of any rectification, the bias introduced by the bandpass differences is as much as 0.25 in daylight illuminants and about 0.4 in fluorescent illuminants in units of ΔE^*_{ab}. The correction of Section 6 reduces the bias to about 0.02 for daylight illuminants and to about 0.04 ΔE^*_{ab} for fluorescent illuminants illuminating typical non-fluorescent surface colors.

9. Keywords

9.1 bandpass rectification; spectral deconvolution

[3] The boldface numbers in parentheses refer to a list of references at the end of this standard.

APPENDIX

(Nonmandatory Information)

X1. BEST PRACTICES FOR THE IMPLEMENTATION OF THE SPECTROPHOTOMETRIC BANDPASS RECTIFICATION

X1.1 Effective with the issuance of the practice, ASTM has changed the standard method for implementing the bandpass rectification of a measured spectrum from the jurisdiction of Practice E308 to the jurisdiction of this separate standard. This involves an implementation model in which both instrument and software manufacturers will have to participate, and it will require the understanding and cooperation of the user community. The following is written to assist both instrument manufacturers and users in selecting the best practices in implementing the new bandpass correction scheme.

X1.1.1 To explain the change in brief, the bandpass rectification was previously most often made at the time of tristimulus integration. Under the jurisdiction of this standard the rectification has been moved to a separate action prior to integration. This assures that the spectral data, as well as the tristimulus values, have been corrected, and leaves no doubt in the users mind as to whether or not the spectrum has been rectified as all spectra will hereafter be rectified.

X1.1.2 *Bulk Rectification of Legacy Files*—It would be a best practice for manufacturers to provide users a utility program to which they could submit their standard, batch record, history, or color measurement files for processing from bandpass unrectified to bandpass rectified. The utility would take each record in turn, process it, and return it to its rightful place in the rectified output file. Processing by such a utility, with the concomitant flagging of the rectified records, will eliminate, once and for all time, any worry about the status of legacy files. Each record so upgraded will need to be flagged as discussed in X1.1.4 and following to avoid the possibility of the record's being duplicatively treated at a later date.

X1.1.3 *Record by Record Rectification of Legacy Files*—Another option among the best practices, is to process each record brought into software after the implementation date and to restore it to its place in the original file rectified and flagged as discussed in the following sections.

X1.1.4 *Flagging of Records that are Rectified*—In any case, it is best practice to flag any record that has previously been rectified by any means in the database as being a record that has already been corrected. Rectifying software may then be programmed automatically to avoid redundantly correcting such a record. This has the capacity to avoid even human error should the user believe a file, or record, has not been previously processed.

X1.1.5 *Suggested Flagging*—Most spectrophotometric database systems will contain a table which describes the geometric conditions under which the spectrum has been measured. At the present time these geometric conditions may be limited to "Specular Included," "Specular Excluded," and "0°/45°" or some other short list of geometries. It would be beneficial to users if manufacturers adopted the practice of extending this list to items such as "Specular Included BP Rectified," "Specular Excluded BP Rectified," etc. This can be done without change in the database definition on the part of the manufacturer, and gives the user a target location in the database where he may expect to find the bandpass rectification flag.

REFERENCES

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(5) Venable, W. H., "Accurate tristimulus values from spectral data," *Color Research and Application*, 1989, 14, pp. 260–267.

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