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INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

PHYSICAL CHEMISTRY DIVISION

COMMISSION ON PHYSICOCHEMICAL MEASUREMENTS AND STANDARDS

· SUBCOMMITTEE ON CALIBRATION AND

TEST MATERIALS

RECOMMENDED REFERENCE MATERIALS FOR REALIZATION OF PHYSICOCHEMICAL PROPERTIES

Recommendations (1976)

EDITOR: E. F. G. HERINGTON

SECTION: ABSORBANCE AND WAVELENGTH

COLLATOR: G. MILAZZO

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CONTENTS

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INTRODUCTION

The use of spectroscopic methods for physicochemical and analytical studies has grown extraordinarily during the last 30 yr and during that time the precision of the results has improved considerably. For the comparison of the results obtained by the use of different spectrometers it is essential that the instruments should be calibrated in the same manner and for this purpose a series of well-defined Reference Materials must be available.

Symbols and Units

The internal transmittance, T, is defined as the ratio of the transmitted to incident radiant or luminous flux of the sample itself disregarding boundary or container influence. The (decadic) absorbance, A, is defined as $-\log_{10}T$. Both T and A are dimensionless but are functions of the wavelength and of the thickness of the sample.

The primary standard of wavelength is that of the radiation corresponding to the transition between the unperturbed levels $2p_{10}$ and $5d_5$ of the krypton-86 atom. Secondary standards are based on other wavelengths of krypton-86, mercury-198 and cadmium-114 atoms; for a summary see Ref. 1. Wavelengths in the u.v. and visible regions are expressed in nanometers (nm) and in the i.r. in micrometers (μm). The reciprocal of the wavelength expressed in cm^{-1} is commonly used for the i.r. region. In this report the values of wavelengths for the u.v. and visible regions are all recorded as measured in air but the conditions for the measurements in the i.r. region are stated on each data sheet.

Reference Materials

Reference Materials for absorbance and wavelength measurements may be solids, liquids, gases or fabricated devices.

Solid Reference Materials are sometimes preferred because they are easy to handle and present no difficulties in transportation from one laboratory to another although there may be difficulties in the sample location in the instrument being calibrated or checked. The solid selected as a Reference Material must not change its optical properties with time or under the influence of light, heat or humidity.

Suitable Liquid Reference Materials are often prepared from solid or liquid reagents. However solutions are liable to change more readily than solids or pure liquids because the solvent may evaporate and dissolved solids may precipitate.

Gases and Vapour Reference Materials are often difficult to transport and handle if they are not constituents of the atmosphere or are not contained in closed and sealed cells.

Fabricated devices used as Reference Materials (e.g. discharge lamps, light sources and rotating sectors) are often expensive and may require special power supplies or other installations. Sometimes equipment has to be built so that the device can be inserted into the spectrometer. Such devices with mechanical parts may also suffer wear when they are used for a long period but nevertheless they are preferred by many investigators because devices often have good reproducibility.

The IUPAC Commission of Molecular Structure and Spectroscopy,I.5, has made extensive recommendations (Refs. 2-6) for Reference Materials for wavelength measurements in the i.r. region and those papers should be consulted for details. One mixture recommended by Commission I.5 is listed here (II/10) with the names of suppliers.

The following provisos apply to information on Reference Materials: (a) the recommended materials, in most instances, have not been checked independently by the IUPAC; (b) the quality of a material may change with time; (c) the quoted sources of supply may not be exclusive sources because no attempt has been made to seek all possible alternative sources; (d) the IUPAC does not guarantee any material that is recommended.

It is the intention of the Sub-Commission to revise from time to time information given in the Recommendations and users are invited to send suggestions for improvements nad extensions of the Recommendations to the Secretary of Commission I.4.

REFERENCES

1. G. W. C. Kaye and T. H. Laby, *Tables of Physical and Chemical Constants*, 4th Edn. Longman, London (1973).
2. Tables for the calibration of grating spectrometers in the range 4300 - 600 cm^{-1}. *Pure Appl. Chem.* 1, 537 (1961).
3. Wavenumbers for the calibration of prism and small grating spectrometers (Resolution 0.5 - 10 cm^{-1}) in the range 3950 - 600 cm^{-1}. *Pure Appl. Chem.* 1, 601 (1961).
4. Tables for the calibration of moderately high resolution spectrometers in the range 600 - 1 cm^{-1}. *Pure Appl. Chem.* 33, 613 (1973).

5. Tables for the calibration of low resolution spectrometers in the range 600 - 15 cm^{-1}. *Pure Appl. Chem.* 35, 639 (1973).
6. Corrigendum, Appendix. Revised spectrum of indene-camphor-cyclohexanone for the calibration of low resolution spectrometers in the range 4000 - 600 cm^{-1}. *Pure Appl. Chem.* 37, 649 (1974).

I/1

Physical property: Absorbance in the ultraviolet region
Unit: Dimensionless
Recommended reference material: Potassium dichromate in aqueous sulphuric acid solution
Range of variables: 235, 257, 313 and 350 nm
Physical state within the range: Liquid
Class: Calibration and Test Material
Contributors: I. Brown, J. P. Cali, G. Milazzo

Intended usage: Calibration of the absorbance scales of spectrometers

Sources of supply and/or methods of preparation: Samples of reagent grade potassium dichromate of purity better than 99.95% are available from many manufacturers. The required solution is prepared by dissolving 0.060 06 g of potassium dichromate in 1 kg of 0.005 M H_2SO_4. Measurements are carried out against a sulphuric acid solution of the same concentration.

Pertinent physicochemical data: The following values of the absorbances at the wavelengths listed refer to a 1.000 cm thickness of the above solution at 20° C: 235 nm, A = 0.748; 257 nm, A = 0.865; 313 nm, A = 0.292; 350 nm, A = 0.640. Minima in the absorbance curve occur at 235 and 313 nm and maxima occur at 257 and 350 nm.

REFERENCES

1. R. W. Burke, E. R. Deardorff and O. Menis, *Accuracy in Spectrophotometry and Luminescence Measurements* (editors R. Mavrodineanu, J. I. Shultz and O. Menis) National Bureau of Standards Special Publication No. 378, p. 95. U.S. Department of Commerce, Washington, DC (1973).
2. G. Milazzo, National Bureau of Standards Special Publication No. 408, p. 127. U.S. Department of Commerce, Washington, DC (1975).

I/2

Physical property: Absorbance in the visible region
Unit: Dimensionless
Recommended reference material: Copper sulphate in aqueous sulphuric acid solution
Range of variables: 15 wavelengths in the region 400 - 750 nm
Physical state within the range: Liquid
Class: Calibration and Test Material
Contributors: I. Brown, J. P. Cali, G. Milazzo

Intended usage: Calibration of the absorbance scales of spectrometers

Sources of supply and/or methods of preparation: Samples of reagent grade copper sulphate pentahydrate with a purity better than 99.9% are available from many manufacturers. The required solution is prepared by dissolving 20g of copper sulphate pentahydrate ($CuSO_4.5H_2O$) in water to which is added 10 cm^3 of sulphuric acid (d = 1.835) and then diluting the resulting mixture to make 1 dm^3 of solution. Measurements are carried out against a sulphuric acid solution of the same concentration.

Pertinent physicochemical data: Data are given in the references listed below but the following information for eight wavelengths at regular intervals and seven wavelengths for the emission lines of mercury (Hg) and helium (He) all refer to the absorbances of a 1.000 cm thickness of the above solution at 25° C.

Wavelength nm	A	Wavelength nm	A
400	0.0023	435.8 (Hg)	0.0013
450	0.0011	491.6 (Hg)	0.0019
500	0.0026	501.6 (He)	0.0028
550	0.0155	546.1 (Hg)	0.0135
600	0.0680	578.0 (Hg)	0.0368
650	0.224	587.6 (He)	0.0487
700	0.527	667.8 (He)	0.319
750	0.817		

REFERENCES

1. K. S. Gibson, National Bureau of Standards Circular No. 484, p. 43. U.S. Department of Commerce, Washington, DC (1949).
2. G. Kortüm, *Kolorimetrie, Photometrie und Spektrometrie*, 4th Edn, p. 303. Springer, Berlin (1962).

I/3

Physical property: Absorbance in the visible region
Unit: Dimensionless
Recommended reference material: Cobalt ammonium sulphate [$CoSO_4(NH_4)_2SO_4.6H_2O$] in aqueous sulphuric acid solution
Range of variables: 16 wavelengths in the region 400 - 750 nm
Physical state within the range: Liquid
Class: Calibration and Test Material
Contributors: G. Milazzo, T. Plebanski

Intended usage: Calibration of the absorbance scales of spectrometers

Sources of supply and/or methods of preparation: Samples of cobalt ammonium sulphate hexahydrate [$CoSO_4(NH_4)_2SO_4.6H_2O$] of purity better than 99.9% are available from many manufacturers. The required solution is prepared by dissolving 14.821 g of the salt and 10 cm^3 of sulphuric acid (d = 1.835) in water and diluting to 1 dm^3. Measurements are carried out against a sulphuric acid solution of the same concentration.

Pertinent physicochemical data: Data can be found in Refs. (1 - 3) but the following values of absorbance are for a 1.000 cm thickness of the above solution at 25° C for eight wavelengths at regular intervals and for eight wavelengths for the emission lines of mercury (Hg) and helium (He).

Wavelength nm	*A*	Wavelength nm	*A*
400	0.0125	404.7 (Hg)	0.0144
450	0.0773	435.8 (Hg)	0.0301
500	0.1635	491.6 (Hg)	0.150
550	0.0775	501.6 (Hg)	0.166
600	0.0137	546.1 (Hg)	0.0901
650	0.0105	578.0 (Hg)	0.0219
700	0.0054	587.6 (He)	0.0167
750	0.0028	667.8 (He)	0.0089

REFERENCES

1. K. S. Gibson, National Bureau of Standards Circular No. 484, p. 43. U.S. Department of Commerce, Washington, DC(1949).
2. G. Kortüm, *Kolorimetrie, Photometrie und Spektrometrie*, 4th Edn, p. 303.Springer, Berlin (1962).
3. A. Michalik, PKNIM, Poland, unpublished work.

I/4

Physical property: Absorbance in the visible region
Unit: Dimensionless
Recommended reference material: Cobalt [Co(II)] and nickel [Ni(II)] nitrates in aqueous perchloric acid solution
Range of variables: 302, 395, 512, 678 nm
Physical state within the range: Liquid
Class: Certified Reference Material
Contributors: J. P. Cali, H. Feuerberg

Intended usage: Calibration of the absorbance scales of spectrometers which normally use glass cuvettes.

Sources of supply and/or methods of preparation: Sets of three solutions and a bottle of solvent are available from supplier (H).

Pertinent physicochemical data: Certificates are provided by the supplier for the absorbances of the solutions at 25° C for the wavelengths 302, 395, 512 and 678 nm.

REFERENCES

1. R. W. Burke, E. R. Deardorff and O. Menis, *Accuracy in Spectrophotometry and Luminescence Measurements* (editors R. Mavrodineanu, J. I. Shultz and O. Menis) National Bureau of Standards Special Publication No. 378, p. 95, (1973).
2. G. Milazzo, National Bureau of Standards Special Publication No. 408, p. 127. U.S. Department of Commerce, Washington, DC (1975).

I/5

Physical property: Absorbance in the visible region
Unit: Dimensionless
Recommended reference material: Coloured glass filters
Range of variables: 400 - 800 nm
Physical state within the range: Solid
Class: Certified Reference Material
Contributors: I. Brown, J. P. Cali, H. Feuerberg

Intended usage: Calibration of the absorbance scales of spectrometers

Sources of supply and/or methods of preparation: Coloured glass filters are available from suppliers (D), (E), (H), (G).

Pertinent physicochemical data: Certified values for absorbance and/or transmittance are provided by the suppliers of the filters whose instructions for the use and handling must be followed strictly.

REFERENCES

1. R. Mavrodineanu, National Bureau of Standards Technical Note No. 584, p. 18. U.S. Department of Commerce, Washington, DC (1971).
2. R. W. Burke, E. R. Deardorff and O. Menis, *Accuracy in Spectrometry and Luminescence Measurements* (editors R. Mavrodineanu, J. I. Shultz and O. Menis), National Bureau of Standards Special Publication No. 378, p. 31. U.S. Department of Commerce, Washington, DC (1973).

I/6

Physical property: Transmittance in the infrared region
Unit: Dimensionless
Recommended reference material: Rotating sectors
Range of variables: Transmittance between 0.04 and 0.96
Physical state within the range: Mechanical device
Class: Calibration and Test Material
Contributors: I. Brown, T. Plebanski, G. Milazzo

Intended usage: Calibration of transmittance scales of spectrometers

Sources of supply and/or methods of preparation: Rotating sectors are available from many suppliers.

Pertinent physicochemical data: Instructions for use and values of transmittance are provided by the suppliers.

REFERENCE

1. R. N. Jones, *Pure Appl. Chem.* 18, 303 (1969).

II/1

Physical property: Wavelength in the ultraviolet region
Unit: nanometers (nm)
Recommended reference material: Low pressure discharge lamps containing cadmium, mercury or zinc
Range of variables: 185 - 400 nm
Physical state within the range: Device
Class: Calibration and Test Material
Contributors: H. Feuerberg, G. Milazzo

Intended usage: Calibration of wavelength scales of spectrometers

Sources of supply and/or methods of preparation: Suitable lamps are available from many manufacturers. Lamps containing other elements are also available.

Pertinent physicochemical data: Sharp maxima occur in the emission spectra at the following wavelengths:

Lamp	Wavelength nm	Lamp	Wavelength nm
Mercury	184.96	Mercury	253.652
Zinc	213.856	Mercury	365.015
Cadmium	228.802	Mercury	404.656

REFERENCE

1. G. R. Harrison, *Wavelength Tables*, M.I.T. Press, Cambridge, Mass. (1969).

II/2

Physical property: Wavelength in the ultraviolet region
Unit: nanometers (nm)
Recommended reference material: Hollow cathode discharge lamps
Range of variables: 203 - 420 nm
Physical state within the range: Device
Class: Calibration and Test Material
Contributor: G. Milazzo

Intended usage: Calibration of the wavelength scales of spectrometers

Sources of supply and/or methods of preparation: Suitable hollow cathode lamps are available from many suppliers.

Pertinent physicochemical data: The wavelengths of emission lines from many lamps are given in the reference quoted below. The following table shows some sharp emission lines obtainable from some selected lamps.

Lamp	Wavelength nm	Lamp	Wavelength nm
Magnesium	202.582	Magnesium	285.213
Zinc	213.856	Zinc	307.590
Lead	216.999	Copper	324.754
Cadmium	228.802	Cadmium	326.106
Mercury	253.652	Rhodium	343.489
Lead	283.307	Tungsten	400.875

REFERENCE

1. G. R. Harrison, *Wavelength Tables*, M.I.T. Press, Cambridge, Mass. (1969).

II/3

Physical property: Wavelength in the ultraviolet region
Unit: nanometers (nm)
Recommended reference material: Holmium (III) ions in aqueous perchloric acid solution
Range of variables: 200 - 400 nm
Physical state within the range: Liquid
Class: Calibration and Test Material
Contributor: G. Milazzo

Intended usage: Calibration of wavelength scales of spectrometers

Sources of supply and/or method of preparation: Suitable samples of holmium sesqui-oxide (Ho_2O_3) are available from many suppliers. The required solution is prepared by dissolving 4g of holmium sesqui-oxide (Ho_2O_3) in 100 g of 1.4 M perchloric acid solution.

Pertinent physicochemical data: G. Milazzo (3) using a recording Cary XVII spectrophotometer calibrated immediately before use with a mercury-discharge lamp found very sharp absorption maxima at the following wavelengths: 241.15; 249.75; 278.2; 287.15; 333.5; 345.6; 361.5 and 385.6 nm.

REFERENCES

1. J. M. Vandenbelt, *J. Opt. Soc. Amer.* 51, 802 (1961).
2. J. McNeirny and W. Slavin, *Appl. Opt.* 1, 365 (1962).
3. G. Milazzo, unpublished work.

II/4

Physical property: Wavelength in the visible region
Unit: nanometers (nm)
Recommended reference material: Low pressure discharge lamps containing cadmium or mercury
Range of variables: 435 - 644 nm
Physical state within the range: Device
Class: Calibration and Test Material
Contributor: G. Milazzo

Intended usage: Calibration of the wavelength scales of spectrometers

Sources of supply and/or methods of preparation: Low pressure discharge lamps containing cadmium or mercury are available from many suppliers.

Pertinent physicochemical data: The following values for the emmission lines obtained from commercial lamps are useful for the calibration of spectrometers.

Lamp	Wavelength nm	Lamp	Wavelength nm
Mercury	435.835	Mercury	546.075
Cadmium	467.816	Mercury	579.065
Cadmium	479.992	Cadmium	643.847

REFERENCES

1. E. J. G. Engelhard and F. Bayer-Helms, *Metrologia* 8, 91 (1972).
2. G. R. Harrison, *Wavelength Tables*, M.I.T. Press, Cambridge, Mass. (1969).

II/5

Physical property: Wavelength in the visible region
Unit: nanometers (nm)
Recommended reference materials: Hollow cathode discharge lamps containing calcium, strontium, sodium, lithium or potassium
Range of variables: 400 - 800 nm
Physical state within the range: Device
Class: Calibration and Test Material
Contributor: G. Milazzo

Intended usage: Calibration of wavelength scales of spectrometers

Sources of supply and/or methods of preparation: Hollow cathode lamps are available from many suppliers

Pertinent physicochemical data: Lamps containing the elements indicated exhibit emission lines with the following values of wavelength/nm: calcium, 422.673; strontium, 460.733; sodium, 588.995; lithium, 670.784; potassium, 766.491.

REFERENCE

1. G. R. Harrison, *Wavelength Tables*, M.I.T. Press, Cambridge, Mass. (1969).

II/6

Physical property: Wavelength in the visible region
Unit: nanometers (nm)
Recommended reference material: Holmium (III) ions in aqueous perchloric acid solution
Range of variables: 400 - 650 nm
Physical state within the range: Liquid
Class: Calibration and Test Material
Contributor: G. Milazzo

Intended usage: Calibration of wavelength scales of spectrometers

Sources of supply and/or methods of preparation: Suitable samples of holmium sesqui-oxide (Ho_2O_3) are available from many suppliers. The required solution is prepared by dissolving 4g of holmium sesqui-oxide (Ho_2O_3) in 100 g of 1.4 M perchloric acid solution.

Pertinent physicochemical data: G. Milazzo (3) using a recording Cary XVII spectrophotometer calibrated immediately before use with a mercury-discharge lamp found very sharp absorption maxima at the following wavelengths: 416.2; 450.7; 452.0; 467.75; 485.25; 536.3; 640.5 nm.

REFERENCES

1. J. M. Vandenbelt, *J. Opt. Soc. Amer.* 51, 802 (1961).
2. J. McNeirny and W. Slavin, *Appl. Opt.* 1, 365 (1962).
3. G. Milazzo, unpublished work.

II/7

Physicochemical property: Wavelength in the infrared region
Unit: micrometers (μm)
Recommended reference material: Lasers
Range of variables: Infrared wavelength range
Physical state within the range: Device
Class: Calibration and Test Material
Contributors: H. Feuerberg, P. Trubirohe

Intended usage: Calibration of wavelength scales of spectrometers

Sources of supply and/or methods of preparation: Various lasers are available from many different suppliers.

Pertinent physicochemical data: Different lasers emit light at different fixed wavelengths, thus a helium - neon laser emits light with sharp lines at 1.1523 and 3.3912 μm in air. Lasers of very good wavelength reproducibility can be made by frequency stabilization by electronic feedback control. Lasers of very much better wavelength reproducibility can be made by stabilization absorption techniques. Measurements of the vacuum wavelength of the i.r. helium - neon laser stabilized by saturated absorption in methane, give a value of 3.392 231 39 μm with a measurement uncertainty of 1 part in 10^8.

REFERENCES

1. D. Ross, *Laser*, Akademische Verlagsgellschaft, Frankfurt/Main (1966).
2. N. Kleen and R. Muller, *Laser*, Springer, Berlin (1969).
3. B. A. Lengyel, *Laser*, Kohlhammer, Stuttgart (1969).
4. G. W. C. Kaye and T. H. Laby, *Tables of Physical and Chemical Constants*, 14th Edn, p. 86. Longman, London (1973).

II/8

Physical property: Wavenumber in the infrared region
Unit: cm^{-1} (vacuum)
Recommended reference material: Air containing water vapour
Range of variables: 600 - 157 cm^{-1}
Physical state within the range: Gas
Class: Calibration and Test Material
Contributors: H. Feuerberg, D. Gross, K. Kienitz, Y. Mashiko, G. Milazzo

Intended usage: Calibration of the wavenumber (wavelength) scales of spectrometers

Sources of supply and/or methods of preparation: Air containing water vapour, relative humidity 32%, path length 60 cm, temperature 20° C.

Pertinent physicochemical data: Blaine *et al.* (1) have recorded spectra and the following values for the wavenumbers (vacuum) of sharp absorption bands.

Absorption bands of water (wavenumbers reduced to vacuum)

Band no. & class	Wavenumber cm^{-1}	Band no. & class	Wavenumber cm^{-1}	Band no. & class	Wavenumber cm^{-1}
1A	600.11	41A	434.83	81B	280.34
2A	594.96	42A	431.16	82B	278.32
3B	591.85	43B	425.34	83B	276.15
4A	584.74	44B	423.04	84A	271.85
5C	580.8	45B	419.86	85B	266.21
6A	576.14	46C	418.5	86B	263.26
7A	571.31	47B	400.38	87B	257.03
8A	569.28	48A	398.97	88B	253.96
9A	567.23	49B	397.48	89B	247.94
10A	554.63	50B	396.45	90C	245.3
11B	550.00	51A	394.24	91A	233.34
12B	547.86	52C	385.1	92C	231.4
13B	546.32	53A	383.83	93B	227.83
14B	545.30	54A	378.56	94B	226.27
15A	536.26	55B	376.23	95A	223.72
16A	525.98	56B	375.35	96B	221.67
17A	519.60	57B	374.54	97B	216.79
18B	517.79	58B	369.96	98C	214.6
19B	516.82	59B	362.76	99B	213.95
20B	510.47	60A	358.50	100B	212.61
21A	506.93	61A	357.29	101A	208.46
22B	504.41	62B	354.38	102C	202.7
23B	502.27	63B	351.86	103C	200.4
24A	494.19	64A	349.79	104B	197.50
25C	492.0	65B	345.85	105A	195.86
26A	486.14	66A	343.21	106B	194.37
27A	483.98	67A	340.55	107B	193.45
28A	481.04	68B	335.16	108A	188.21
29A	476.39	69C	327.6	109A	183.46
30C	472.5	70B	323.80	110A	181.40
31A	470.49	71B	315.03	111C	179.0
32B	468.76	72A	311.72	112A	177.55
33B	467.96	73A	309.51	113B	176.05
34A	461.44	74C	303.0	114B	173.45
35C	457.8	75A	298.40	115B	170.37
36A	452.87	76B	290.74	116C	166.6
37B	446.80	77A	289.46	117A	161.79
38A	443.71	78B	285.04	118A	160.20
39B	441.96	79B	284.61	119B	158.89
40A	436.46	80B	282.25	120B	157.82

Class A Bands are reliable to ± 0.03, Class B Bands are reliable to ± 0.1 and Class C Bands are reliable to ± 0.3 cm^{-1}.

REFERENCE

1. L. R. Blaine, E. K. Plyler and W. S. Benedict, *J. Res. Nat. Bur. Std.* 66A, 223 (1962).

II/9

Physical property: Wavenumbers in the infrared region
Unit: cm^{-1} (vacuum)
Recommended reference material: Polystyrene film
Range of variables: 3000 - 700 cm^{-1}
Physical state within the range: Solid
Class: Calibration and Test Material
Contributors: I. Brown, H. Feuerberg, D. Gross, Y. Mashiko

Intended usage: Calibration of wavenumber (wavelength) scales of spectrometers

Sources of supply and/or methods of preparation: Purified polystyrene is used as a cast or drawn film with a thickness of about 0.025 mm.

Pertinent physicochemical data: Sharp absorption bands occur at the following wavenumbers (vacuum)/cm^{-1}: 3026; 2851; 1946; 1802; 1603; 1495; 1154; 1028; 06; 700.

REFERENCES

1. E. K. Plyler and C. W. Peters, *J. Res. Nat. Bur. Std.* 45, 462 (1950).
2. E. K. Plyler, L. R. Blaine and M. Novak, *J. Res. Nat. Bur. Std.* 58, 195 (1957).
3. A. E. Martin, *IR Instrumentation and Techniques*, p. 58. Elsevier, Amsterdam (1966).
4. K. N. Rao, C. J. Humphreys and D. H. Rank, *Wavelength Standards in IR*, Academic Press, New York (1966).
5. R. G. I. Miller, *Laboratory Methods in IR Spectroscopy*, 2nd Edn, Heyden, London (1965).
6. S. Krimm, *Fortschr. Hochpolym. Forsch.* 2, 51 (1960).

II/10

Physical property: Wavenumber in the infrared region
Unit: cm^{-1} (vacuum)
Recommended reference material: Indene (98.4%), camphor (0.8%), cyclohexanone (0.8%), the percentages are by weight (Table 1), or the same components in equal proportions (Table 2)
Range of variables: 4000 - 690 cm^{-1} (Table 1) and 600 - 300 cm^{-1} (Table 2)
Physical state within the range: Liquid
Class: Calibration and Test Material
Contributors: H. Feuerberg, D. Gross, Y. Mashiko, G. Milazzo

Intended usage: Calibration of the wavenumber (wavelength) scales of spectrometers

Sources of supply and/or methods of preparation: Samples are available from suppliers (A), (B), (C), (F), (I) and (J).

Pertinent physicochemical data: The recommended calibration bands (wavenumbers in vacuum) shown in Tables 1 and 2 are taken from Ref. 1.

Table 1. Indene (98.4%), camphor (0.8%) and cyclohexanone (0.8%)

Band no.	Wavenumber cm^{-1}	Band no.	Wavenumber cm^{-1}	Band no.	Wavenumber cm^{-1}
1	3927.2±1.0	33	2172.8	55	1361.1
2	3901.6	34	2135.8±1.0	57	1312.4
3	3798.9	35	2113.2	58	1288.0
5	3660.6±1.0	36	2090.2	60	1226.2
8	3297.8±1.0	39	1943.1	61	1205.1
9	3139.5	40	1915.3	62	1166.1
10	3110.2	41	1885.1	64	1122.4
12	3025.4	42	1856.9	66	1067.7±1.0
15	2887.6	44	1797.7±1.0	67	1018.5
17	2770.9	44α	1741.9	69	947.2
19	2673.3	44β	1713.4	70	942.4
20	2622.3	47	1661.8	71	914.7
21	2598.4±1.0	48	1609.8	72	861.3
23	2525.5	49	1587.5	73	830.5
28	2305.1	51	1553.2	74	765.3
29	2271.4	53	1457.3±1.0	76	718.1
30	2258.7	54	1393.5	77	692.6±1.0

Values are accurate to ±0.5 cm^{-1} unless otherwise indicated.

Cell thickness: 0.2 mm for the regions 4000 - 3100, 2800 - 1500 cm^{-1}; 0.03 mm for the regions 3100 - 2800, 1650 - 1600, 1400 - 800 cm^{-1}; contact film for the region 800 - 690 cm^{-1}. Band No. 44α is from camphor and Band No. 44β is from cyclohexanone. This mixture was also investigated by Lukasiewicz-Ziarkowska (2) whose results differ from those in Table 1 by 1.1 cm^{-1} at 4000 cm^{-1} and by 0.2 cm^{-1} at 600 cm^{-1}; the differences vary linearly from 4000 to 600 cm^{-1}.

Table 2. Equimixture of indene, comphor and cylohexanone; wavenumber (vacuum)

Band no.	Wavenumber cm^{-1}	Band no.	Wavenumber cm^{-1}	Band no.	Wavenumber cm^{-1}
1	592.1	4	490.2±1.0	7	381.6
2	551.7	5	420.5	8	301.4
3	521.4	6	393.1		

Values are accurate to ±0.5 cm^{-1} unless otherwise indicated.

Cell thickness 0.05 mm. Bands No. 3 and 8 are from camphor and Band No. 4 is from cyclohexanone.

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Physical property: Wavenumbers in the infrared region
Unit: cm^{-1} (vacuum)
Recommended reference material: 1,2,4-trichlorobenzene
Range of variables: 4700 - 4100 cm^{-1}; 600 - 400 cm^{-1}
Physical state within the range: Liquid
Class: Calibration and Test Material
Contributors: G. Milazzo, T. Plebanski

Intended usage: Calibration of the wavenumber (wavelength) scales of spectrometers

Sources of supply and/or methods of preparation: Samples are available from supplier (J).

Pertinent physicochemical data: Absorption bands occur at the following wavenumbers (vacuum) when the path lengths indicated are used, for a 0.5 mm thickness 4645.6; 4324.1, 4161.4; 4102.7 cm^{-1} and for a 0.025 thickness 574.8; 550.7; 458.7; 439.4 cm^{-1}.

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