Designation: E1791 – 96 (Reapproved 2021)

Standard Practice for Transfer Standards for Reflectance Factor for Near-Infrared Instruments Using Hemispherical Geometry[1]

This standard is issued under the fixed designation E1791; 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.

INTRODUCTION

The internationally accepted standard of reflectance is the perfect reflecting diffuser. This ideal reflecting surface reflects 100 % of the radiant power incident on it, such that the radiance is the same for all directions within the hemisphere of solid angles. No physical realization of this standard exists. Optical properties of standards prepared from pressed plaques of barium sulfate ($BaSO_4$) or polytetrafluoroethylene (PTFE), as well as commercially available samples of sintered PTFE (**1-4**),[2] can approximate those of a white material. For further information, see Commission Internationale de L'Eclairage (CIE) Publication No. 46 (**5**). Additional transfer standards are required that have a very stable reflectance factor that is constant with wavelength and that have a range of values from near zero to close to that of the perfect reflecting diffuser. Such materials as carbon-black doped sintered PTFE (**6-8**) fulfill this requirement. The principle uses of a reflectance factor standard are for transferring an absolute scale of reflectance to a more durable material or for calibrating near-infrared (NIR) spectrophotometers for linearity of reflectance scale. In theory, this transfer, conducted from first principles, should be quite easy. In practice, values are likely to be required for parameters that are unknown, proprietary, or require a highly sophisticated level of skill. Some, but not all, of these parameters are discussed in this practice.

1. Scope

1.1 This practice covers procedures for the preparation and use of acceptable transfer standards for NIR spectrophotometers. Procedures for calibrating the reflectance factor of materials on an absolute basis are contained in CIE Publication No. 44 (**9**). Both the pressed powder samples and the sintered PTFE materials are used as transfer standards for such calibrations because they have very stable reflectance factors that are nearly constant with wavelength and because the distribution of flux resembles closely that from the perfect reflecting diffuser.

1.2 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.3 *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.*

1.4 *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:*[3]

E131 Terminology Relating to Molecular Spectroscopy
E259 Practice for Preparation of Pressed Powder White Reflectance Factor Transfer Standards for Hemispherical and Bi-Directional Geometries
E284 Terminology of Appearance

3. Terminology

3.1 *Definitions*—Terms and definitions in Terminology E284 are applicable to this practice.

[1] This practice is under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Separation Science and is the direct responsibility of Subcommittee E13.03 on Infrared and Near Infrared Spectroscopy.

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[2] The boldface numbers in parentheses refer to the list of references at the end of this practice.

[3] 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.

3.2 *Descriptions of Terms Specific to This Standard*—The following definitions are particularly important to this practice.

3.2.1 *linearity*—the ability of a photometric system to yield a linear relationship between the radiant power incident on its detector and some measurable quantity provided by the system. (**E131**)

3.2.2 *near-infrared, adj*—the region of the electromagnetic spectrum for radiation of wavelengths between 780 and 2500 nm (0.78 and 2.50 µm).

3.2.3 *perfect reflecting diffuser*—ideal reflecting surface that neither absorbs nor transmits light, but reflects diffusely, with the radiance of the reflecting surface being the same for all reflecting angles, regardless of the angular distribution of the incident light.

3.2.4 *reflectance, r, n*—ratio of the reflected radiant or luminous flux to the incident flux in the given conditions (**1**).

3.2.4.1 The term reflectance is often used in a general sense or as an abbreviation for reflectance factor. Such usage may be assumed unless the definition is specifically required by the context.

3.2.5 *reflectance factor, R, n*—ratio of the flux reflected from the specimen to the flux reflected from the perfect reflecting diffuser under the same geometric and spectral conditions of measurement (**2**).

4. Summary of Practice

4.1 Procedures for the preparation of packed powder samples of barium sulfate and PTFE can be found in Practice E259. Sintered PTFE samples are commercially available. Reflectance data for this material are given in Table 1. These materials provide close approximation to the optical properties of the perfect reflecting diffuser and may be used to transfer a scale of reflectance factor to another material or instrument.

4.2 Sintered carbon-black doped PTFE samples are also commercially available and are described in Table 2. These materials provide close approximation to the optical properties of a perfect reflecting diffuser with spectrally neutral absorbance features and may be used to transfer a scale of linearity in reflectance factor to another material or instrument.

5. Significance and Use

5.1 Most commercial reflectometers and spectrophotometers with reflectance capability measure relative reflectance. The instrument reading is the ratio of the measured radiation reflected from the reference specimen to the measured radiation reflected by the test specimen. That ratio is dependent on specific instrument parameters.

5.2 National standardizing laboratories and some research laboratories measure reflectance on instruments calibrated from basic principles, thereby establishing a scale of absolute reflectance as described in CIE Publication No. 44 (**5**). These measurements are sufficiently difficult and of prohibitive cost that they are usually left to laboratories that specialize in them.

5.3 A standard that has been measured on an absolute scale could be used to transfer that scale to a reflectometer. While such procedures exist, the constraints placed on the mechanical properties restrict the suitability of some of the optical properties, especially those properties related to the geometric distribution of reflected radiation. Thus, reflectance factor standards that are sufficiently rugged or cleanable to use as permanent transfer standards, with the exception of the sintered PTFE standards, depart considerably from the perfect diffuser in the geometric distribution of reflected radiation.

TABLE 1 6°/Typical Diffuse Reflectance for Sintered PTFE

Wavelength, nm	Reflectance Factor
250	0.940
300	0.977
400	0.991
500	0.991
600	0.991
700	0.990
800	0.991
900	0.991
1000	0.990
1100	0.990
1200	0.989
1300	0.988
1400	0.986
1500	0.988
1600	0.987
1700	0.984
1800	0.984
1900	0.978
2000	0.970
2100	0.950
2200	0.963
2300	0.955
2400	0.944
2500	0.940

Density = 1500 kg/m^3; thickness ≥7 mm

TABLE 2 6°/Typical Diffuse Reflectance for Three Sintered Carbon-Black Doped PTFE

Wavelength, nm	80 % Standard	10 % Standard	2 % Standard
250	0.774	0.106	0.015
300	0.793	0.099	0.016
400	0.795	0.097	0.017
500	0.796	0.099	0.017
600	0.797	0.101	0.017
700	0.799	0.103	0.017
800	0.802	0.105	0.018
900	0.803	0.105	0.017
1000	0.805	0.106	0.018
1100	0.806	0.108	0.017
1200	0.807	0.109	0.018
1300	0.808	0.111	0.018
1400	0.808	0.112	0.018
1500	0.810	0.113	0.020
1600	0.811	0.114	0.021
1700	0.812	0.115	0.023
1800	0.813	0.116	0.024
1900	0.811	0.118	0.026
2000	0.814	0.117	0.027
2100	0.809	0.114	0.030
2200	0.812	0.110	0.032
2300	0.813	0.110	0.035
2400	0.809	0.103	0.034
2500	0.809	0.101	0.038
	thickness ≤7 mm	thickness ≤5 mm	thickness ≤3 mm