

Spectrophotometer Calibration and Certification

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This report describes a verification procedure for spectrophotometers used in process control based on trend analysis. This analysis is more valuable if the instrument's drift is tightly monitored, so it can be unequivocally established that any detected drift is in the process under observation and not in the instrument used for the measurements. The difference to practice in traditional color metrology is that instrument precision is much more important than accuracy.

We recommend a much more frequent calibration certification that is usual for spectrophotometers used in color matching applications. To make this feasible the procedure must be very simple and quick to perform; our procedure fulfills this requirement.

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1 Introduction

Like all instruments used for measuring physical quantities, spectrophotometers need to be calibrated and characterized periodically. The procedure itself must be certified, also periodically, to validate the use of the instrument. ISO 9000 — a series of quality management and quality assurance standards — recommends the documentation of these procedures to maintain a history trail of a process. Since many people are unfamiliar with ISO 9000, the original standards in the series are outlined in a table:

ISO Number	Scope	Comment
9000	Quality management and assurance standards—guidelines for selection and use	Roadmap for the series. Provides the user with guidelines for selection and use of ISO 9001, 9002, 9003, and 9004
9001	Model for quality assurance in design, development, production, installation, and servicing	For use when conformance to specified requirements is to be assured by the supplier during several stages, including design, development, production, installation, and servicing
9002	Model for quality assurance in production and installation	For use when conformance to specified requirements is to be assured by the supplier during production and installation
9003	Model for quality assurance in final inspection and testing	For use when conformance to specified requirements is to be assured by the supplier solely at final inspection and test
9004	Quality management and quality system elements—guidelines	Describes a basic set of elements by which quality management systems can be developed and implemented. There is heavy emphasis on “meeting company and customer needs”

TABLE 1. Overview of the main ISO 9000 standard series
There are more standards in this evolving series.

1.1 Terminology

Before proceeding any further, we need to agree on the terminology. Often we use interchangeably terms like calibration, characterization, certification, qualification, and validation. However, these terms are all different.

Calibration. To correlate the readings of an instrument with a standard. After a calibration procedure the output of the instrument may be different (closer to the standard).

Characterization. To relate the readings of an instrument to a standard. The characterization procedure does not change the instrument's output. The characterization of a (calibration) standard, e.g., a reference tile, consists in determining a physical property of the standard based on a physical observation. If the characterization instrument has been calibrated with respect to a natural constant or a primary standard, then the characterization is absolute, otherwise it is relative.

Certification. The creation of a document attesting that performance of an instrument is within a pre-specified tolerance. The certification requires three elements: an authority (person or apparatus skilled in the art), a characterization, and the presence of a tolerance.

Qualification. The verification that an instrument can be used to fulfill a specified task. The steps required to certify an instrument for a particular task.

Validation. Confirmation that an instrument or procedure performs as certified. Validation occurs through peer review or through signature of a certificate after the assertion has been verified.

Traceability. The ability to relate an instrument to a natural constant or a primary standard by transferring a calibration from one tile to another [9].

Precision. Random error in measurement.

Accuracy. Systematic error in measurement.

1.2 Manufacturing issues

Most commonly CIE colorimetry is employed to determine whether the color of a sample is a match to the aim-color of a product for an average observer under specified viewing conditions. The tolerance of an instrument can then be just slightly lower than a just noticeable difference (jnd). In a different application, some drifts in manufacturing processes can be detected more easily with a colorimetric measurement than measuring a different parameter, e.g., temperature* or acidity. In these cases jnds are irrelevant and precision is much more important than accuracy.

This report describes a verification procedure for spectrophotometers used in process control based on trend analysis. This analysis is more valuable if the instrument's drift is tightly monitored, so it can be unequivocally established that any detected drift is in the process under observation and not in the instrument used for the measurement. Verification implies a two step process:

* For example, blood banks measure body temperature with a disposable thermometer based on thermochromism, where a scale marks patches with different thermochromism thresholds. Similar paints are routinely used also in prototyping electronic components.

a calibration to adjust the instrument's scale, and the measurement of a sample of known color to validate the calibration within a predetermined tolerance.

We recommend a much more frequent calibration certification than is usual for spectrophotometers used in color matching applications. To make this feasible, the procedure must be very simple and quick to perform; our procedure fulfills both requirements.

In support of ISO 9001 procedures we publish all data relevant to our instruments. We make recommendations for a working methodology and record-keeping that significantly facilitate the introduction of ISO 9001 compliant procedures.

1.3 Previous work

Today's spectrophotometers can be easily calibrated making a single quick measurement of a white reference tile that is traceable to an absolute standard. This procedure is sufficient for routine work, but periodically the instrument's calibration must be verified by measuring a number of different tiles. Unfortunately this verification is often ignored.

In today's world of contract manufacturing, where parts are progressively manipulated by a number of suppliers and then assembled, quality control can be a nightmare if it is not designed very meticulously. This is the main goal of the ISO 9000 standards series mentioned earlier. The prescribed procedures for a spectrophotometer can consist for example in a verification with a single color tile each three months and a larger set each year. This larger set usually consists in a number of gray samples to determine linearity and various vivid samples.

For process control we need a more frequent verification. If possible, we would like to use the verification data to increase the precision of the measurement data.

Most research in this direction has been to improve the calibration of instruments. The techniques (see e.g., [9]) consist in modeling the various errors, such as white reference, black reference, wavelength errors. A set of reference samples characterized with an absolute instrument by a standards body is measured with the instrument under consideration. The obtained data is used to estimate the parameters for the error model. The analyst can then measure a sample and apply the model to the measurement data to obtain a characterization that is traceable to a primary standard.

Such a procedure is quite difficult and requires a very high commitment. Fortunately it is necessary only when calibration standards are manufactured, because in calibration a scale is zeroed and accuracy is therefore very impor-

tant. An example is the standard for a corporate color that is used in all goods manufactured or distributed by a company. In most applications of spectrophotometry accuracy is less important than precision, the ability to repeat a certain measurement.

The focus of the work in this report is to design a validation procedure that is as simple as a calibration. Such a procedure does not need a high commitment.

1.4 Roadmap

This report is structured as follows: Section 2, “Tools,” on page 13 lists the required material, how to handle it, and explains the difference between absolute and relative certification. It also describes the instruments used for the experiments in this report.

Section 3, “Color-difference and hue angle evaluation,” on page 23 enumerates the calculation steps for CIE 1994 (ΔL^* ΔC^*_{ab} ΔH^*_{ab}) color difference model and the canonical formula for the hue angle.

Trend analysis requires the on-line availability of as much time data as possible. To support ISO 9001 requirements, it is better to use a database system than to just append individual measurement records to a sequential disk file. We have developed an example of such a database and describe it in Section 4, “Software,” on page 25. The metadata is described in the appendices, so that the database can easily be re-implemented using a different vendor’s system.

Section 5, “Procedures,” on page 39 places the various calibration and characterization procedures in context and walks the user through each procedure step-by-step. The information in this section represents the recommended qualification procedures, to which each analyst is required to adhere.

The largest environmental problem in manufacturing is the temperature both in the instrument and of the sample when a measurement is taken. Section 6, “Thermal issues,” on page 53 describes the problems and the results of our experiments.

This report does not cover the analysis of the collected measurement data. Methods are process-specific and can be designed consulting the published literature, such as [2].

2 Tools

2.1 Preparation

The procedures in this report are tailored to the SPM-100 and Spectrolino spectrophotometer families by Gretag-Macbeth. In these instruments the measurement geometry is $45^\circ/0^\circ$ with ring optics and a 4 mm measuring aperture. We provide sufficient information to easily adapt the procedure to other spectrophotometers.

2.1.1 Material

The certification set consists of the following elements:

- a white reference ceramic tile (part of the spectrophotometer kit)
- a green reference ceramic tile
- a thermometer with a Celsius scale
- a database with the measurements of the green reference
- the instructions contained in this report

2.1.2 Absolute vs. relative certification

Usually, spectrophotometer certifications are *absolute* and serve the purpose of verifying the mutual correspondence of a number of instruments of the same type used in one or several plants. This is achieved by circulating one or more ceramic tiles such as the BCRA-NPL* Ceramic Color Standards, Series II (CCS II). The tiles are characterized in a standards laboratory and each instrument must produce the same measurement result within a given tolerance, e.g., $\Delta E = 0.8$. The characterization of the tiles can be quite expensive, not only when ISO 9001 procedures are followed for traceability to a primary standard.

In a *relative* certification, the nominal colorimetry of the tiles is not known and the performance of an instrument is compared to an aim value obtained with the instrument itself. In this case the required tolerance depends on the process being monitored; an instrument that meets or exceeds this tolerance is employed, and the certification verifies this tolerance over time. Ceramic tiles that have not been characterized following procedures for traceability to a primary standard are relatively inexpensive.

* BCRA: British Ceramic Research Association. NPL: National Physical Laboratory

In trend analysis it is important to keep all historical data of the certification process. If the instrument error is not random, an incorrect trend may be predicted. When this fact is recognized, the instrument drift can be taken into account in the trend analysis and the precision can be increased or the confidence interval can be reduced.

In our procedure the relative certification is performed with a single green ceramic tile. Since each instrument is frequently calibrated with its own white tile, verifying the measurement of one chromatic color yields a good degree of confidence in the instrument at a small cost.

More elaborated procedures can be conceived. In order of increased sophistication and effort they are:

1. use statistical methods to verify that the variations of the green tile measurements are indeed random
2. use three gray tiles to assess the linearity of the instrument
3. measure the full CCS II set to assess independence from hue
4. maintain traceability to an absolute standard instrument

The reader who wishes to embark in this adventure should start by studying the excellent article [1] by Roy Berns and Lisa Reniff. This article also has an exhaustive bibliography.

2.2 Reference tiles

Each spectrophotometer has its own *white reference tile*. The absolute spectrum of the tile is stored in the instrument; during the calibration the spectral response is adjusted so that it matches the stored spectrum within a specified tolerance. A white calibration tile is “married” to an instrument; if a white tile is lost or damaged, the instrument must be returned to the manufacturer to marry the instrument with a new white tile.

We recommend a separate *color reference tile* for each geographic location. For the color we recommend green. Other authors have suggested the cyan CCS II tile because of its range of reflectance factor, multiple well-defined inflection points, and low sensitivity to temperature changes [1]. Fig. 1 shows the spectral reflectance data for the green and cyan master tiles measured at 25°C over the wavelength range 320–780 nm for 0°/45° geometry, published in [8]. The green tile has more inflection points than the cyan tile. As Fig. 1 illustrates, the green tile has also steeper slopes which are in a more sensitive spectral range and improve the detection of spectral shifts in the instrument’s scale. The colorimetric data can be found in Appendix VI on page 77.

In global companies it has long been customary to circulate one expensive absolute reference tile set among all locations to allow for inter-instrument

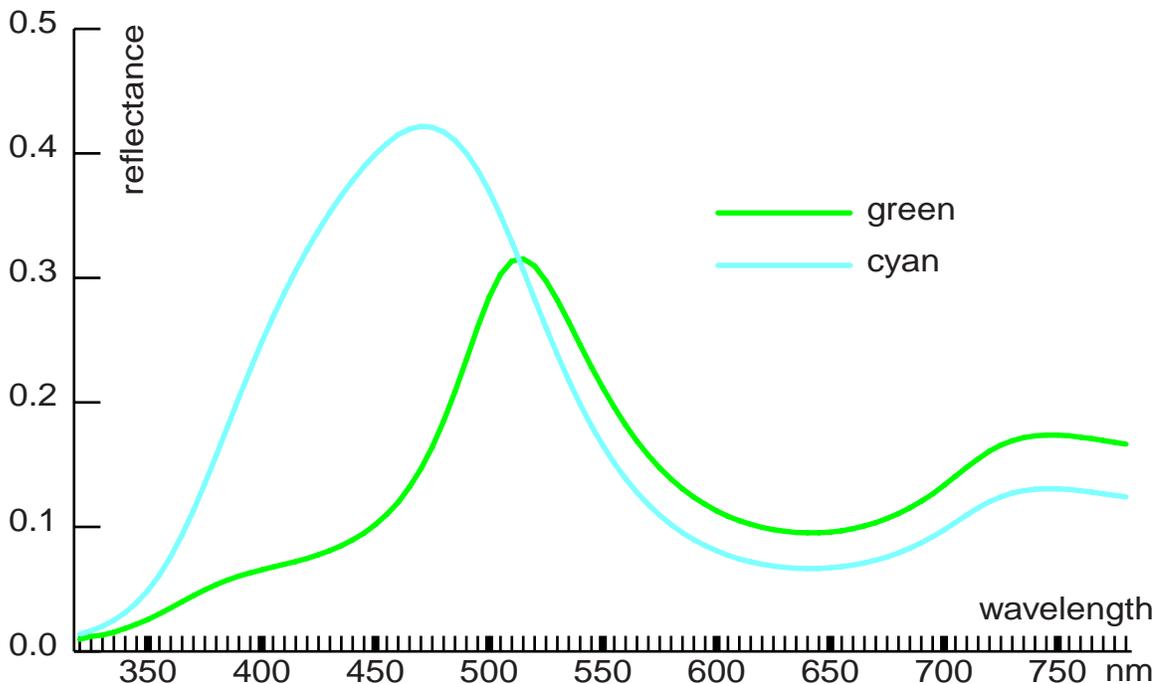


FIGURE 1. Reflectance of the green and cyan master tiles
 Measured by the National Physical Laboratory at $25\pm 1^\circ\text{C}$ for $0^\circ/45^\circ$ geometry.

comparisons, but experience teaches that it is difficult to enforce a circulation schedule. Since tiles used for relative certification are not characterized by a standards authority, they are inexpensive and can easily be afforded in multiple quantities. The local availability of a number of tiles allows frequent re-certification.

The green color reference is not married to a particular instrument and only one tile is required at each location. For each spectrophotometer it is necessary to perform an initial characterization. The initial calibrations for various instruments used in a location are unrelated and the database must allow searching by the serial number of an instrument.

2.2.1 Panic reference tile

From experience it is known that sooner or later every color engineer will come to a point when he or she no longer trusts his or her instrument. For this situation we keep one green tile that has been characterized absolutely. The data for this tile is recorded in every site's certification database. In the case of a panic situation, this tile can quickly be sent to the engineer in distress.

The next three tables list the colorimetric values for the panic tile that can be borrowed from HP Laboratories; in the meantime, other tiles may be available. This tile is mounted on a calibration plate for the SPM-100. With a Spec-

trolino, use the positioning foot (see Figure 3 on page 19) after removing the sliding lock (3).

Illuminant	Observer	L*	a*	b*	C*	h _{ab}
A	2°	50.79	-27.56	8.53	28.85	162.80
C	2°	52.96	-34.48	16.76	38.33	154.08
D ₆₅	2°	53.24	-35.03	16.78	38.84	154.41
D ₅₀	2°	52.76	-33.06	14.73	36.19	155.98
A	10°	50.92	-25.89	10.94	28.11	157.09
C	10°	52.94	-32.32	18.45	37.22	150.28
D ₆₅	10°	53.23	-32.75	18.59	37.66	150.42
D ₅₀	10°	52.81	-30.92	16.73	35.16	151.59

TABLE 2. Tile 221, no filter

Absolute values for the Green reference tile serial number 221, calibrated by Gretag-Macbeth on 8 June 1998. The tile was measured at 22±2°C without filter.

Illuminant	Observer	L*	a*	b*	C*	h _{ab}
A	2°	50.79	-27.56	8.53	28.85	162.80
C	2°	52.96	-34.48	16.76	38.33	154.08
D ₆₅	2°	53.24	-35.03	16.78	38.84	154.41
D ₅₀	2°	52.76	-33.06	14.73	36.19	155.98
A	10°	50.92	-25.89	10.94	28.11	157.09
C	10°	52.94	-32.32	18.45	37.22	150.28
D ₆₅	10°	53.23	-32.75	18.59	37.66	150.42
D ₅₀	10°	52.81	-30.92	16.73	35.16	151.59

TABLE 3. Tile 221, D65 filter

Absolute values for the Green reference tile serial number 221, calibrated by Gretag-Macbeth on 8 June 1998. The tile was measured at 22±2°C with D65 filter. Note how the values are close to those in the previous table.

Illuminant	Observer	L*	a*	b*	C*	h _{ab}
A	2°	51.28	-28.48	8.71	29.78	162.99
C	2°	53.52	-35.59	17.22	39.54	154.18
D ₆₅	2°	53.81	-36.16	17.24	40.06	154.51
D ₅₀	2°	53.31	-34.13	15.12	37.33	156.10
A	10°	51.41	-26.76	11.21	29.02	157.27
C	10°	53.51	-33.38	18.99	38.41	150.37
D ₆₅	10°	53.80	-33.82	19.12	38.85	150.51
D ₅₀	10°	53.37	-31.94	17.20	36.28	151.70

TABLE 4. Tile 221, polarization filter
Absolute values for the Green reference tile serial number 221, calibrated by Gretag-Macbeth on 8 June 1998. The tile was measured at 22±2°C with POL filter. Note how the values are different from those in the previous tables.

2.2.2 Validity

The *white* reference tile can be used for ten years from the date the manufacturer has performed the absolute spectral characterization. In the SPM-100 this date can be retrieved from the “specials” menu in the “SW-Release” sub-menu; for the Spectrolino it is safe to consider the original purchase date.

The *relative green* reference tile can be used for 5 years from the initial characterization. Currently there is research in progress to determine whether this limit can be extended, so this rule should be revisited in a few years.

The *absolute green* tile can be used for 5 years from the date the manufacturer has performed the absolute spectral characterization. This date is recorded in the certificate supplied with the tile. This rule should also be revisited in a few years.

2.2.3 Handling and cleaning

The ceramic surfaces must not be scratched and shall not be exposed to permanent direct sunlight.

The tiles should be protected from soiling. Avoid all chemical substances that attack plastics, because they change the reflectance properties. In practice the most dangerous substance is acetone, because it is widely used for cleaning purposes. Acetone will destroy the calibration target.

If a reference tile is soiled, it can be cleaned with a soft cloth and a mild soap water or ethanol. If a white calibration tile is damaged, the instrument has to be sent to the manufacturer so it can be married to a new tile. If a color reference is damaged, it can be replaced with a new tile; for long-term analysis, a new series must be started.

2.2.4 Construction

Even under the most rigorous manufacturing conditions, a ceramic tile is never completely uniform. It is therefore essential to always measure exactly the same spot on the tile. All three the SPM-100, the hand-held Spectrolino, and the Spectrolino with SpectroScan have special provisions for ensuring the measurement of the same spot.

For the SPM-100 the ceramic tile is mounted permanently in a calibration plate (part number 34.67.89). For the Spectrolino the ceramic tile (part number 36.65.25) is mounted in a clip (7) that can be inserted either in a calibration plate (hand-held, see Fig. 2) or in an apposite bay in the SpectroScan stage. For hand-held use, the calibration plate is equipped with positioning pins (6). In the SpectroScan, the software implementor must always position the instrument in the same xy position for calibration.

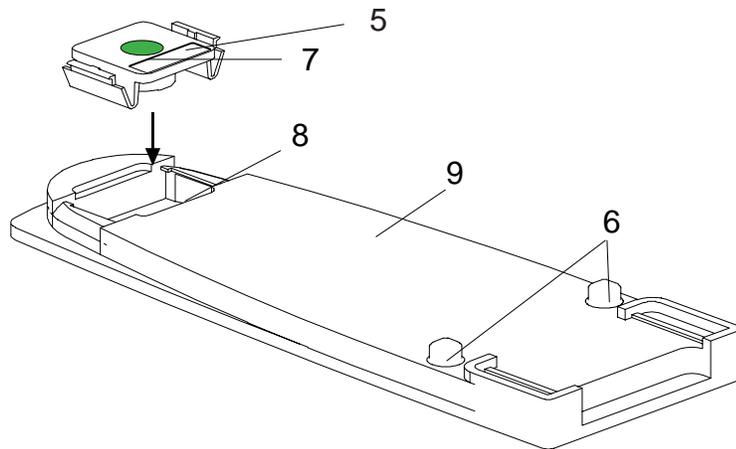


FIGURE 2. Calibration plate with green reference
5 label with serial number, 6 positioning pins, 7 clip with reference tile, 8 slit for mounting clip, 9 calibration plate.

Because of lateral diffusion, it is essential that the optical axis is perfectly perpendicular to the ceramic tile. The most difficult step in the fabrication of calibration targets is to mount them perfectly even and parallel in the clip or calibration plate.

When the positioning foot (see Fig. 3) is left on the Spectrolino, neither the exact location nor the exact perpendicularity can be controlled. Therefore, during verification is mandatory to remove the positioning foot from the instrument. When the panic tile is used, that tile may not be available with the proper mount; in this case, and only in this case, you can leave the positioning foot on.

A frequent error when the BCRA tiles are used, is to slightly tilt the instrument. This will create incorrect measurements, especially for the orange tile, which is very translucent. Analysts often use a second tile to avoid tilting the instrument; it should be noted, however, that not all BCRA tiles have the same thickness and this stratagem does not entail perpendicularity.

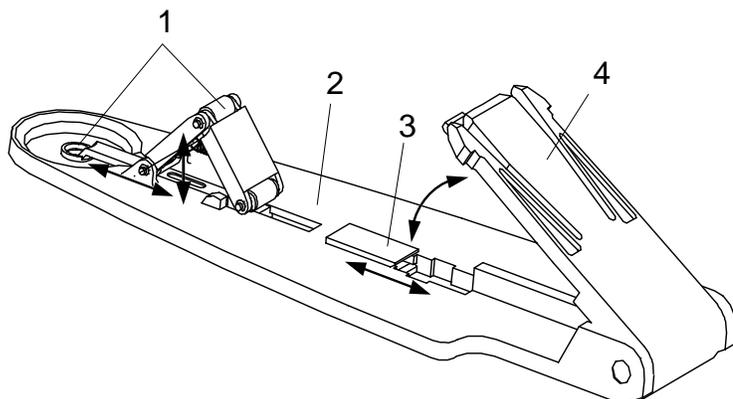


FIGURE 3. Positioning foot
1 measuring diaphragm with folding mechanism, 2 positioning foot, 3 sliding lock, 4 folding tab.

Except when you are in a panic situation, always use a ceramic tile manufactured for your instrument type. This is the only way you can be sure you measure the same spot and your instrument is not tilted.

2.3 Thermometer

The spectral reflectance of ceramic tiles changes linearly with temperature, an effect known as thermochromism. For this reason the tiles should be kept at the same ambient temperature as the instrument during its normal use; if the tiles are kept in a box or drawer, it should be opened half an hour prior to use [8].

Any thermometer with a tolerance smaller or equal the tolerance indicated in the reference database can be used. A calibrated mercury in glass thermometer graduated in 0.5°C intervals and placed near the instrument will be adequate for normal operation. For each measurement performed for certification purposes, the analyst shall record both the current temperature and the thermometer's tolerance.

The thermometer used in our experiments is an Omega HH-21 hand-held microprocessor digital thermometer with a NiCr-NiAl thermocouple sensor. The sensor is a surface probe with a flexible tip made from RTV silicone rubber to avoid damaging the ceramic tiles. The RTV silicone rubber allows for good thermal contact.

The serial number of our unit is T-198789 and it has been calibrated by the vendor. In the 18°C to 28°C ambient temperature range of interest in this application, the thermometer accuracy (excluding thermocouple error) is $\pm(0.1\% \text{ rdg} + 0.6^\circ\text{C})$. With the thermocouple the accuracy is $\pm 0.7^\circ\text{C}$, but for simplicity we will indicate the tolerance as $\pm 1^\circ\text{C}$.

2.4 Spectrophotometer

In compliance with ISO 9001 recommendations, we report the specifications of the spectrophotometer used in the experiments described in this report. Since this is an older unit, its performance may be slightly inferior to a unit purchased more recently.

The instrument is a Gretag-Macbeth Spectrolino unit with serial number 10255. Before the measurements reported here were performed, we replaced optics with a new design that reduces lateral diffusion problems in the case of translucent samples (e.g., ceramic tiles). This modification was carried out by the manufacturer and the instrument has been calibrated very carefully. The instrument had also a motherboard replacement due to a fissure.

The calibration and characterization was performed by the manufacturer on 24 June 1998, 11:24 in a room with very tight climatic control and a temperature of 23°C. The illuminant was D₆₅ and the color-matching functions were the 2° CIE observer. Table 5 shows the instrument's deviation from the absolute values for a set of ceramic tiles. Note that knowledge of these deviations is not sufficient to transfer a standard and build traceable standards (see [9] for details).

Tile	Measured CIELAB			Absolute deviation CIELAB			ΔE
	L*	a*	b*	ΔL^*	Δa^*	Δb^*	
Green	51.70	-34.97	19.17	-0.24	0.44	-0.16	0.52
Orange	63.06	39.61	60.03	-0.01	0.56	0.05	0.56
Red	32.97	52.81	38.40	-0.07	0.00	-0.60	0.60
Light blue	49.65	-14.19	-31.37	-0.21	0.02	0.05	0.22
Dark blue	8.68	23.76	-33.75	-0.17	0.02	0.00	0.17
Yellow	80.80	-3.76	83.53	0.18	0.73	-0.03	0.75
Pink	39.11	30.27	5.16	-0.18	0.26	-0.01	0.31
Light gray	82.64	-0.15	0.45	-0.03	0.28	0.04	0.28
Medium gray	56.01	-2.46	2.49	-0.21	0.29	-0.09	0.37
Difference gray	55.72	-0.12	0.20	-0.18	0.29	0.03	0.34
Dark gray	26.24	-0.32	0.54	-0.43	0.13	-0.11	0.46
MRS							0.45

TABLE 5. Absolute characterization unit 10255

Calibration data for Spectrolino unit 10255, obtained 24 June 1998, 11:24 at 23°C. Tiles characterized absolutely 21 April 1997, 17:30 with reference SPM 9001 at 23°C. The conditions were illuminant D₆₅ and the 2° standard observer.

If we assume (we do not know as a fact) the reference tiles are the BCRA CCS II and they were traced through the NPL tiles (the certification was performed in Europe), then according to Eq. (A1) in reference [1] for the cyan tile with illuminant D_{65} and the 10° observer we can assess systematic errors by evaluating the linear system

$$\begin{bmatrix} E_w \\ E_k \\ E_\lambda \end{bmatrix} = \begin{bmatrix} -2.79 & 1.52 & 2.94 \\ -0.32 & -0.47 & -0.41 \\ 0.09 & -0.81 & 0.67 \end{bmatrix} \cdot \begin{bmatrix} \Delta L^* \\ \Delta a^* \\ \Delta b^* \end{bmatrix} \quad (\text{EQ 1})$$

where E_w is the systematic photometric error for white calibration, i.e., the spectrophotometer performance with respect to reference white (% reflectance). Similarly, E_k is with respect to black (%) and E_λ with respect to wavelength (nm). We do not have the data for the cyan tile and insert the values for the light blue tile instead (it might actually be the same tile, allowing for the possible German translation of the color term cyan into Hellblau):

$$\begin{bmatrix} E_w \\ E_k \\ E_\lambda \end{bmatrix} = \begin{bmatrix} -2.79 & 1.52 & 2.94 \\ -0.32 & -0.47 & -0.41 \\ 0.09 & -0.81 & 0.67 \end{bmatrix} \cdot \begin{bmatrix} -0.21 \\ 0.02 \\ 0.05 \end{bmatrix} = \begin{bmatrix} 0.76 \\ 0.04 \\ 0.00 \end{bmatrix} \quad (\text{EQ 2})$$

This results should be considered with caution, since we made several assumptions about the tiles and the data, like our data is for the 2° observer while the values in (EQ 1) are for the 10° observer (the fact that E_w is much larger than ΔE is suspicious). The error for the white calibration seems to be the critical step for this particular spectrophotometer. Hence the Spectrolino should be frequently calibrated according to the procedure in Section 5.2 on page 43.

To assess the inter-instrument repeatability, it is useful to compare the values with those averaged from a number of instruments of the same model. In this case 10 instruments were used.

Tile	Measured CIELAB			Spectrolino deviation CIELAB			ΔE
	L^*	a^*	b^*	ΔL^*	Δa^*	Δb^*	
Green	51.70	-34.97	19.17	-0.01	0.16	-0.23	0.28
Orange	63.06	39.61	60.03	0.12	0.32	0.60	0.69

TABLE 6. Relative comparison unit 10255
Comparison data for Spectrolino unit 10255, obtained 24 June 1998 at 23°C . Average computed 21 April 1997 from 10 Spectrolinos (serial numbers 109xx) at 23°C . The conditions were illuminant D_{65} and the 2° standard observer.

Tile	Measured CIELAB			Spectrolino deviation CIELAB			ΔE
	L*	a*	b*	ΔL^*	Δa^*	Δb^*	
Red	32.97	52.81	38.40	-0.16	-0.04	0.09	0.19
Light blue	49.65	-14.19	-31.37	-0.12	0.20	-0.12	0.26
Dark blue	8.68	23.76	-33.75	-0.21	-0.11	0.20	0.31
Yellow	80.80	-3.76	83.53	0.09	0.07	0.34	0.36
Pink	39.11	30.27	5.16	-0.13	-0.04	0.16	0.21
Light gray	82.64	-0.15	0.45	-0.18	0.09	0.11	0.23
Medium gray	56.01	-2.46	2.49	-0.14	0.06	0.08	0.17
Difference gray	55.72	-0.12	0.20	-0.12	0.08	0.08	0.17
Dark gray	26.24	-0.32	0.54	-0.19	0.00	0.08	0.21
MRS							0.31

TABLE 6. Relative comparison unit 10255

Comparison data for Spectrolino unit 10255, obtained 24 June 1998 at 23°C. Average computed 21 April 1997 from 10 Spectrolinos (serial numbers 109xx) at 23°C. The conditions were illuminant D₆₅ and the 2° standard observer.

Finally, Table 7 shows the short term reproducibility of our unit.

Measurement	L*	a*	b*	ΔE
1	95.80	-1.07	1.96	0.044
2	95.80	-1.07	1.97	0.031
3	95.80	-1.06	1.98	0.024
4	95.80	-1.06	2.00	0.008
5	95.80	-1.06	2.00	0.007
6	95.80	-1.05	2.00	0.003
7	95.80	-1.05	2.01	0.012
8	95.80	-1.05	2.02	0.023
9	95.80	-1.05	2.03	0.033
10	95.80	-1.04	2.04	0.042
Average	95.80	-1.06	2.00	0.023

TABLE 7. Reproducibility unit 10255

Short term reproducibility for Spectrolino unit 10255, obtained 24 June 1998 at 23°C. This data shows how accurately a measurement can be repeated with the same instrument. The conditions were illuminant D₆₅ and the 2° standard observer.

3 Color-difference and hue angle evaluation

3.1 Color difference

The color-difference shall be evaluated according to the CIE 1994 (ΔL^* , ΔC^*_{ab} , ΔH^*_{ab}) color difference model with symbol ΔE^*_{94} and abbreviation CIE94. This evaluation is described in CIE Technical Report 116-1995 [5] and in the following we only mention the calculation steps necessary to compute the color difference value.

$$\Delta L^* = L^*_1 - L^*_2 \quad (\text{EQ 3})$$

$$C^*_{ab} = \sqrt{a^{*2} + b^{*2}} \quad (\text{EQ 4})$$

$$\Delta C^*_{ab} = C^*_{ab,1} - C^*_{ab,2} \quad (\text{EQ 5})$$

$$\Delta E^*_{ab} = \sqrt{(\Delta L^*)^2 + (\Delta a^*)^2 + (\Delta b^*)^2} \quad (\text{EQ 6})$$

$$\Delta H^*_{ab} = \sqrt{(\Delta E^*_{ab})^2 - (\Delta L^*)^2 - (\Delta C^*_{ab})^2} \quad (\text{EQ 7})$$

$$\Delta E^*_{94} = \sqrt{\left(\frac{\Delta L^*}{k_L \cdot S_L}\right)^2 + \left(\frac{\Delta C^*_{ab}}{k_C \cdot S_C}\right)^2 + \left(\frac{\Delta H^*_{ab}}{k_H \cdot S_H}\right)^2} \quad (\text{EQ 8})$$

with

$$\begin{aligned} S_L &= 1 \\ S_C &= 1 + 0.045 \cdot C^*_{ab} \\ S_H &= 1 + 0.015 \cdot C^*_{ab} \end{aligned} \quad (\text{EQ 9})$$

and

$$k_L = k_C = k_H = 1 \quad (\text{EQ 10})$$

In formulæ (EQ 9), the value for chroma is the one from the reference measurement stored in the reference table of the certification database (not the geometric mean of the two chroma values, as is customary).

3.2 Hue angle

In conformity with CIE Publication 15.2 [3], h_{ab} lies between 0° and 90° if a^* and b^* are both positive, between 90° and 180° if a^* is negative and b^* is posi-

tive, between 180° and 270° if a^* and b^* are both negative, and between 270° and 360° if a^* is positive and b^* is negative.

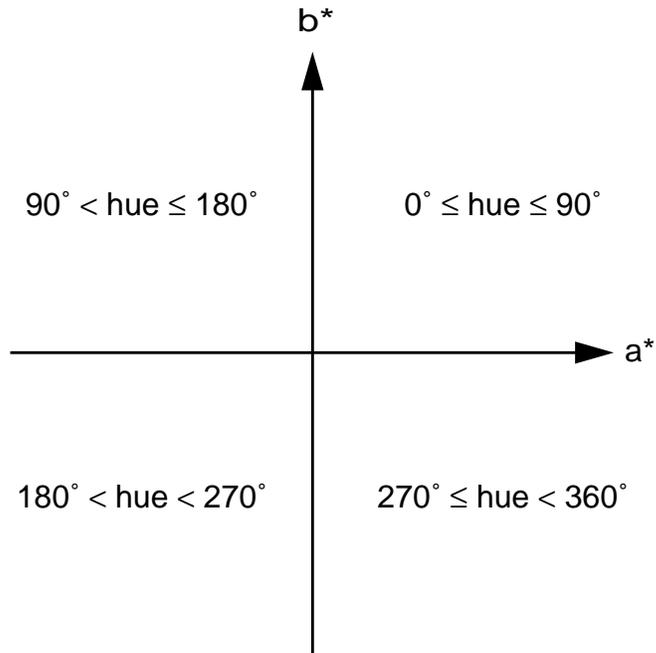


FIGURE 4. CIE convention for the hue angle value

4 Software

The software described in this report is only for demonstration purposes. Although it provides all the required functionality, for operational use custom software such as the KoolTool [11] is necessary, which integrates in the other operations software (e.g., the Grade Book). In this demonstration all program parameters, including spectrophotometer settings, database schemata and layouts can be changed by the user; in a production system these parameters would have to be locked to avoid unintended operator mistakes.

4.1 Spectrophotometer interface

In this demonstration, the spectrophotometer is accessed through the KeyWizard program from Gretag-Macbeth. The general settings are specified according to the viewing conditions under which the instrument is operated and certified, for example:

Condition	Value
Illuminant	D ₆₅
Observer angle	2°
Density standard	DIN
White base	Abs
Filter	D ₆₅
Measuring mode	Reflectance

TABLE 8. General settings for the KeyWizard

In the program settings, we recommend the following functions:

Function	Validation
Measuring conditions	required
CIE Lab	required
CIE LCh(ab)	required
Spectrum R	optional

TABLE 9. Program settings for the KeyWizard

We recommend to require the measuring conditions as a redundancy to test for operator error. The cylindrical coordinates are required for simplicity in the implementation; they are necessary to calculate the CIE94 color difference

and are more readily calculated by the spectrophotometer firmware than having to resort to an external function in our simple database.* Like the measuring conditions, also storing the colorimetric values in both Cartesian and cylindrical coordinates provides redundant information for the case of data corruption or operator error.

Recording the reflectance spectrum is not necessary, because the targeted application makes use only of colorimetric data. However, for the initial measurement of the Green reference tile for the relative certification we recommend to record the entire spectrum. If an instrument fails the certification procedure, the spectral data can be useful to quickly diagnose the problem with the instrument.

The choices for the separators are mandatory and cannot be changed for the database system used in this demonstration. This is different than the flexibility possible in a spreadsheet application or in a production database. The separators are as follows:

Program setting	Separator
block separator	none
function separator	tabulator
value separator	tabulator
label	none (do not label)

TABLE 10. Separators for the KeyWizard

Again, for production deployment we recommend the integration with a tool like the KoolTool for the user interface and a robust database like the Grade Book for persistent storage.

4.2 Database

4.2.1 What is a database?

A *database system* consists of a database and an administration system. The *database* is used to store *application data* and *descriptive data*, also called *metadata*. An example of application data is the record of a measurement, which contains fields such as the date, the analyst's name, the instrument's serial number, a specimen description, as well as the actual measurement result, i.e. the CIELAB values and the reflectance spectrum. An example of

* For the case it is really needed, there is a script to perform the calculation, see Figure 15 on page 36.

metadata is a list of fields, their type, and syntactic rules for their validation or computation.

The *administration system* usually consists of the software necessary to declare the metadata and manage the operations on the application data. In addition the system also comprises a language for defining, manipulating, and evaluating the data.

The metadata together with the relations among the data are called the database's *schema*.

There are four common ways to represent the real world data through a *data model* in a database system. In *hierarchical* and *network* database systems the data sets are represented as trees or general graphs, and the respective database languages have operations to navigate, manipulate, and operate on graphs. In *relational* database systems the data is represented as tables (homogeneous data records) and relations among tables; related data is looked up dynamically. Finally, in *object-oriented* database systems (OODBS) the data is represented as objects and the language is object oriented; database elements are not accessed directly, but through their class methods.

4.2.2 Database product used for the demonstration

Simple database packages for small applications have a graphical user interface (GUI) that allows the designers to define interactively the fields and the layout for the end-user GUI. In addition these packages have a scripting language to perform simple operations on the database. This scripting language makes it also possible to implement simple WWW hosted databases controlled by scripts embedded in HTML code generated dynamically by a servlet.

For this demonstration we chose FileMaker, which is very simple relational database system, yet sufficiently powerful for the application at hand. Since we are not developing an end-user application, we implemented the demonstration with the basic “lite” version of the package.

In FileMaker each table is implemented as a disk file (often incorrectly referred to as a database). The user interface to manipulate the records in the table is stored in the same file, as are the metadata and the scripts. When the file for a table is opened through the operating system, the user is presented with a window* to manipulate the last record accessed in the database. Related files are opened in iconic (Windows) or hidden (MacOS) form.

* Sporadically the window size is reset to a standard size at program execution. As a temporary fix, in this demonstration each opening window has a gray background rectangle; resize each window to the extent of this rectangle.

4.2.3 Description of the schema

The certificate database is organized in four tables: certificates, color references, measurements, and measurement sets. The certificate table is the main table and therefore all other tables can be accessed through the opening menu that is presented when this table is opened.

In a small laboratory that performs only sporadic measurements, the database can also be used to record measurements other than for the certification, e.g., for the quarterly Collaborative Test Service (CTS) results or individual measurements (see “Quarterly certification” on page 44). In general, for production use it is a good practice to keep only measurements related to instrument certification in this database; for other measurements it is recommended to clone the database* to keep separate things separate. In our demonstration database we have included a number of useful data† to simplify its distribution; an example is the data from the initial characterization of all tiles with our certified spectrophotometer described in Section 2.4 on page 20.

The metadata for the *certificate table* is fully described in Appendix I on page 65. The fields in this table include such information as: the certificate number, a link to the reference tile, a link to a set of measurements, the CIE94 error, and the pass/fail result.

The relations associated with this table are:

Relationship name	Relationship		Related table
	Key	Related key	
Reference SN	Color Reference	Serial No	colorreference
Measure Set	Certificate Number	Set	measureset
Measurement	Certificate Number	SetNumber	measurement

TABLE 11. Relations from the certificate table

* When cloning simple relational databases, it is necessary to rename the files and redeclare the relations and the scripts that open other tables, otherwise they will refer to the original tables and the database will be inconsistent. In an effort to make things simple for casual users, simple database packages implement tables as separate files with relative path names. When a database system opens a related table, it issues to the underlying operating system an “open” command with the table name. The operating system uses the path environment variable or a canonical directory enumeration order and opens the first file with the table’s name.

† There appears to be a small difference in binary files between Windows NT and 95. The database can be transferred from Windows NT to Windows 95, but not the other way around. The original database was created under Windows NT; to move the database from 95 to NT, reinstall the original database on NT, delete all records, export all records in the 95 database, move the files, and reimport the records in NT.

The metadata for the *color reference table* is fully described in Appendix II on page 67. The fields in this table include such information as the serial number and characterization date of a color reference tile and the colorimetric data for the various filters. This table does not use any related data.

The metadata for the *measurement table* is fully described in Appendix III on page 69. The fields in this table include such information as: the measurement conditions, the analyst, and the spectral and colorimetric data. To make the database useful for situations where the cylindrical CIELAB coordinates are not available, this table has a provision to calculate these values and insert them in the table (this can also be useful to test a coordinate system transformation routine). This table does not use any related data.

The metadata for the *measurement set table* is fully described in Appendix IV on page 73. It aggregates a number of related measurements and contains statistical fields for the average and standard deviation in the set. This table implements the user interface for data collection. The relation associated with this table is:

Relationship name	Relationship		Related table
	Key	Related key	
Measurement	Certificate Number	SetNumber	measurement

TABLE 12. Relation from the measurement set table

4.2.4 Description of the user interfaces

In this section we show the various views of the certificate database. The views are grouped by relational table, since this is the way they are implemented in our demonstration system. In the subsequent sections on the various applications of the database, the views will be discussed briefly in the order they are accessed by users. For each view we just mention briefly some salient features. The best way to get accustomed with the database is to explore it while looking up the field definitions in the appendices of this report.

One problem creating cross-platform graphical user interfaces is the availability of fonts. This database was created in Windows NT 4.0, where the Gill Sans typeface is a standard component of the distribution. It was only in the final testing that we discovered this font is not part of the Windows 95 distribution, where it gets substituted by the Helvetica typeface. Since the Helvetica character boxes are wider than Gill Sans character boxes, in some views the graphical elements overlap when the database is used on a Windows 95 system.

The main window for the database is the *Menu* view in the *certification* table shown in Fig. 5. It has buttons for the certification process, to access all tables, and to quit the application. Normally, when users perform a new task, they will come back to this window and start from here.



FIGURE 5. Table: certification. View: Menu

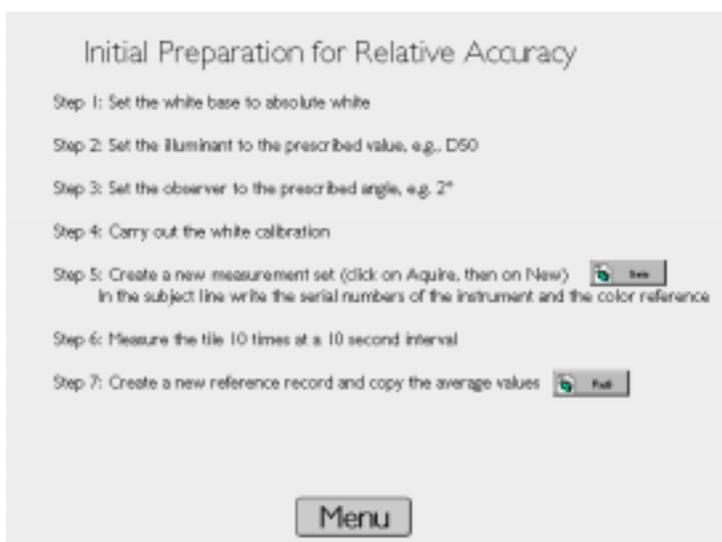


FIGURE 6. Table: certification. View: Preparation

The first button in this view is labelled *Initial* and brings the user to the view *Preparation* shown in Fig. 6, where the relative certification is set up. It is used only once when a new spectrophotometer is added to the program and stores the initial spectral and colorimetric data of a color reference tile for that site or instrument. The procedural steps are detailed in Section 5.5 on page 48. This view has two buttons: *Sets* to navigate to the data acquisition

view of the measurement set and *Refs* to the *reference table* where the newly obtained data can be recorded. The menu button at the bottom takes the user back to the main view shown in Fig. 5 above.

The screenshot shows the 'Accuracy Check' interface in 'Test' mode. At the top, the title 'Accuracy Check' is followed by a value '22'. Below this is a 'New' button and a date/time field 'Fri, Oct 16, 1998 16:32:42'. The interface is divided into nine steps:

- Step 1: Click to create a new record (New button)
- Step 2: Enter the filter on the spectrophotometer (D65, OK button)
- Step 3: Enter the serial number of the color reference (221-D65-2, View button)
- Step 4: Carry out the white calibration and enter the temperature (22.9°C, OK button)
- Step 5: Check your color reference for cleanliness and place it in the receptacle
- Step 6: In the line below write the serial numbers of the instrument and the color reference (A white box contains: 10255, Q881 Spectralno 3.257.10255, green reference 221)
- Step 7: Measure the tile 10 times waiting 10 seconds between measurements (Go button, (Click on Acquire if necessary))
- Step 8: Click in the next two fields to refresh them (Viewing Angle: 2°, OK; Base: ABS, OK; Beam: D65, OK; Bead on: 124, View button)
- Step 9: Print a certificate and file it (Print button)

 At the bottom, the 'Result of the instrument check' is displayed as 'E94 = 0.26 Pass'. A 'Menu' button is located at the very bottom of the interface.

FIGURE 7. Table: certification. View: Test

performs a number of consistency checks by requiring the specification of redundant data and comparing it with the expected data in the appropriate related record in the color reference table. For each consistency check there is an individual field that displays the status, so that in case of an operator error is easy to pin-point the problem and resolve it.

When the possible values for a field are restricted, the user is presented with a pop-up menu. In particular, when the user proceeds into the field for the color reference, the database system looks up the related color reference table and dynamically constructs a list of the available search keys (therefore, it is recommended not to distribute unnecessary reference tile data). This method is necessary not only as a convenience, but also because during an accuracy check the user cannot jump to a related color reference table using the *View* button; at this point in the process, the new record cannot be committed because only a few fields have been entered. The *View* button is part of the interface because it can be convenient when the user is browsing the accuracy check.

The white rectangle in step 6 (Fig. 7) is a portal to a related record in the measurement set database. If the user is creating a new record, then by typing

data into a field in the portal automatically created a new record in the measurement set database.

The *View* button at the lower right of the *Test* view (after “Based on”) takes the user to the measurement on which the consistency checks are based. If any field is flagged as wrong, then this button allows the user to quickly determine the actual value returned by the spectrophotometer and compared it with the expected value.

Since the database system normally computes the calculated fields when a new record is created, the result fields contain bogus values. By clicking in the field the user can trigger the recalculation of the values.

The *Print* button at the bottom of the *Test* view actually prints the current record using the *Certificate* view shown in Fig. 8. This view must conform to the particular ISO 9001 procedures in use at the site, i.e., it is necessary to edit the layout of this view to bring it in conformance with the adopted documentation rules.

The first two buttons at the bottom of the certificate view can be used to browse through all certificates in the database. The *Print* button is used to generate a hardcopy of the currently displayed certificate. These three buttons are on this view because when users click on the *Certs* button on the main view (Fig. 5) to browse the certificates, they are taken to this view.

The data on the color reference tiles is in the *colorreference* table. Most user will never access this table directly; the only ones to add data to this table are analysts putting in service a instrument and performing the initial color tile characterization for that instrument (see “Initial characterization of the Green tile” on page 48). Note that the system verifies that the temperature during certification is in the range specified in the *colorreference* table.

Calibration Certificate 22 Absolute
Spectrophotometer S/N 10255
Subject: GBB's Spectrolino 3257.10255, green reference 221

Color Reference Field No.	221-D65-2	Color	Green
Date	Friday, October 16, 1998	Time	16:52:42
Analyst	Giordano Beretta	Ambient Temp.	22.9°C
White Tile	ABS	Chamber Path	2"
Standard	D65	Filter	D65

	L*	a*	b*	C*	h
Measurement	53.31	-34.79	17.11	38.77	153.81
Reference	53.24	-35.03	16.78	38.84	154.41
Difference	-0.07	-0.24	-0.33	0.07	0.40

CIE94 Error 0.26 Pass

Back Forward Print Menu

FIGURE 8. Table: certification. View: Certificate

FIGURE 9. Table: colorreference. View: Main

from the instructions in Section 5.5, “Initial characterization of the Green tile,” on page 48. The temperature tolerance prescribes the interval in which the ambient temperature must lie when the measurement is made.

Color-Reference Database

Reference	III	Cbr.	L*	No Filter			h	L*	Pol Filter			L*	D65 Filter				
				a*	b*	C*			a*	b*	C*		a*	b*	C*	h	
221-A-2	A	2°	50.79	-27.56	8.53	28.85	162.80	51.28	-28.48	8.71	29.78	162.99	50.79	-27.56	8.53	28.85	162.80
221-C-2	C	2°	52.96	-34.48	16.76	38.33	154.08	53.52	-35.59	17.22	39.54	154.18	52.96	-34.48	16.76	38.33	154.08
221-D45-2	D45	2°	53.24	-35.03	16.78	38.84	154.41	53.81	-36.16	17.24	40.06	154.51	53.24	-35.03	16.78	38.84	154.41
221-D50-2	D50	2°	52.76	-33.06	14.73	36.19	155.98	53.31	-34.13	15.12	37.33	156.10	52.76	-33.06	14.73	36.19	155.98
221-A-10	A	10°	50.92	-25.89	10.94	28.11	157.09	51.41	-26.76	11.21	29.02	157.27	50.92	-25.89	10.94	28.11	157.09
221-C-10	C	10°	52.94	-32.32	18.45	37.22	150.28	53.51	-33.38	18.99	38.41	150.37	52.94	-32.32	18.45	37.22	150.28
221-D45-10	D45	10°	53.23	-32.75	18.59	37.66	150.42	53.80	-33.82	19.12	38.85	150.51	53.23	-32.75	18.59	37.66	150.42
221-D50-10	D50	10°	52.81	-30.92	16.73	35.16	151.59	53.27	-31.94	17.20	36.28	151.70	52.81	-30.92	16.73	35.16	151.59

FIGURE 10. Table: colorreference. View: List

Fig. 9 shows the main view into the color reference table. At the top is a row of buttons to create a new record, to search the database, a pair of buttons to browse the found* records (note the current record number between these two buttons), to sort all found records by any field, to print the contents, and a close button to close this table. The various fields are obvious

The *Print* button on the main view triggers a script that uses a hidden view to generate a compact printed compilation of the currently found records. This view is shown in Fig. 10 and fits the essential data stored in each record on a single line.

To encourage averaging several measurements for each experiment, we have designed a summarizing table whose records are related to all measurements in a a set for each record. Other than the relation, this table essentially contains only the statistical parameters for the set, as can be seen in Appendix IV on page 73. The certificates are always based on a set, not on an individual measurement. We encourage to average over at least three measurements, but not more than ten. The number three comes from personal experience with the instruments and the number ten comes from ASTM standard practice E 1345-90.

The measurement set table — which can be accessed from the main view of the database shown in Figure 5 on page 30 by clicking on the *Sets* button — has two distinct views for data acquisition and to evaluate the measurements in a set. Fig. 11 on the next page shows the acquisition view. At the bottom, the view contains detailed instructions on how to make measurements with the KeyWizard software from Gretag-Macbeth. These instructions are more

* Perform the *Find All* command in the *Select* menu to browse the entire database.

generic than for the purposes describes in this report, so this portion of the database system can be easily re-purposed for other application without requiring any editorial changes.

The temperature tolerance in this table is different from that in the color reference table. The tolerance in this table is the one of the thermometer used when the measurement is made, for example 0.7°C or 1°C in the case of our thermometer. The temperature tolerance in the color reference table instead prescribes the interval in which temperature at measurement time must by contained and depends on thermochromism.

The central portion in the acquisition view (Fig. 11) is a portal containing up to ten related records from the measurement table. The first column is a read-only running record number included for orientation purposes. When the cursor is placed in the first field of a blank column, a new related measurement record is automatically created. The intention is that the measurement record is entered with the aid of a program, but the data can also be typed in manually.

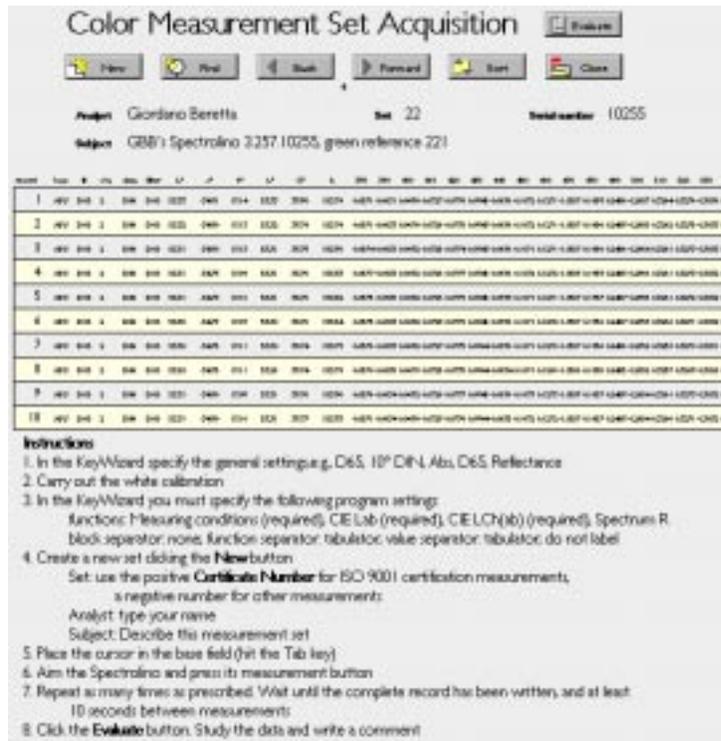


FIGURE 11. Table: measureset. View: Acquisition

The first group of fields in each row of the portal holds the measurement conditions. This redundant data is collected for integrity check purposes: it can be used to verify that the data returned by the spectrophotometer is for the viewing conditions intended by the analyst and specified in the record relating to each measurement set (e.g., in the certificate database).

The second group of fields hold the colorimetric data, both in Cartesian and in cylindrical CIELAB coordinates. Finally, there are optional fields for recording the spectral reflectance data.

When the last measurement has been performed, the analyst will click on the *Evaluate* button at the top right of the acquisition view, just after the title. This will switch the window to the evaluation view, shown in Fig. 12, which

presents the colorimetric data in the related record and the statistical information.

The screenshot shows the 'Color Measurement Set Evaluation' interface. At the top, there are navigation buttons: Find, Back, Forward, Sort, Print, and Close. Below these are input fields for 'Analyst' (Giordano Baretta), 'Age' (22), and 'Serial number' (10255). The 'Subject' field contains 'G88's Spectrolno 3.257.10255, green reference 221'. The main part of the interface is a table with columns: record, time, #, size, filter, filter, L*, a*, b*, L*, C*, h, and match. The table contains 10 rows of data. Below the table, there is a 'summary' section with values for L*, a*, b*, L*, C*, and h. At the bottom, there is a 'standard deviation' section and a 'comments' text area.

record	time	#	size	filter	filter	L*	a*	b*	L*	C*	h	match
4	485	D65	2"	DF4	D65	50.02	-04.01	17.14	50.02	30.86	150.79	41875
485	D65	2"	DF4	D65	50.02	-04.00	17.13	50.02	30.79	150.79	41805	
485	D65	2"	DF4	D65	50.01	-04.00	17.13	50.01	30.76	150.80	41894	
485	D65	2"	DF4	D65	50.01	-04.79	17.09	50.01	30.76	150.82	41104	
485	D65	2"	DF4	D65	50.01	-04.79	17.10	50.01	30.76	150.82	41115	
485	D65	2"	DF4	D65	50.00	-04.79	17.09	50.00	30.76	150.84	41125	
485	D65	2"	DF4	D65	50.00	-04.75	17.11	50.00	30.74	150.79	41135	
485	D65	2"	DF4	D65	50.29	-04.75	17.11	50.29	30.74	150.79	41145	
485	D65	2"	DF4	D65	50.01	-04.00	17.08	50.01	30.76	150.86	41156	
485	D65	2"	DF4	D65	50.01	-04.00	17.10	50.01	30.77	150.82	41165	

summary: L* 50.01, a* -04.79, b* 17.11, L* 50.77, C* 150.81
 standard deviation: L* 0.01, a* 0.02, b* 0.02, L* 0.02, h 0.01
 comments: [text area]

FIGURE 12. Table: measureset. View: Evaluation

In the portal, the last column (Fig. 12) contains the measurement record's time stamp in seconds. In the case of data entered programmatically, this allows the analyst to verify that the minimal wait time between measurements has been respected; this is important when measuring ceramic tiles with a significant thermochromism effect.

At the bottom of the view there is a scrollable text field to enter free text comments. It should be used to record any unusual situations or comments on the

measurement set. It is always better to have too many rather than too few comments; performing measurements is a tedious task and minds tend to wander, rendering it difficult to produce good recollections of what might have happened during an unusual measurement.

Between the portal and the comment field are the fields with the statistical data. This data is used in the certificate table to perform the accuracy check. When a new color reference record is created, this data should be transferred manually in the newly created record in that database.

Last but not least are the views in the measurement table. This table can be accessed from the main view of the database shown in Figure 5 on page 30 by clicking on the *Browse* button. The main view *Colorimetry* is shown in Fig. 13. The various fields have been described in the discussion of the measurement

The screenshot shows the 'Color Measurement Database' interface. At the top, there are navigation buttons: New, Find, Back, Forward, Sort, Print, and Close. Below these are input fields for 'Material' (ABS), 'Method' (D65), 'Observer' (10°), 'Geometry' (DF4), and 'Filter' (D65). The 'Measurement' field contains '95', 'Set' contains '-106 D61', and 'Date' contains 'Fri, Oct 16, 1998'. The 'Time' field contains '16:41:30'. Below these are fields for 'L*' (52.14), 'a*' (-9.58), 'b*' (-6.95), 'L*' (52.14), 'C*' (11.94), and 'h' (215.95). At the bottom, there is a 'Comment' text area.

Material: ABS, Method: D65, Observer: 10°, Geometry: DF4, Filter: D65
 Measurement: 95, Set: -106 D61, Date: Fri, Oct 16, 1998, Time: 16:41:30
 L*: 52.14, a*: -9.58, b*: -6.95, L*: 52.14, C*: 11.94, h: 215.95
 Comment: [text area]

FIGURE 13. Table: measurement. View: Colorimetry

set table. Of note is a text field to record comments on a specific measurement. As we noted on the previous page, analysts should be encouraged to make good use of this field.

For example, if there is a problem with a measurement and it is decided to exclude it from a measurement set, the measurement itself should be kept in the database for further reference. To exclude the measurement from the set, it is sufficient to alter the relating field, which in this case is the set field of the color measurement record, to a new value not occurring in any other set (there has to be a policy for this).

When a printed document of a number of measurements is required, this can be generated by first performing a find operation, then sorting the resulting records, and finally clicking on the *Print* command. This command uses the *List* view shown in Fig. 14 to generate a compact document. This view can also

ID	Document	C*	a*	b*	Comment
-106 D81 94		52.09	-9.59	-6.98	11.86 216.04
-106 D81 95		52.14	-9.58	-6.95	11.84 215.95
-106 D81 96		52.17	-9.58	-6.92	11.82 215.84
-106 D81 97		52.24	-9.58	-6.90	11.80 215.76
-106 D81 98		52.05	-9.59	-6.98	11.86 216.03
-106 D81 99		52.20	-9.55	-6.89	11.78 215.83
-106 D81 100		52.13	-9.58	-6.93	11.82 215.87
-106 D81 101		52.08	-9.59	-6.93	11.83 215.85
-106 D81 102		52.05	-9.57	-6.96	11.83 216.04
-106 D81 103		52.10	-9.57	-6.95	11.83 215.97
-106 D82 104		53.22	-9.55	-6.92	11.80 215.91
-106 D82 105		53.17	-9.55	-6.91	11.79 215.90

FIGURE 14. Table: measurement. View: List

be obtained for on-line browsing; to examine a particular record, click in any field of that record and click on the *Show Detail* button, which brings up that record in the *Colorimetry* view (Fig. 13).

	L*	C*	h
Current	52.14	11.84	215.95
Recomputed	52.14	11.84	215.96

FIGURE 15. Table: measurement. View: Correlates

Both the *Colorimetry* view and the *List* view have a button labelled *Recompute*. Clicking on it brings the user to a special view to recompute the correlates. This view is shown in Fig. 15. Sometimes the cylindrical coordinate values for a measurement are not readily available. How-

ever, this database requires the chroma and hue correlates. The solution is to temporarily enter bogus values in these two fields. Then the analyst can switch to this recalculation view.

In this view the CIELAB coordinates are presented twice: as recorded in the database, and as computed from the L^* , a^* , b^* coordinate values. When the user clicks on the *Replace* button, the recorded values are replaced by the

recomputed values. The number at the right of the *Replace* button indicates the serial number of the measurement. The serial number is labelled *Measurement* in the *Colorimetry* view (see Figure 13 on page 35).

In a final note, reflect on the significance of relations in a relational database. There is a number of tables and relations are defined dynamically by comparing search keys defined in a relation. In the application described in this report, related records are often created automatically. If a data entry mistake is made and needs to be corrected, then it is necessary to verify whether the corrected field is a search key.

The search keys are listed in Section 4.2.3, “Description of the schema,” on page 28. If the corrected field is such a search key, the records in both tables must be edited, otherwise the relations are broken.

5 Procedures

5.1 Overview

Each of the sub-sections in this section is a self-contained step-by-step description of a qualification procedure. This sub-section is an overview outlining how the various procedures fit together. It shall also clarify why the procedures have been defined and what benefits they provide. We generally follow the recommendations of Christopher Burgess [3] and of Gretag-Macbeth [10].

It was not so many years ago, that the standard instrumentation for color measurements consisted of a spectroradiometer, a set lamps, and a BaSO₄ (barium sulfate) cake. The instrument's sensor was cooled with a Peltier element, which caused condensation, requiring a silicagel cake in the instrument that had to be baked periodically in an oven. A careful log had to be maintained on the lamp's "on" time so they could be renewed when a certain usage time had past. Finally, the barium sulfate cake had to be inspected carefully and sanded when necessary.

Setting up the instruments was also a challenge, because the geometry had to be calibrated for each measurement session. The instruments were connected to a minicomputer running simple software that could compute the colorimetric quantities and sometimes could produce simple diagrams or histograms.

Today's spectrophotometers are simpler to use than the remote controller for a television set, are completely self-contained, ruggedized, and have a sophisticated embedded software system that can compute a plethora of quantities, evaluate them statistically, and plot them.

Unfortunately this can mislead users in thinking that measuring color is as easy as flipping a light switch. The fundamental physics on which color measurements are based have not changed; color has not become easier to measure, and modern instruments merely provide more comfort and convenience.

The main area of concern in practical colorimetry is the validation of color measurements. As outlined by Burgess, this consists of the following points:

- the fitness for purpose of the spectrophotometer for the task
- demonstrable compliance with the manufacturer's performance criteria
- demonstrable compliance with established standards and practices
- documented evidence for continued operability and data integrity

These requirements for validation are met with the qualifications for design, installation, operation, and performance. These qualification steps are summarized in the following sections.

5.1.1 Design qualification

The design qualification is a *specification* for the instrument:

- photometric requirements
- environmental conditions
- sample presentation
- data acquisition and presentation needs
- operability factors; health & safety issues
- cost/benefit analysis

The photometric requirements include such parameters as precision, accuracy, uniformity with respect to color, aperture, reading frequency, and geometry. Color metrology is still a field of active study in the basic sciences; the colorimetric calculations are still being improved considerably and standardization bodies such as the ASTM, CIE, and ISO/IEC regularly update the recommended procedures. The instrument should be current with the latest progress in the technology, such as color matching function interpolation and color difference evaluation.

The environmental conditions cover parameters such as operational limits for temperature and humidity, ruggedness, orientation in space, electrical supply stability, and the generation of heat and noise by the instrument.

The sample presentation refers to the instrument's ability to reliably measure the sample. This is not limited to the physical size of the sample, but also covers considerations such as the ability to measure liquids, wet samples, cockled samples, and to select the appropriate backing. If the sample is ink on a substrate, the substrate can be opaque, translucent, or transparent; it can be glossy or opaque.

The data acquisition needs usually are a serial RS-232 or USB connection and a full specification of the protocol. In the past years there has been increased demand for support of the http data transfer protocol. Depending on the user's skills and time, there are varying demands on a client implementation of the protocol, which can range from a simple driver to a class library or a specialized application.

The operability factors include documentation and training. Color is an illusion and colorimetry is the art to predict an illusion from a physical measurement. Each analyst using the instrument must be thoroughly trained in the

basics of colorimetry and in the operation of the equipment. Refresher courses must be given periodically, and a supervisor must be responsible for the analyst's training.

5.1.2 *Installation qualification*

The second qualification is the compliance with the above specification, i.e., does the instrument work the way the manufacturer claims it should? This reports provides methods and guidance for the following qualification steps:

- written test protocol with acceptance criteria
- certification from the installation engineer
- full written records
- adequate documentation and manuals
- health and safety information from manufacturer

Regardless of their exterior ruggedness and environmental specifications, internally spectroradiometers are very delicate instruments that should never be opened or disassembled.

The installation engineer has also to assure that the analysts using the instrument fully understand the operation of the instrument and the procedures. Especially in the collection of historical data for process control, meticulous adherence to procedures and accurate records are essential for the ability to perform time series analyses.

When several sites use the same process, then the procedures must be the same, so it is possible to compare the data.

5.1.3 *Operational qualification*

The operability items ensure that the instrument works for the specific applications:

- training for staff
- testing protocols for standards
- testing protocols for subsystems
- calibration procedure and defined test methods and procedures
- challenging the system with known standards
- record what is done and why it is done
- ensure data transfer integrity to external software

In essence, the operational qualification requires that the procedures in this report be followed and that the described tools be used. If the application changes, then this report must be revised as necessary, historical data must be safeguarded as necessary, and the analysts must be retrained.

The major immediate change is to port the database aspect from the simple demonstration application described in this report to a database that is fully integrated with the existing data storage and management system.

Another major change will be to upgrade the procedures to full ISO 9001 compliance. Such a compliance does not only facilitate the business transactions with suppliers and customers. It also entails a critical review of all procedures and eventually leads to improved product quality, higher manufacturing yields, and improved profits.

Accumulating data by itself does not serve any useful purpose. The linchpin of the process is the design of data analysis algorithms that allow the data's use to provide a feedback mechanism in the manufacturing line to keep the process within specified tolerances. The quality of the collected data directly determines the statistical confidence intervals for the correlation between col-orimetric data and manufacturing drifts.

Once sufficient historical data is available and data analysis algorithms are designed, the tolerances described in this report will have to be reconsidered. This reconsideration will produce a different set of qualifications.

5.1.4 Performance qualification

The performance qualification regulates the ongoing compliance, ensuring that the instrument continues to work in the intended manner. The items in this qualification include:

- regular service program
- performance monitoring with warning and action limits
- individual log books and databases for spectrophotometers
- regular peer review
- simple change procedure

The essence of this report is to define a good set of procedures for the performance qualification, and the following sections will describe each procedure in detail. These procedures ensure that each instrument performs within certain limits and assures the validity of the data generated.

While the database designed for this demonstration deals only with measurements per se, there should also be a database table to log all other events that impact the data, such as

- lamp changes
- problems and service calls
- instrument substitutions
- firmware upgrades
- optical upgrades
- procedure changes
- manufacturing line changes impacting the colorimetry
- manufactured good changes (e.g., ink formulation)
- environmental changes
- personnel changes
- peer reviews

With the last item we imply that each site is visited on a regular basis and the procedures and data be reviewed by a peer or a consultant. This ensures that the data of the various sites is fully exchangeable and the sites do not drift away from each other.

Changes in ink formulation are important because they can lead to metameric matches. Metameric matches require accuracy, i.e., absolute certification, while the procedures described in this report are based on relative certification, i.e., only precision is certified. This aspect may have to be reconsidered.

The log should not only exist digitally in a database, but should also exist in printed form, because it is more convenient and robust to use during peer reviews. For this reason, when we designed our demonstration database we took care to design a printable form layout of each record, allowing physical collection in a log book.

5.2 White calibration

The white calibration must be performed when one of the following events has occurred:

- begin a new measurement session
- end of a pause
- 10 consecutive measurements have been performed
- the ambient temperature has changed by more than 5°C

Frequent white calibration is important in the case of process control, because a drift in the instrument might be interpreted as a drift in the process. When an automatic stage such as the SpectroScan is used, the controller software must be programmed to perform the periodic calibration automatically. With the SpectroScan, the reference tiles should be lodged permanently in one of the apposite receptacles in the stage and the entire set-up should be shielded from direct sun light.

When the instrument is used manually, the white calibration must be performed in the following steps:

1. set the white reference parameter to “absolute”
2. set the filter wheel to the desired position (SPM-100) or apply the required filter (Spectrolino)
3. check the white reference for cleanliness and place it on an even surface; for the Spectrolino, always insert the reference tile in the special calibration base (see Figure 2 on page 18)
4. adjust the spectrophotometer to the white reference and initiate the white calibration

Using the calibration plate (9) and ensuring the instrument fits perfectly in the positioning pins (6) is important. Ceramic tiles are never uniform and the purpose of the base is to ensure you always measure the same spot of the tile. For this reason it is necessary to remove the positioning foot (see Fig. 3) from the Spectrolino and measure directly on the calibration plate holding the clip (7) with the white reference. For details, see “Construction” on page 18.

If you have several instruments, make sure that the serial number on the instrument’s identification plate is the same as that on the white reference (5).

5.3 Quarterly certification

Instrument error is not the only source of incorrect measurements. More often the error is in the measurement procedure. This can have many causes, such as documentation error, personnel changes, etc. The best insurance against this type of problems is to participate in the *CTS Collaborative Reference Program for Color and Appearance*.

5.3.1 Background

Collaborative Testing Services Inc. (CTS) is an organization that conducts interlaboratory tests. In such a test, the performance of a laboratory is not compared to an absolute reference. Instead, multivariate comparative statistical methods developed in conjunction with the National Institute of Standards and Technology (NIST) are used to gauge performance.

With these techniques a consensus value among a large number of participating laboratories using a variety of instruments and methods is determined. The values of each laboratory are then compared with this consensus value. Such an analysis is also known as a “real world” analysis.

The concept of formalized, large-scale interlaboratory testing was developed in the late 1960s by NIST (then known as the National Bureau of Standards, NBS). In the mid 1970s, full responsibility for the laboratory proficiency testing program was transferred to CTS. CTS maintains compliance with *ISO Guide 43-1996: Development and Operation of Laboratory Proficiency Testing*.

It is important to understand that proficiency testing does not gauge the performance of an instrument. Rather, as the name implies, it assesses the proficiency of a laboratory.

5.3.2 Color and color difference

Analysts measure a set of three opaque color paint chips made by Munsell Color, Macbeth Division. The colors are selected from throughout the full color spectrum. The chips consist of a metameric and nonmetameric match with small color differences.

The measurements are performed according to ASTM E 1349 immediately after opening the sealed moisture-free barrier bag containing the specimens. Each specimen is backed with the other specimens when making measurements.* Each specimen is measured twice, rotating the specimen 90° for the second measurement. This latter step is very important for the Gretag instruments, because they are based on 45°/0° geometry, which is susceptible to polarization.

When you receive the report with the results, use your lab code to find the data you have contributed. You will find one of two data flags: 0 or X. If the data flag is 0, your results are consistent with those of the other participants and you may proceed. If the data flag is X, stop work immediately and consult an expert to review your data and your testing procedure. This review will consist of four steps, as delineated in the decision tree in Fig. 16.

In the first step repeat the performance test and verify that you can approximately reproduce the results in the report. With this you check for gross errors, such as using the paint chips from an old test or measuring the chips from the back side. We strongly recommend a peer review if this happened.

In the second step perform the certification procedure with your Green reference tile. If this test fails, you probably have a defective instrument and

* Be careful not to tilt the instrument!

should repeat the CTS test with the backup instrument. If you would have passed the test with the backup instrument, follow the procedure to replace a defective instrument (not described in this document).

If the certification with your reference tile passes, proceed as follows with step three. Request the panic reference tile (see Section 2.2.1 on page 15) and use the certification database to perform an absolute certification. If this certification passes, you made a procedural error in performing the CTS test. You should obtain training in ASTM procedure E 1349–90 and the CTS test in particular. All procedures in your laboratory should be reviewed by an expert.

Step four. If the absolute certification fails but the relative certification failed, your laboratory is set up incorrectly and an expert should review all operations.

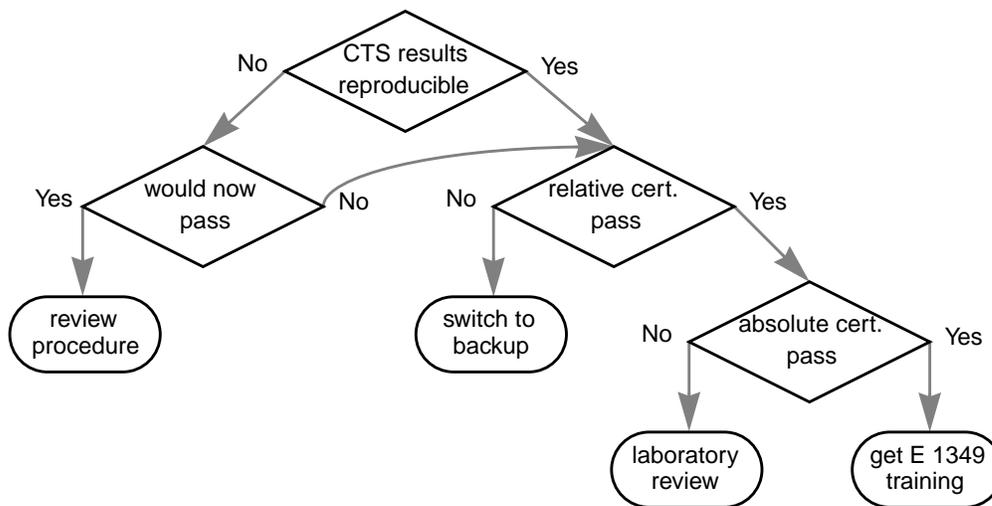


FIGURE 16. Decision tree in case of failure of the CTS test

Returning to the CTS report, after reviewing the data flag, examine the column labelled ΔE^* . If the result is followed by an * your ΔE is greater than 2 but less than 3 standard deviations from the grand mean. You should review your procedure and perform the relative certification procedure to establish if you can continue working.

If the result is followed by an X, your ΔE is greater than 3 standard deviations from the grand mean. In this case you should follow the decision tree in Fig. 16.

5.3.3 Spectrophotometric analysis

In this test analysts report the reflectance data at 16 selected wavelengths in the 400–700 nanometer range (i.e., at 20 nm intervals) on one of the opaque color chips. The same backing rule as in the previous test is followed. Also in this test it is important to repeat the measurement after rotating the specimen by 90° because of polarization in the instrument.

The results are evaluated as in the color & color difference test by examining the data flag and the procedure explained in the previous section can be followed. The reflectance values at single wavelengths can also be flagged. Since our intended use of the spectrophotometer is just colorimetry, a few errors in the reflectance values are not a cause for alarm.

5.3.4 Useful aids

One of the advantages of the CTS program is that it takes only a few minutes each quarter to complete. There are a few tools to make this work even easier.

Copying the results from the screen into the CTS form is tedious and can introduce errors. If you have the KeyWizard, download a convenient Acrobat form from <http://chroma.hpl.hp.com/Acrobat/Notebook/Colorimetry/cts.pdf> (if you are viewing this document on-line, the link is active and you can click on it). JavaScript is used to calculate the data required in the CTS form from the data provided by the SMP-100 or Spectrolino.

If you have an older version of the Acrobat Reader, you may have to download the free Acrobat Forms Fill-in Plug-in 3.5 Update from the Adobe Web site. This two-page form will automatically fill out the CTS form, which can be printed and sent to CTS.

If you have Acrobat Exchange, you can save the blank form after you have edited the laboratory number and analyst name. You can also save the completed form for future retrieval or to submit it to a document repository. In any case, keep a hard copy in the log book.

If you want to further examine the data, there is an Excel spreadsheet to tabulate the data, plot the spectra, and compute the resultant ΔE of your laboratory. This spreadsheet is available from <http://chroma.hpl.hp.com/color/CTS1098D65.xls>.

Finally, the historical CTS data for Spectrolino serial number 10255 in Palo Alto can be found at <http://chroma.hpl.hp.com/color/cts.html>.

5.4 Yearly calibration

Once a year the instrument should be sent to the manufacturer for the following operations:

- install firmware and hardware updates (this is to ensure that all instruments are comparable and interchangeable)
- measure the full set of color ceramic tiles, each mounted in the calibration base
- compute the error compared to an absolute instrument traceable according to ISO 9001
- compute the error compared to the average of 10 instruments of the same construction
- measure 10 times the white tile to assess the short term repeatability

The manufacturer will return the instrument with a calibration certificate that must be stored in the document repository. An example of the yearly calibration certificate can be found on the intranet at <http://chroma.hpl.hp.com/color/absCal98.html>. This is the same data as in Section 2.4, “Spectrophotometer,” on page 20.

5.5 Initial characterization of the Green tile

We have discussed earlier (Section 2.1.2 on page 13) the distinction between absolute and relative certification. For the relative certification, when you receive a new spectrophotometer you must first determine the aim values of the green tile for this instrument. We refer to this preparation as the *initial characterization*.

Since the color reference tile has a life time of 5 years, we recommend to collect the data for a number of illuminants and filters, because it is possible that during such a long period of time the viewing conditions chosen as a Corporate standard can change. We suggest to characterize at least for two illuminants, D₅₀ and D₆₅, and two filter settings, no filter (U for unfiltered) and D₆₅ filter. The observer angle is 2° and the color space is CIELAB.

Although it is sufficient to record the L^* , a^* , and b^* coordinate values, for convenience we require to record also the correlates for chroma and hue. We suggest to also keep a record of the reflectance spectrum of the reference tile measured with the various filters. The benefit of recording the entire spectrum is with the CTS test (see Section 5.3.3 on page 47). When there are several flagged values, it is a good idea to compare the values at those wavelength for the color reference with the initial values. Finally, the spectral data can be useful for diagnostic purposes when an instrument fails.

The steps are similar to those discussed earlier for the white calibration. In the demonstration database, select *Set up relative certification* for an on-line guide.

1. set the white reference parameter to “absolute”
2. set the first illuminant
3. set the observer angle
4. carry out the white calibration as described in Section 5.2 on page 43
5. create a new measurement set in the certification database
6. measure the color reference tile 10 times at a 10 second interval
7. record the color coordinates in the *colorreference* table of the database
8. repeat for each filter and illuminant
9. back up all database files

In step 6, we recommend to use the *Color Measurement Set Acquisition* view in the *measureset* table of the database. If you cannot make 10 measurements, we encourage to make at least 3 measurements at 10 second intervals and to enter the average values in the color reference table. The average values are displayed in the evaluation view of the measurement set table.

There is no command to transfer by program the color coordinates from the measurement set table to the color reference table. This is intentional, so the color reference table is a database by itself that can be easily redistributed within the Company any time it is necessary. For example, this table could be maintained in a central location and made available on the intranet through a servlet. Depending on the platform, the color coordinates can be transferred from one table to another using copy & paste or drag & drop.

In the color reference database, the part number for the clip with the green tile that fits in the Spectrolino calibration plate is 36.65.25. It is important to record the serial number because even if the ceramic tiles are from the same batch, the uniformity is not perfect.

Always record the current ambient temperature. If the tile is stored in a closed container, the container should be opened half an hour prior to use. The temperature tolerance depends on the effect of thermochromism (see Section 6.4 on page 55) for the particular tile and the planned tolerance for the certification.

For example, the Green tile in the BCRA CCS II standard exhibits a change of $0.68 \Delta E^*_{ab}$ units when the temperature changes by 10°C , the measurement geometry is spinc $0^\circ/t$, and the illuminant is D_{65} with the CIE 10° observer [8]. A tolerance of $\pm 2^\circ\text{C}$ in this case translates to a measurement uncertainty of $0.68 * 0.4 = 0.27$ CIELAB units. This is a large error in the case of process con-

trol, but it seems to be realistic in the real world. If the temperature excursion can be reduced, then a smaller interval should be specified for the temperature tolerance. The raw data in Table 16 on page 57 should be used to compute the colorimetric differences for the particular instrument geometry and viewing conditions prescribed.

Conceptually, we treat a reference tile as a different color reference for each viewing condition. In the database we store a separate record for each combination of illuminant and observer angle. Since the serial number must be a unique identifier, we have followed the convention of creating a serial number by combining the serial number on the clip label (see Figure 2 on page 18, item 5) with the illuminant and the observer angle.

For example, the colorimetric data for reference tile 221 measured for illuminant A and the 2° CIE observer is stored in the record with the serial number field 221-A-2. This convention is only a pro memoria and does not have to be followed. (See Table 2 on page 16 for the colorimetric data.)

In Appendix VI on page 77 we reproduce the colorimetric values from the initial characterization of five Green tiles with instrument 10255. These values are just examples and cannot be used with other instruments.

5.6 Accuracy check

The accuracy check is a simple verification that must be repeated at the beginning at every working shift for instruments that are used in process control. For instruments used in less critical applications, such as color reproduction or ICC profile creation, the verification must be repeated at least every three months.

The first preparatory step in this procedure is to start the certification database and browse the references until the relevant reference record is found. Check the current room temperature and verify that it lies within the limits indicated in the record, taking into account the tolerance of your thermometer.* Complete all preparatory steps:

1. check room temperature
2. set the white reference parameter to absolute white
3. set the illuminant
4. set the observer angle
5. apply the desired filter (Spectrolino) or set the desired filter wheel position (SPM-100)

* The tiles should be stored at ambient temperature and if they are in a closed container the container should be opened 30 minutes before the measurement.

Return to the certification window and select the view *Perform certification*. In this view follow the instructions on the screen:

1. click on the *New* button to create a new record. The system generates a new sequential certificate number and fills in the fields with the current date and time
2. enter the filter on the spectrophotometer. When you proceed to the next field, on the right of the filter designation you will see the warning *WRONG*. Ignore this warning for the moment; at the end of the certification it will indicate if the unit has detected the same filter as you indicated. This is a consistency check
3. enter the serial number of the color reference tile. The pop-up menu shows the entries in your color reference database
4. carry out the white calibration as described in Section 5.2 on page 43. Enter the current room temperature. The system will instantly verify that it lies within the limits; the instrument check will fail if the temperature is outside the limits
5. check the color reference for cleanliness and place it in the receptacle
6. enter the instrument's serial number and a description of the instrument and the reference
7. click the *Go* button to jump to the measurement set window and make sure it is set to the data acquisition view. On the bottom on the screen are the instructions for the KeyWizard; you have already performed the white calibration and a new record has already been created, so these two steps must be omitted
 proceed to step 5 in the instructions on the screen and perform the prescribed number of measurements. This number is usually the same as the number of repetitions you normally perform in the instrument's operation
 at the end go to the evaluation view and verify that the standard deviation is small. If necessary, you can add a comment for future reference
8. return to the certification window, where you will notice that the system has verified the settings on the instrument against the values in the color reference database
 click in the next two fields to refresh them
 the first field shows the CIE94 color difference and the second field shows the pass/fail message. Currently the tolerance for absolute measurements is 0.8 and for relative measurements it is 0.3
9. Click on the *Print* button to print a certificate and file it in the log book

If the test fails, check for the following conditions:

- is the room temperature correct?
- are the white reference and the color reference both clean?

- do the reference tiles have the correct serial numbers?
- if you are using the SpectroScan, are the two clips in the correct bays?
- if you are using the Spectrolino in hand-held mode, did you remove the positioning foot?
- is the filter clean?

After checking all conditions, repeat the accuracy check. If it fails again, follow the rules for a failed quarterly certification summarized in Figure 16 on page 46.

6 Thermal issues

In a manufacturing situation it is not always possible to control the room temperature. For example, in a factory that has been built in four copies, the following temperature ranges have been measured:

Location	Low temperature	High temperature
Dublin	19°C	23°C
Puerto Rico	21°C	22°C
Corvallis	22°C	23°C
Singapore	24°C	26°C

TABLE 13. Room temperature in various factories

At first glance, these ranges seem to quite benign, especially when compared to the typical operating temperature range for spectrophotometers, which is from -10°C to 40°C . However, there are four important issues, especially when ceramic tiles are measured: noise in the sensor, dimensional stability of the monochromator, heating the sample, and thermochromism in the sample.

6.1 Sensor noise

CCDs have a temperature-dependent leakage current that flows even when no light impinges upon the element. This signal is called *dark current*. Modern instruments no longer require cooling with a Peltier element and instead dissipate heat produced by the light source with passive systems.

Because customers want small instruments and short measurement intervals, instrument designers tend to dimension the cooling elements small and the measurement intervals short. In a well-balanced system, the noise will be just under the precision stated in the instrument specifications.

The instrument specifications are tailored to the market in which the instrument is sold. For example, an instrument sold in the graphic arts market will not require a precision larger than 0.5 units. Since this is a relatively large market, such instruments are inexpensive, and since the target users are not technicians, the user interfaces tend to be very user-friendly.

If an isolated measurement is taken with such an instrument, the precision is typically much better than stated in the specifications. This leads us use graphic arts instruments in process control applications. The important point is not to perform measurements and the maximum rate allowed by the instru-

ment, but to delay measurements until the heat generated by the lamp has completely dissipated. In the case of the Spectrolino, this interval is 10 seconds. This is why in the validation procedures we prescribe to wait for 10 seconds between measurements and why we log the time of each measurement.

6.2 Optics stability

Heat also causes the optics in the instrument to expand. A common device used as a monochromator is a holographic diffraction grating. When the grating expands, the spectrum interval detected by the sensor moves and the instrument's calibration is no longer valid. The instrument designer can minimize this effect by choosing a material that has a very good dimensional stability, but there is a cost trade-off.

The user has two choices to avoid this problem. The first choice is to recalibrate the instrument frequently, say every 10 measurements. The second choice is to wait between measurements until the instrument has completely cooled, which in the case of the Spectrolino is 10 seconds.

To err on the safe side, in our procedures we have recommended to do both, wait for 10 seconds and recalibrate every 10 measurements. It is now clear to the reader that the calibration can be much less frequent. We have not performed experiments to determine the exact required calibration frequency, but it might be an order of magnitude larger.

In the specific case of the Spectrolino, in the models designated as "Rev. A" or newer the diffraction grating is on a new glass type that is dimensionally very stable under temperature changes.* With this improvement it will be worthwhile to relax the calibration requirements.

6.3 Sample heating

A typical light source for spectrophotometers is a gas filled tungsten lamp. Such a lamp has a strong radiation in the infrared part of the spectrum, which can heat up the sample. In the Spectrolino, for example, the filament heats to 3000°K on a surface of 1.5 mm × 0.5 mm.

If the measurement time is kept very short to minimize this effect, then only a small number of photons will be available at the sensor and the dark current will cause a very poor signal to noise ratio. The classical solution to this problem is to keep the light on until the sensor saturates, and then to determine the spectral power from the integration time of the radiant flux. With dark samples this time can be quite long and considerably heat the sample.

* In the Spectrolino S/N 10255 used to obtain the data for this report we have upgraded the grating to the new type.

We do not know how the Spectrolino and the SPM-100 work, so we have assessed the problem with an experiment. We set the Spectrolino with serial number 10255 to the following conditions:

- illuminant D₆₅
- 2° observer
- no filter
- no data transfer

We measure the temperature of a green reference tile (serial number GBB-1), then we perform 30 measurements at the maximal speed allowed by the instrument and immediately measure the tile's temperature again. The result of three repetitions is shown in the table below.

Ceramic tile condition	Temperature 1	Temperature 2	Temperature 3	Average
Initial	22.7±1°C	22.7±1°C	22.7±1°C	
After 30 measurements	22.9±1°C	22.9±1°C	22.9±1°C	
Difference	0.2°C	0.2°C	0.2°C	0.2°C

TABLE 14. Heating of green ceramic tile by Spectrolino lamp

The error due to thermochromism would be approximately 0.01 CIELAB units. Given that in the certification procedures the tile is measured at most 10 times and there is a 10 second wait between measurements, heating of the ceramic reference tile by the instrument during a measure is not a problem.

6.4 Thermochromism

Thermochromism refers to a color change with temperature change. Among others, it occurs with some tiles that contain selenium. Anne Compton reported [6] that when a tile is heated from 25 to 35°C — a typical temperature change in the instruments using prolonged polychromatic irradiation common at that time — the effect is a small reduction in reflectance with an increase in temperature. She observed that in general thermochromism occurs on steep spectral profiles. The largest value of ΔE^*_{ab} occurred for the dark green tile and was 0.9, a difference that is larger than the tolerances in our procedures. The instrument geometry was diffuse/0°.

Mark Fairchild and Frank Grum [7] conducted a similar experiment* with an instrument of 0°/45° geometry. For the same temperature change they observed a ΔE^*_{ab} value of 0.7 for a green tile. However, they observed much

* Compton's data is for the original series of BCRA tiles. The second series was launched at the 20th CIE session in 1983.

larger changes for the Orange (1.6) and Red (1.5) BCRA Series II (CCS II) tiles.

More recently the National Physical Laboratory (NPL) has released a comprehensive collection of spectral reflectance and thermochromism data [8] on the NPL Master Set of the BCRA CCS II tiles. The colorimetric data for the green tile is shown in Table 15 for spex and spinc geometry; unfortunately no data is provided for 0°/45° geometry, but the interested reader can calculate it from the data provided in the article. Some data for the other tiles is in Table 17.

Green tile	specular excluded 0°/d	specular included 8°/t	10255 inter-instrument
Δx	-0.0016	-0.0013	
Δy	0.0008	0.0008	
$\Delta Y\%$	0.18	0.17	
ΔL^*	0.20	0.18	-0.01
Δa^*	-0.75	-0.66	0.12
Δb^*	0.03	0.04	-0.23
ΔC^*	0.68	0.64	
ΔH	0.32	0.28	
ΔE^* (CIELAB)	0.77	0.68	0.28
ΔE (CMC(1:1))	0.40	0.37	

TABLE 15. Colorimetric differences caused by a 10° change in temperature
Green tile, illuminant D₆₅, 10° observer, Δ = value at 25°C minus value at 35°C.

In the last column is the deviation of Spectrolino S/N 10255 from the average values obtained from 10 Spectrolinos and reported in Table 6 on page 21. Thermochromism is linear, so if we take from Table 13 on page 53 the maximum temperature span of 7°C, for the spinc measurement we would obtain a difference of 0.48 ΔE^*_{ab} . This value is almost twice the inter-instrument agreement, i.e., if ambient temperature is ignored during measurements, a significant error is introduced and the data is less valuable.

Remember also that the tolerance for the relative accuracy check in Section 5.6 on page 50 is 0.3. Hence, a temperature difference of 4°C is by itself the limit to pass the validation, assuming the instrument is perfect. With the 2°C temperature tolerance prescribed in that procedure, a 0.12 unit error is already introduced by the temperature uncertainty, leaving 0.18 units for drifts in the instrument. The Dublin factory, with a temperature excursion from 19°C to 23°C, will have a challenging time to pass the instrument's qualification. In reality, the procedure described in this report is more lenient, because it is based on the CIE94 color difference, which is closer to CMC.

In time series analysis we examine a long series of measurements and try to find trends. For highly significant assertions the analyst will always use the same instrument. If the operation is very meticulous, then the repeatability will be close to the short-term repeatability, which for Spectrolino S/N 10255 is $0.023 \Delta E^*_{ab}$ units. This number is an order of magnitude smaller than the effect of thermochromism with the 2°C tolerance, hence temperature variations will limit the usability of the calibration data.

This last qualification is important. Ink on paper most likely does not suffer the thermochromism problem, so the measurements by themselves do not limit the precision of time series analysis. The limitation is when the measurements of the green tile are used to calibrate the data in the time series. What we have seen is that this calibration is limited by the uncertainty of the temperature.

If the temperature is stable for a period of 30 minutes (the time for a ceramic tile to adapt to a small temperature change) or longer, and an accurate thermometer is available, for example a mercury in glass thermometer graduated in 0.1°C intervals, then highly accurate measurements can be made by correcting the spectral data for the temperature difference before the colorimetric quantities are computed.

The correction data is listed in the following table listing the differences in reflectance caused by a 10°C (25 to 35°C) change in temperature for the Green tile in the Master Set of the BCRA CCS II tiles:

Wavelength [nm]	difference
380	0.0003
390	0.0002
400	0.0002
410	0.0001
420	0.0001
430	0.0002
440	0.0003
450	0.0005
460	0.0009
470	0.0017
480	0.0030
490	0.0049
500	0.0065

TABLE 16. Thermochromism data for Green tile

Wavelength [nm]	difference
510	0.0064
520	0.0048
530	0.0033
540	0.0020
550	0.0009
560	0.0006
570	0.0002
580	-0.0001
590	-0.0004
600	-0.0005
610	-0.0006
620	-0.0006
630	-0.0007
640	-0.0007
650	-0.0007
660	-0.0007
670	-0.0007
680	-0.0006
690	-0.0005
700	-0.0003
710	0.0001
720	0.0002
730	0.0004

TABLE 16. Thermochromism data for Green tile

Fig. 17 shows the spectral reflectance data of the green reference tile S/N GBB-11 measured at $24.4 \pm 1^\circ\text{C}$ with Spectrolino S/N 10255 without filter. The gray curve plots the NPL data for the difference in reflectance caused by a 10°C (25 to 35°C) change in temperature (units on right axis) tabulated in Table 16 above.

Table 17 from reference [8] shows the colorimetric differences caused by a 10°C temperature change. From this data one might assume that the cyan or even the deep blue tile would be a better choice for the problem at hand. However, as we noted in the discussion of Figure 1, "Reflectance of the green and

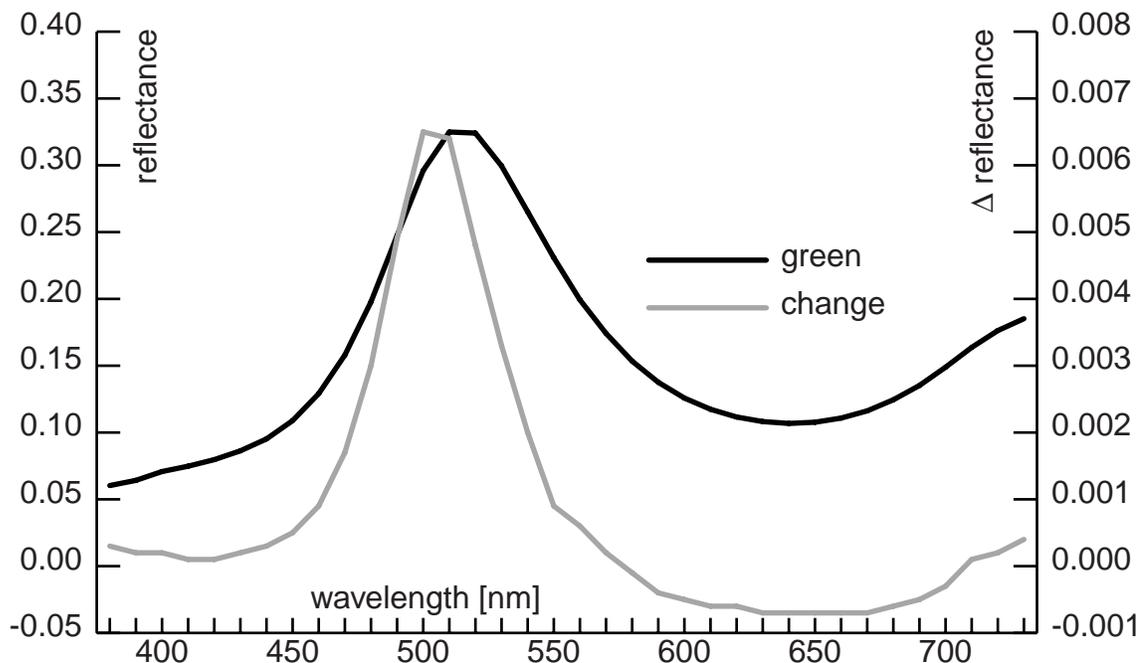


FIGURE 17. Difference in reflectance due to thermochromism
Spectral reflectance of green tile GBB-1 measured with Spectrolino 10255 at $24.4 \pm 1^\circ\text{C}$ (left ordinate) and difference in reflectance caused by a 10° change in temperature from 35°C (right ordinate).

cyan master tiles,” on page 15, the green tile with its sloped spectral distribution curve is better suited for detecting the critical shift of the instrument’s scale.

The deep blue tile exhibits the lowest thermochromism, but with its flat spectral distribution curve, by itself it is not useful at all to certify an instrument’s calibration. In summary, the green tile is the most suitable tile for certifying a spectrophotometer’s calibration; due to its thermochromic properties, ambient temperature must be controlled and recorded.

Tile	ΔE^*_{ab}	$\Delta E_{CMC} (1:1)$
Pale gray	0.04	0.05
Mid gray	0.05	0.07
Difference gray	0.06	0.07
Deep gray	0.01	0.01
Deep pink	0.48	0.30

TABLE 17. NPL thermochromism data for all tiles [8]
Colorimetric differences caused by a 10°C change in temperature for spinc 8°/t geometry and illuminant D65 with the 10° observer (Δ = value at 25°C minus value at 35°C); NPL data [8]. The CMC color difference evaluation is more similar to the CIE94 evaluation recommended in this report.

Tile	ΔE^*_{ab}	ΔE CMC (1:1)
Red	1.01	0.56
Orange	0.97	0.85
Bright yellow	0.76	0.44
Green	0.68	0.37
Difference green	0.72	0.39
Cyan	0.32	0.22
Deep blue	0.06	0.04

TABLE 17. NPL thermochromism data for all tiles [8]

Colorimetric differences caused by a 10°C change in temperature for spinc 8°/t geometry and illuminant D65 with the 10° observer (Δ = value at 25°C minus value at 35°C); NPL data [8]. The CMC color difference evaluation is more similar to the CIE94 evaluation recommended in this report.

7 Acknowledgements

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Thomas Senn and Markus Weidmann have patiently demonstrated and explained the calibration equipment and procedures at Gretag-Macbeth in Regensdorf (Switzerland) and given special care to our unit S/N 10255. Thomas Senn has organized the manufacture of the green reference tiles for us. Ernst Hohmann of Automation Engineering in Philadelphia (Pennsylvania) has been very helpful explaining how spectrophotometers are certified in the field and shared a sample database.

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Last but not least, this project was managed by Cormac Herley, with Neerja Raman Department Manager. Edith Sandoval has helped manufacturing the reference tiles.

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Appendix I Metadata for the certificate table

The keys are fields “Color Reference” and “Certificate Number.”

Field Name	Field Type	Formula / Entry Option
Color Reference	Text	Required value Indexed
Date	Date	Auto- enter the: “Creation Date” Do not allow user to override validation Required value Indexed
Time	Time	Auto- enter the: “Creation Time” Prevent data that is automatically entered from being changed. Indexed
Filter	Text	Value List (Custom Values): No, Pol, D65, Repro
Certificate Number	Number	Serial Number with Current Value: “23” Increment: “23” Indexed
RefLstar	Calculation (Number)	Unstored calculation = Case(Exact(Filter, “NO”), Reference SN:: FilterNo Lstar, Exact(Filter, “Pol”), Reference SN:: FilterPol Lstar, Exact(Filter, “D65”), Reference SN:: FilterD65 Lstar, -1)
RefaStar	Calculation (Number)	Unstored calculation = Case(Exact(Filter, “NO”), Reference SN:: FilterNo aStar, Exact(Filter, “Pol”), Reference SN:: FilterPol aStar, Exact(Filter, “D65”), Reference SN:: FilterD65 aStar, -1)
RefbStar	Calculation (Number)	Unstored calculation = Case(Exact(Filter, “NO”), Reference SN: FilterNo bStar, Exact(Filter, “Pol”), Reference SN:: FilterPol bStar, Exact(Filter, “D65”), Reference SN:: FilterD65 bStar, -1)
RefChroma	Calculation (Number)	Unstored calculation = Case(Exact(Filter, “NO”), Reference SN:: FilterNo Cstar, Exact(Filter, “Pol”), Reference SN:: FilterPol Cstar, Exact(Filter, “D65”), Reference SN:: FilterD65 Cstar, -1)
RefHue	Calculation (Number)	Unstored calculation = Case(Exact(Filter, “NO”), Reference SN:: FilterNo hStar, Exact(Filter, “Pol”), Reference SN:: FilterPol hStar, Exact(Filter, “D65”), Reference SN:: FilterD65 hStar, -1)

Field Name	Field Type	Formula / Entry Option
DeltaLStar	Calculation (Number)	Unstored calculation = RefLStar - Measure Set::LStarAve
DeltaaStar	Calculation (Number)	Unstored calculation = RefaStar - Measure Set::aStarAve
DeltabStar	Calculation (Number)	Unstored calculation = RefbStar - Measure Set::bStarAve
DeltaChroma	Calculation (Number)	Unstored calculation = RefChroma - Measure Set::chromaAve
DeltaE76	Calculation (Number)	Unstored calculation = Sqrt(Sum((DeltaLStar * DeltaLStar), (DeltaaStar * DeltaaStar), = Sqrt(Sum((DeltaLStar * DeltaLStar), (DeltaaStar * DeltaaStar), (DeltabStar * DeltabStar)))
DeltaHue	Calculation (Number)	Unstored calculation = Sqrt(DeltaE76 * DeltaE76 - DeltaLStar * DeltaLStar - DeltaChroma * DeltaChroma)
CIE94	Calculation (Number)	Unstored calculation = Sqrt(DeltaLStar * DeltaLStar + (DeltaChroma / (1.0+ 0.045 * RefChroma)) * (DeltaChroma / (1.0+ 0.045 * RefChroma)) + (DeltaHue / (1.0 + 0.015 * RefChroma)) * (DeltaHue / (1.0 + 0.015 * RefChroma)))
Pass	Calculation (Number)	Unstored calculation = If(Exact("Absolute", Reference SN:: Reference), (CIE94 <= 0.8), (CIE94 <= 0.3))
FilterOK	Calculation (Number)	Unstored calculation = Exact(Filter, Measurement:: Filter)
TemperatureOK	Calculation (Number)	Unstored calculation = (Measure Set::Temperature >= Reference SN:: Ambient temperature - Reference SN:: Temperature tolerance) and (Measure Set::Temperature <= Reference SN:: Ambient temperature + Reference SN:: Temperature tolerance)
WhiteBaseOK	Calculation (Number)	Unstored calculation = Exact(Reference SN:: White base, Measurement:: WhiteBase)
IlluminantOK	Calculation (Number)	Unstored calculation = Exact(Reference SN:: Illumination, Measurement:: Illuminant)
ObserverOK	Calculation (Number)	Unstored calculation = Exact(Reference SN:: Viewing angle, Measurement:: ObserverAngle)

Appendix II Metadata for the reference table

Field Name	Field Type	Formula / Entry Option
Color	Text	Auto-enter: "Green"
Part	Text	
Date	Date	Auto-enter the: "Creation Date"
Serial No	Text	Required value Unique values only Unique values only
Ambient temperature	Number	Auto-enter: "23"
Temperature tolerance	Number	
FilterNo Lstar	Number	
FilterNo aStar	Number	
FilterNo bStar	Number	
FilterNo Cstar	Number	
FilterNo hStar	Number	
FilterPol Lstar	Number	
FilterPol aStar	Number	
FilterPol bStar	Number	
FilterPol Cstar	Number	
FilterPol hStar	Number	
FilterD65 lstar	Number	
FilterD65 aStar	Number	
FilterD65 bStar	Number	
FilterD65 Cstar	Number	
FilterD65 hStar	Number	
White base	Text	Auto-enter: "Abs"
Illumination	Text	Auto-enter: "D50"
Viewing angle	Number	Auto-enter: "2"

Field Name	Field Type	Formula / Entry Option
Reference	Text	Value List (Custom Values): Absolute, Relative Do not allow user to override validation Required value Message: "Reference field cannot be empty. Enter "Absolute" if this data was obtained from a primary instrument. Otherwise enter the serial numbers of the instruments from which the data was averaged"
Reference Comment	Text	
Reference Instrument	Text	
Analyst	Text	Auto-enter the: "Creator Name"

Appendix III Metadata for the measurement table

Field Name	Field Type	Formula / Entry Option
WhiteBase	Text	Auto-enter value from previous record Do not allow user to override validation Required value
Illuminant	Text	Auto-enter value from previous record Do not allow user to override validation Required value
ObserverAngle	Number	Auto-enter value from previous record Do not allow user to override validation Required value Only allow values of type: "Number"
DensityStd	Text	Auto-enter value from previous record
Filter	Text	Auto-enter value from previous record Do not allow user to override validation Required value
lStar	Number	Do not allow user to override validation Required value
aStar	Number	Do not allow user to override validation Required value
bStar	Number	Do not allow user to override validation Required value
lStar2	Number	
chroma	Number	Do not allow user to override validation Required value Message: "If you do not have the chroma value, enter any number and then press the recompute button"
hue	Number	Do not allow user to override validation Required value Message: "If you do not have the hue value, enter any number and then press the recompute button"
nm380	Number	
nm390	Number	
nm400	Number	

Field Name	Field Type	Formula / Entry Option
nm410	Number	
nm420	Number	
nm430	Number	
nm440	Number	
nm450	Number	
nm460	Number	
nm470	Number	
nm480	Number	
nm490	Number	
nm500	Number	
nm510	Number	
nm520	Number	
nm530	Number	
nm540	Number	
nm550	Number	
nm560	Number	
nm570	Number	
nm580	Number	
nm590	Number	
nm600	Number	
nm610	Number	
nm620	Number	
nm630	Number	
nm640	Number	
nm650	Number	
nm660	Number	
nm670	Number	
nm680	Number	
nm690	Number	
nm700	Number	
nm710	Number	

Field Name	Field Type	Formula / Entry Option
nm720	Number	
nm730	Number	
SerialNumber	Number	Serial Number with Current Value: "134" Increment: "134" Indexed
SetNumber	Number	Indexed
Date	Date	Auto-enter the: "Creation Date"
Time	Time	Auto-enter the: "Creation Time"
Comment	Text	
epsilon	Global (Number)	
lStarTmp	Calculation (Number)	= lStar
chromaTmp	Calculation (Number)	= Sqrt(aStar * aStar + bStar * bStar)
hueTmp	Calculation (Number)	Unstored calculation = Case((Abs(aStar) < epsilon), If(bStar >= 0, 90.0, 270.0), ((bStar >= 0) and (aStar >= 0)), Degrees(Atan(bStar / aStar)), ((bStar >= 0) and (aStar < 0)), Degrees(Atan(bStar / aStar)) + 180.0, ((bStar < 0) and (aStar < 0)), Degrees(Atan(bStar / aStar)) + 180.0, ((bStar < 0) and (aStar >= 0)), Degrees(Atan(bStar / aStar)) + 360.0, 999999)

Appendix IV Metadata for the measurement set table

Field Name	Field Type	Formula / Entry Option
Set	Text	Required value Unique values only Indexed
Analyst	Text	Auto-enter the: "Creator Name"
lStarAve	Calculation (Number)	Unstored calculation = Average(measurement::lStar)
aStarAve	Calculation (Number)	Unstored calculation = Average(measurement::aStar)
bStarAve	Calculation (Number)	Unstored calculation = Average(measurement::bStar)
chromaAve	Calculation (Number)	Unstored calculation = Average(measurement::chroma)
hueAve	Calculation (Number)	Unstored calculation = Average(measurement::hue)
lStarVar	Calculation (Number)	Unstored calculation = StDev(measurement::lStar)
aStarVar	Calculation (Number)	Unstored calculation = StDev(measurement::aStar)
bStarVar	Calculation (Number)	Unstored calculation = StDev(measurement::bStar)
chromaVar	Calculation (Number)	Unstored calculation = StDev(measurement::chroma)
hueVar	Calculation (Number)	Unstored calculation = StDev(measurement::hue)
Subject	Text	
Comments	Text	
Serial number	Text	Required value
Temperature	Number	Required value Only allow values of type: "Number" Only allow values in the range from "18" to "28" Message: "You must enter the temperature in °C. The range must be within 18 and 28° C"

Field Name	Field Type	Formula / Entry Option
TTolerance	Number	

Appendix V Metadata for the correlates table

Field Name	Field Type	Formula / Entry Option
measurement	Number	
chroma	Number	Auto-enter calculation = Sqrt(Measurement:: aStar * Measurement:: aStar + Measurement:: bStar * Measurement:: bStar)
hueTmp	Number	Auto-enter calculation = Degrees(Atan(Measurement:: bStar / Measurement:: aStar))
hue	Number	Auto-enter calculation = if (hueTemp >= 0, hueTemp, hueTemp + 180)

Appendix VI Green tile examples

The “mother” of the Green CCS II tiles is the one at the National Physical Laboratory [8]. Its colorimetric values at 25°C for the 0°/45° geometry, illuminant D₆₅, and the CIE 10° observer are tabulated below. These values are absolute, but they are only valid for this particular tile, not the one to you might have access. For future use we also include the data for the Cyan tile.

Tile	x	y	Y	L*	a*	b*	C*	hue
Green	0.2834	0.4307	19.56	51.33	-33.28	17.19	37.45	152.7
Cyan	0.1992	0.2572	19.56	51.33	-18.95	-29.42	35.00	302.2

The colorimetric values for the initial characterization of the Green tile (see Section 5.5 on page 48) are different for every instrument because it is a relative procedure. To give a frame of reference, we reproduce the initial data for the Spectrolino unit with serial number 10255. The tolerance for the temperature is 1°C.

Tile label	Illuminant	CIE Observer	Filter	Temperature [°C]	L*	a*	b*	C*	h _{ab}
GBB-1	A	2°	D65	23.7	50.876	-27.372	8.498	28.664	162.756
			Pol	23.7	50.886	-28.338	8.34	29.538	163.596
			No	23.4	50.594	-27.492	8.01	28.636	163.752
	D65		23.7	52.856	-32.772	14.584	35.872	156.004	
	Pol		23.8	53.126	-33.87	14.766	36.95	156.446	
	No		23.5	52.546	-32.858	14.148	35.776	156.708	
	D ₅₀	10°	D65	23.6	53.298	-32.346	18.326	37.176	150.466
			Pol	23.8	53.624	-33.434	18.702	38.308	150.778
			No	23.4	53.032	-32.474	17.932	37.092	151.092
	D ₆₅	2°	D65	23.7	53.318	-34.65	16.526	38.39	154.5
			Pol	23.8	53.642	-35.814	16.824	39.568	154.838
			No	23.4	53.044	-34.67	16.074	38.212	155.126

Tile label	Illuminant	CIE Observer	Filter	Temperature [°C]	L*	a*	b*	C*	h _{ab}
GBB-2	A	2°	D65	23.7	50.884	-27.336	8.45	28.614	162.828
			Pol	23.7	50.666	-28.204	8.286	29.396	163.628
			No	23.5	50.572	-27.444	8.064	28.604	163.62
	D65		23.7	52.862	-32.744	14.462	35.796	156.166	
	Pol		23.7	53.124	-33.806	14.634	36.838	156.594	
	No		23.5	52.544	-32.83	14.216	35.776	156.588	
	D ₅₀	10°	D65	23.6	53.254	-32.312	18.282	37.128	150.496
			Pol	23.8	53.622	-33.354	18.688	38.232	150.734
			No	23.5	53.016	-32.444	17.958	37.08	151.04
		D ₆₅	D65	23.6	53.32	-34.61	16.53	38.354	154.472
			Pol	23.8	53.628	-35.722	16.846	39.494	154.748
			No	23.5	53.04	-34.718	16.174	38.304	155.022
GBB-3	A	2°	D65	23.6	50.884	-27.448	8.446	28.718	162.896
			Pol	23.7	50.59	-28.254	8.26	29.438	163.706
			No	23.5	50.64	-27.536	8.086	28.7	163.636
	D ₅₀		D65	23.7	52.874	-32.816	14.59	35.916	156.03
			Pol	23.8	53.128	-33.826	14.794	36.92	156.376
			No	23.5	52.594	-32.914	14.216	35.854	156.638
	D ₆₅	10°	D65	23.6	53.318	-32.382	18.348	37.218	150.46
			Pol	23.9	53.65	-33.372	18.658	38.23	150.788
			No	23.4	53.056	-32.48	17.932	37.104	151.096
		2°	D65	23.7	53.336	-34.752	16.578	38.506	154.502
			Pol	23.8	53.672	-35.774	16.85	39.544	154.776
			No	23.4	53.064	-34.792	16.208	38.382	155.024

Tile label	Illuminant	CIE Observer	Filter	Temperature [°C]	L*	a*	b*	C*	h _{ab}	
GBB-4	A	2°	D65	23.6	51.09	-27.638	8.606	28.948	162.702	
			Pol	23.7	50.792	-28.436	8.502	29.682	163.356	
			No	23.5	50.842	-27.728	8.218	28.916	163.496	
	D65		23.7	53.106	-33.07	14.772	36.218	155.93		
	Pol		23.7	53.35	-34.08	15.002	37.234	156.238		
	No		23.5	52.812	-33.142	14.404	36.138	156.51		
	D ₅₀	10°	D65	23.6	53.528	-32.624	18.516	37.512	150.422	
			Pol	23.9	53.87	-33.64	18.93	38.604	150.634	
			No	23.4	53.282	-32.75	18.178	37.458	150.968	
	D65		23.8	53.562	-34.978	16.778	38.792	154.37		
	Pol		23.7	53.894	-36.058	17.066	39.888	154.674		
	No		23.5	53.284	-35.036	16.4	38.686	154.916		
GBB-5	A	2°	D65	23.7	50.84	-27.36	8.428	28.628	162.88	
			Pol	23.7	50.45	-28.174	8.298	29.372	163.588	
			No	23.5	50.58	-27.446	8.006	28.59	163.74	
	D ₅₀		10°	D65	23.7	52.826	-32.744	14.538	35.822	156.062
				Pol	23.8	53.042	-33.764	14.758	36.85	156.392
				No	23.5	52.544	-32.806	14.232	35.758	156.544
	D ₆₅	2°		D65	23.7	53.27	-32.29	18.302	37.116	150.456
				Pol	23.9	53.596	-33.336	18.656	38.202	150.768
				No	23.5	53.012	-32.428	17.882	37.028	151.128
	D65		23.7	53.282	-34.62	16.534	38.368	154.472		
	Pol		23.7	53.592	-35.73	16.816	39.49	154.798		
	No		23.5	53.044	-34.86	16.184	38.436	155.092		

The colorimetric data for the Green reference tile 211 is in Table 2 on page 16 and the following two tables.

