BRITISH STANDARD

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1557 : 1997

Surface active agents — Colorimetric characterization of optically clear coloured liquids (products) as *X*, *Y*, *Z* tristimulus values in transmission

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ICS. 71.100.40

Committees responsible for this British Standard

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British Association for Chemical Specialities
Chemical Industries Association
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Laboratory of the Government Chemist
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National foreword

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Cross-references

Publication referred to	Corresponding British Standard
ISO 4630 : 1981	BS 6782 : *Binders for paints* Part 5 : 1987 *Method for estimation of colour of clear liquids by the Gardner colour scale*
ISO 7724-1 : 1984	BS 3900 : *Methods of test for paints* Group D : *Optical tests on paint films* Part D8 : 1986 *Determination of colour and colour difference: principles*

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Summary of pages

This document comprises a front cover, an inside front cover, pages i and ii, the EN title page, pages 2 to 10, an inside back cover and a back cover.

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EN 1557

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English version

Surface active agents — Colorimetric characterization of optically clear coloured liquids (products) as *X*, *Y*, *Z* Tristimulus values in transmission

Agents de surface — Caractérisation colorimétrique des liquides (produits) colorés optiquement clairs par composantes trichromatiques *X*, *Y*, *Z* en transmittance

Grenzflächenaktive Stoffe — Farbmetrische Charakterisierung von optisch klaren, gefärbten Flüssigkeiten (Produkten) als *X*-, *Y*-, *Z*-Transmissions-Farbwert

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European Committee for Standardization
Comité Européen de Normalisation
Europäisches Komitee für Normung

Central Secretariat: rue de Stassart 36, B-1050 Brussels

Foreword

This European Standard has been prepared by the Technical Committee CEN/TC 276, Surface active agents, the secretariat of which is held by AFNOR.

This European Standard shall be given the status of a national standard, either by publication of an identical text or by endorsement, at the latest by March 1997, and conflicting national standards shall be withdrawn at the latest by March 1997.

Annexes A, B, C and D are informative.

According to the CEN/CENELEC Internal Regulations, the national standards organizations of the following countries are bound to implement this European Standard: Austria, Belgium, Denmark, Finland, France, Germany, Greece, Iceland, Ireland, Italy, Luxembourg, Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, United Kingdom.

Contents

0 Introduction

The basic disadvantage of visual subjective comparisons of coloured solutions is that individuals differ in their perception of colour ; added to this is the difficulty of describing shade variations verbally with reference to agreed scales for coloured liquids.

1 Scope

This European Standard specifies a method for the colorimetric characterization of optically clear, slightly tinted liquids (products) by broad-band measurement of pure transmittance with tristimulus value measuring filters as T_X, T_Y and T_Z.

Since the tristimulus value measuring filters of simple tristimulus colorimeters meet the Luther condition to a limited extent only it is necessary to deliberately restrict the liquids (products) to slightly tinted ones in order to be able to measure them sufficiently exactly with a single calibration against uncoloured distilled water.

If the colour of heavily coloured solutions is measured with simple tristimulus colorimeters, it is necessary to calibrate the instrument with a spectrometrically measured standard of very similar colour.

2 Normative references

This European Standard incorporates by dated or undated reference, provisions from other publications. These normative references are cited at the appropriate places in the text and the publications are listed hereafter. For dated references, subsequent amendments to or revisions of any of these publications apply to this European Standard only when incorporated in it by amendment or revision. For undated references the latest edition of the publication referred to applies.

ISO 4630 : 1981	*Binders for paints and varnishes — Estimation of colour of clear liquids by Gardner colour scale*
ISO 6271 : 1981	*Clear liquids — Estimation of colour by the platinum-cobalt scale*
ISO 7724-1 : 1984	*Paints and varnishes - Colorimetry - Part 1 : Principles*

3 Principle

The principle of the method is the broad-band transmission measurement with *X*, *Y*, *Z*- tristimulus value measuring filters in simple tristimulus colorimeters with special equipped spectral photometers.

The tristimulus colorimeter is calibrated with the tristimulus value measuring filters in each case of 100,0 with a 1 cm square cuvette filled with distilled water.

The slightly tinted, optically clear liquid is measured in the calibrated filter photometer in 1 cm square cuvette with *X*, *Y*, *Z*- tristimulus value measuring filters.

The T_N (N = *X*, *Y* and *Z*) transmittance characterizes the sample directly.

NOTE 1. Different types of colour numbers are compared in annex A.

NOTE 2. Measurement with other layer thicknesses and conversion by the Bouguer-Lamber-Beer law is permissible (with optically clear, i.e. non-diffusing, solutions), provided that the light passes through the solutions at a specific angle and the law is applicable to the solution in question.

Conversion to the CIE tristimulus values *X*, *Y* and *Z* is also possible (see clause **7**).

4 Apparatus and reagents

4.1 *Tristimulus colorimeter*, equipped with *X*, *Y*, *Z*-tristimulus value measuring filters for the 2° standard observer and CIE illuminant C or suitable spectral photometer.

4.2 *1 cm glass or plastics cuvettes.*

NOTE. It is possible and advantageous to use cheap disposable plastics cuvettes.

4.3 *Distilled water or water of equivalent purity.*

5 Preparation of the test sample

The slightly tinted, optically clear liquid shall be filled into 1 cm cells. Air bubbles shall be prevented from adhering to the cell walls. Bubbles can be eliminated by allowing the liquid level to rise slowly, e.g. by filling through (plastic disposable) pipettes.

Pastes or solids shall be melted first. Turbid liquids shall be filtered until they are clear.

If it is not desirable or possible to filter an optically turbid liquid the diffusing solutions shall be measured under special conditions, usually with an Ulbricht sphere (integrating sphere).

Conversion to other layer thicknesses is not possible in this case.

NOTE. The temperature during the sample preparation has an influence on the colour, depending on the chemical composition of the sample. In practice because of the short time of sample preparation this effect can be neglected.

6 Procedure

Equip the tristimulus colorimeter with a 1 cm cell, which is filled with bubble-free distilled water (**4.3**). Insert the tristimulus filter (e.g. for T_Z) and calibrate the display to 100,0. Carry out the same procedure for filters T_X and T_Y if required.

Insert the 1 cm cuvettes containing the optically clear liquids to be investigated and measure the T_Z transmittances (if necessary T_X and T_Y as well) for the CIE 2° Standard observer and CIE illuminant C.

NOTE 1. For better differentiation very pale, optically clear solutions should be measured in a thicker layer, for example in a 5 cm cell, so as to obtain a reliable reading. The results are then converted to those for a 1 cm thick layer at the evaluation stage.

NOTE 2. Results of a ring test of APHA-measurements are given in annex D.

State every deviation from these conditions in the test report.

7 Calculation

The instrument readings T_N ($N = X$, Y or Z) measured with a 1 cm path length can be used directly. For examples of instrument readings see table 1.

Those measured with a layer of any other thickness shall be converted to those for a 1 cm thick layer by equation (1):

$$T_N = 100 \left[\frac{T_{N,d}}{100}\right]^{\frac{1}{d}} \quad (1)$$

where:

d is the layer thickness in centimetres ;

T_N is the transmittance in percent.

The transmittances T_N relative to the 1 cm layer thickness can be used either directly or after conversion to the decimal absorbency (also known as extinction/absorbence A) according to equation (2) :

$$A = \lg \frac{100}{T_N} \quad (2)$$

The T_N ($N = X$, Y or Z) transmittances can be converted to the CIE tristimulus values X, Y and Z for CIE illuminant C according to the following equations[1)]:

$$X = 0{,}7832\ T_X + 0{,}1975\ T_Z \quad (3)$$

$$Y = T_Y \quad (4)$$

$$Z = 1{,}1822\ T_Z \quad (5)$$

From these the CIE chromaticity co-ordinates can be calculated by using equation (6) :

$$x = \frac{X}{X + Y + Z} \text{ or } y = \frac{Y}{X + Y + Z} \quad (6)$$

NOTE. In calculating the CIE tristimulus value X from equation (3) it is assumed that in the tristimulus colorimeter the CIE spectral tristimulus value $X(\lambda)$ is formed a long-wave T_X-filter and a short-wave T_Z-filter, as is usually the case in practice.

Further conversions of the CIE tristimulus values into colour difference systems with almost uniform colour difference scale, e.g. the CIELAB system, can be realized in accordance with ISO/CIE 10526, ISO/CIE 10527 and ISO 7724-1.

Table 1. Examples of instrument readings T_N ($N = X, Y, Z$)

Liquid	Transmittances		
	T_X	T_Y	T_Z
Pale yellowish beer	93,7	89,1	61,0
White wine	97,5	96,4	86,1
Red wine	49,2	27,9	10,6
(Blue) copper sulfate solution (20 %) (solution of 20 g $CuSO_4.5\ H_2O$ in 100 ml water)	26,1	59,6	98,2
(Green) nickel sulfate (20 %) (solution of 20 g $NiSO_4.6\ H_2O$ in 100 ml water)	32,1	62,7	45,2

1) See CIE Publication N° 15.2 (1986).

8 Test report

The test report shall state the following information:

a) type and identification of the sample;

b) transmittance T_X, T_Y and T_Z and corresponding X, Y, Z-tristimulus values;

c) deviations from the cuvette layer thickness of 1 cm, the standard illuminant C and the 2° (small-field) standard observer;

d) date of test.

Annex A (informative)

Colour numbers in comparison

Hazen numbers, iodine colour numbers, Gardner numbers, or other colour numbers may be determined as X, Y, Z-tristimulus values of products if the tristimulus values lies exactly on the colour scale curve in the x-y diagram. These agreed scales may be used in those cases, when the definition of colour gives no ambiguity or does not need a sharp evaluation. When there are variations in shade, the indication of such a colour number is not possible.

For pale yellow liquids (products) it may suffice, for orientation purposes, to determine only the transmittance T_Z, which is measured with a Z tristimulus filter.

In order to permit correlation with some colour scales used, the transmittance, extinction/absorbence A (and CIE chromaticity co-ordinates) of the iodine colour numbers, the Hazen (APHA) colour scale and the Gardner colour scale are compared in tables A.1 to A.3 ; some of these were checked by 'round-robin' tests conducted under the supervision of CESIO (Comité Européen des Agents de Surface et leurs Intermédiaires Organiques). In accordance with these tests the tolerances relative to pale colour numbers, can be indicated with $\pm$10 APHA units and $\pm$0,3 iodine colour number units.

Table A.1 Iodine colour number ; Illuminate C ; 2° standard observer ; 1 cm cuvette

Iodine colour number	*X* Filter		*Y* Filter		*Z* Filter		Chromaticity co-ordinates	
	Extinction/ absorbence A	Transmittance T_X	Extinction/ absorbence A	Transmittance T_Y	Extinction/absorbence A	Transmittance T_Z	x	y
Achromatic Locus		100		100		100	0,3101	0,3162
0,5	0,001	99,8	0,002	99,5	0,023	94,8	0,3141	0,3226
1,0	0,001	99,8	0,004	99,0	0,046	89,9	0,3185	0,3287
1,5	0,002	99,5	0,007	98,4	0,068	85,5	0,3222	0,3344
2,0	0,003	99,3	0,008	98,2	0,090	81,3	0,3256	0,3408
3,0	0,005	98,9	0,013	97,1	0,132	73,8	0,3330	0,3513
4,0	0,006	98,6	0,016	96,4	0,170	67,6	0,3394	0,3612
5,0	0,008	98,2	0,021	95,3	0,210	61,7	0,3462	0,3703
7	0,014	96,8	0,030	93,3	0,311	48,9	0,3613	0,3944
10	0,020	95,5	0,044	90,4	0,424	37,8	0,3785	0,4159
15	0,028	93,8	0,065	86,1	0,585	26,0	0,4022	0,4406
20	0,036	92,0	0,084	82,4	0,723	18,9	0,4198	0,4564
30	0,054	88,3	0,124	75,2	0,954	11,1	0,4468	0,4710
50	0,088	81,7	0,198	63,4	1,317	4,8	0,4846	0,4731

Table A.2 Hazen number in accordance with ISO 6271 Illuminant C, 2° standard observer, measured with 5 cm rectangular cuvette, calculated to 1 cm square cuvette

Hazen number	*X* Filter		*Y* Filter		*Z* Filter		Chromaticity co-ordinates	
	Extinction/ absorbence	Transmittance	Extinction/ absorbence	Transmittance	Extinction/ absorbence	Transmittance	x	y
	A	T_X	A	T_Y	A	T_Z		
Achromatic Locus		100		100		100	0,3101	0,3162
10	0,0000		0,0006	99,9	0,0024	99,4		
20	0,0000		0,0010	99,8	0,0050	98,9		
30	0,0000		0,0014	99,7	0,0076	98,3		
40	0,0000		0,0018	99,6	0,0098	97,8		
50	0,0002	99,95	0,0022	99,5	0,0122	97,2	0,3125	0,3190
60	0,0002	99,95	0,0028	99,4	0,0148	96,6		
70	0,0004	99,9	0,0032	99,3	0,0172	96,1		
80	0,0006	99,9	0,0036	99,2	0,0196	95,6		
90	0,0006	99,9	0,0040	99,1	0,0220	95,1		
100	0,0006	99,9	0,0044	99,0	0,0246	94,5	0,3150	0,3218
120	0,0006	99,9	0,0052	98,8	0,0292	93,5		
150	0,0008	99,8	0,0062	98,6	0,0366	91,9	0,3173	0,3248
180	0,0010	99,8	0,0072	98,4	0,0440	90,4		
200	0,0012	99,7	0,0080	98,2	0,0486	89,4	0,3195	0,3277
250	0,0018	99,6	0,0098	97,8	0,0610	86,9	0,3218	0,3307
350	0,0028	99,4	0,0138	96,9	0,0852	82,2		
500	0,0048	98,9	0,0186	95,8	0,1218	75,5	0,3330	0,3453
750	0,0064	98,5	0,0260	94,2	0,1814	65,9	0,3438	0,3592
1000	0,0080	98,2	0,0326	92,8	0,2372	57,9	0,3540	0,3718

Table A.3 Gardner colour scale ; measurements with an *X*, *Y*, *Z* filter photometer ; liquid colour standards in accordance with ISO 4630 ; illuminant C, 2° standard observer, 1 cm square cuvette

Gardner number	*X* Filter		*Y* Filter		*Z* Filter		Chromaticity co-ordinates	
	Extinction/ absorbence A	Transmittance T_X	Extinction/ absorbence A	Transmittance T_Y	Extinction/ absorbence A	Transmittance T_Z	x	y
Achromatic Locus		100		100		100	0,3101	0,3162
1	0,000		0,004	99,1	0,047	89,7	0,3189	0,3290
2	0,002	99,5	0,007	98,4	0,076	83,9	0,3235	0,3369
3	0,003	99,3	0,012	97,3	0,117	76,4	0,3311	0,3469
4	0,003	99,3	0,017	96,2	0,182	65,8	0,3428	0,3634
5	0,004	99,1	0,025	94,4	0,267	54,1	0,3580	0,3827
6	0,004	99,1	0,033	92,7	0,367	43,0	0,3750	0,4037
7	0,005	98,9	0,046	89,9	0,548	28,3	0,4024	0,4356
8	0,006	98,6	0,052	88,7	0,667	21,5	0,4165	0,4535

Annex B (informative)

Bibliography

Tenside detergents vol. 23, (1986) n° 4, p. 213-219.

Seifen, Öle, Fette, Wachse vol. 114, n° 8/1988, p. 336-338.

Proc. European Brewery Convention (EBC) Congress, 1989, Berlin : *Diskrepanzen bei der Farbmessung an Würzen und Bieren* nach der EBC-Farbskala, p. 145-159.

CIE publication N° 15.2 (1986)	*Colorimetry* : second edition
ISO/CIE 10526 : 12.91	*CIE Standard colorimetric illuminants*
ISO/CIE 10527 : 12.91	*CIE Standard colorimetric observers*

Annex C (informative)

Notes on procedure

X, *Y*, *Z* tristimulus value measuring filters are filters with which colours according to ISO/CIE 10526, ISO/CIE 10527 and ISO 7724-1 can be measured in tristimulus colorimeters. The spectral transmittance of the filters shall be adapted to the course of the CIE spectral tristimulus values of the desired standard observer taking into consideration the spectral transmittance of the optical components and the spectral sensitivity of the detector of the tristimulus colorimeter. This is termed adherence to the Luther condition in ISO/CIE 10526, ISO/CIE 10527 and ISO 7724-1. The CIE spectral colour matching functions $\overline{x}$ (λ), $\overline{y}$ (λ) and $\overline{z}$ (λ) of the 2°(small field) standard observer in accordance with ISO/CIE 10526, ISO/CIE 10527 and ISO 7724-1 are recommended here. At least three different tristimulus filters are required for measuring the CIE tristimulus values *X*, *Y* and *Z*.

Since in practice it is often difficult to simulate the double-peaked CIE spectral colour matching function $\overline{x}$ (λ) with only one filter, this is frequently done with two filters. In this case the long-wave *X* filter is identified either by the suffix a (= amber) or l (= long) or by no suffix at all. The short-wave filter is given the suffix b (= blue) or k (= short [kurz in German]) or is substituted by the tristimulus value measuring filter *Z*, which is sufficiently similar for practical purposes.

Illuminants are standardized with their relative spectral power distributions S_λ. The CIE illuminant C recommended here is a daylight type. Its spectral power distribution $(S_\lambda)c$ will be found in ISO/CIE 10526. The source of radiation (incandescent lamp) in the tristimulus colorimeter shall simulate this spectral power distribution as well as best it can by means of appropriate filters.

The spectral pure transmittance

$$\tau_i(\lambda) = \frac{(\Phi_\lambda)\text{ex}}{(\Phi_\lambda)\text{in}} \qquad (7)$$

of a solution is defined on the basis of ISO/CIE 10526, ISO/CIE 10527 and ISO 7724-1 as the ratio of the directional spectral radiant flux (Φ_λ)ex, which reaches the exist surface of a homogeneous non-scattering layer of the solution, to the spectral radiant flux (Φ_λ)in, which has passed through the entry surface of this layer. The mean path length l of the radiation in the layer, which does not necessarily have to be identical with the layer thickness d of the solution, shall be quoted.

The T_N ($N = X, Y, Z$) transmittance :

$$T_N = 100 \times \lambda \times \frac{\int (S_\lambda)c \times (\tau_i(\lambda))\, sol \times \tau_N(\lambda) \times \tau_{opt}(\lambda) \times s(\lambda)d\lambda}{\int (S_\lambda)c \times (\tau_i(\lambda))H_20 \times \tau_N(\lambda) \times \tau_{opt}(\lambda) \times s(\lambda)d\lambda} \qquad (8)$$

is the spectral pure transmittance of the solution being investigated as assessed by tristimulus colour measurement, which is related to the spectral pure transmittance of a layer of distilled water of identical mean optical path length that is assessed in the same way by colour measurement.

In formula (8) the following symbols are used :

$(S_\lambda)c$	spectral power distribution of CIE illuminant C ;
$(\tau_i(\lambda))$ *sol*	spectral pure transmittance of the solution at a given optical path length ;
$(\tau_i(\lambda))$ H_2O	spectral pure transmittance of distilled water of the same optical path length;
$\tau_N(\lambda)$	spectral transmittance of the tristimulus value measuring filter under consideration of the ;
$\tau_{opt}(\lambda)$	spectral transmittance of the optical components and ;
$s(\lambda)$	relative spectral sensitivity of the detector in the tristimulus colorimeter.

Annex D (informative)
Results of a ring test of APHA-measurements

Solution number	1	2	3	4	5	6	7	8
APHA-number	20	40	60	80	100	150	200	300
Mean value of the colour numbers of 10 laboratories	98,96	97,92	96,78	95,72	94,74	92,10	89,55	84,75
Precision range	± 0,11	± 0,15	± 0,17	± 0,12	± 0,16	± 0,17	± 0,14	± 0,17
Precision in APHA-number units	± 2,0	± 2,7	± 3,2	± 2,2	± 3,0	± 3,5	± 3,1	± 3,6

List of references

See national foreword.

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