INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

PHYSICAL CHEMISTRY DIVISION

COMMISSION ON PHYSICOCHEMICAL MEASUREMENTS AND STANDARDS
SUB-COMMISSION ON CALIBRATION AND TEST MATERIALS

RECOMMENDED REFERENCE MATERIALS FOR REALIZATION OF PHYSICOCHEMICAL PROPERTIES

EDITOR: E. F. G. HERINGTON

SECTION: DENSITY

COLLATORS: I. BROWN and J. E. LANE

PERGAMON PRESS
OXFORD · NEW YORK · PARIS · FRANKFURT

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CONTENTS

NOMENCLATURE AND UNITS

Absolute density (Masse volumique) Symbol, ρ; Unit, $kg\,m^{-3}$. Relative density (Densité relative) Symbol, d, where d is the ratio of the absolute density of a material to the absolute density of a specified reference material. The conditions, pressure, temperature, etc. may be different for the two materials. In the section on water in this report d_t refers to the ratio of the absolute density, ρ_t, of a given sample of water at a temperature $t°C$, relative to its maximum value ρ_{max} which is reached at a temperature close to 4°C, the water being free from dissolved gases and under a pressure of 101 325 Pa. Temperatures refer to the International Practical Temperature Scale of 1968.

INTRODUCTION

The U.S. National Bureau of Standards has determined the densities of four silicon objects to a standard deviation of 0·25 ppm with a systematic error of 0·7 ppm. These objects will be used as in-house reference standards in the determination of densities of liquids and solid objects. The densities of liquid reference materials will be in the range of about 800–2000 $kg\,m^{-3}$. At the present time the NBS, co-operating with other national standards laboratories, will compare the densities of suitable solid artifacts with the single-crystal, in-house silicon density standards of NBS. The uncertainty in such a comparison is *no more* than three parts per million. This number represents three standard deviations plus 1·4 ppm systematic uncertainty in the silicon crystal standards. However in the measurements of density a liquid reference material will frequently be required. Water and mercury are highly suitable substances for the calibration of apparatus used for density measurement and the determination of the volume of apparatus. Samples of a small number of other liquids of certified density are also required for use when water or mercury are unsuitable.

METHODS OF MEASUREMENT

A good general description of the apparatus and of methods for the measurement of density is given by Bauer and Lewin[1] and by Bowman and Schoonover.[2] The most

precise methods are the pycnometric,[1,3] hydrostatic weighing,[1,4] magnetic float[1,2,5] and temperature flotation[6] methods.

At the present time methods are available for the determination of the density of a liquid relative to that of a reference liquid with a precision of 1×10^{-3} kg m^{-3} or better. However it is not possible to take full advantage of this precision in absolute density determinations because of uncertainty in the absolute density of water, and the uncertainty in the meniscus volume of mercury resulting from variations in its surface properties.

WATER AS A REFERENCE MATERIAL

In spite of the problems of isotopic variation between samples of carefully purified water from various sources, water is still the most suitable material for use as a density reference material. Recent work at BIPM and the Institute of Oceanography in France has enabled variations in the densities of samples of water to be related to the isotopic compositions.

Standard Mean Ocean Water (SMOW)

To allow for small variations in absolute density between samples of purified water due to variations in their isotopic composition it is necessary to have a reference datum. It has been recommended by Girard and Menaché[7] that Standard Mean Ocean Water (SMOW) be used as a reference datum for precise density determinations.

Standard Mean Ocean Water is a pure water obtained from the ocean which was prepared by Craig,[8] who proposed it as a universal isotopic standard for reporting deuterium and ^{18}O concentrations in natural waters. SMOW is kept by the International Atomic Energy Agency which is responsible for its distribution in small quantities to laboratories who specialize in isotope ratio measurements by mass spectrometry.

The isotopic composition of SMOW has been determined by Craig[8] (^{18}O) and Hagemann et al.[9] (D), the values found are as follows:

$$r_{18}(\text{SMOW}) = [^{18}\text{O}]/[^{16}\text{O}] = (1993\cdot4 \pm 2\cdot5) \times 10^{-6}$$

$$r_{\text{D}}(\text{SMOW}) = [\text{D}]/[\text{H}] = (155\cdot76 \pm 0\cdot05) \times 10^{-6}$$

where r_{18} and r_{D} are the ratios of the numbers of the specified atoms in the sample.

Variation in density of water as a function of isotopic composition

The isotopic composition of any given sample of water is usually determined by comparison with SMOW using mass spectrometry. The results of this comparison are expressed by the relative differences δ_{18} and δ_{D}, which are defined by the following relations:

$$\delta_{18} = \left(\frac{r_{18}(\text{sample})}{r_{18}(\text{SMOW})} - 1 \right) \times 10^3$$

$$\delta_{\text{D}} = \left(\frac{r_{\text{D}}(\text{sample})}{r_{\text{D}}(\text{SMOW})} - 1 \right) \times 10^3. \quad (1)$$

The variation in density of water with isotopic concentration has been investigated by Girard and Menaché[10-12] over a density interval of 2×10^{-2} kg m^{-3}. The isotopic density correction may be determined from the following provisional relation which was obtained from

their experimental measurements

$$[\rho(\text{sample}) - \rho(\text{SMOW})] \times 10^3/\text{kg m}^{-3}$$
$$= 0\cdot211\delta_{18} + 0\cdot0150\delta_{\text{D}}. \quad (2)$$

This relation applies to absolute densities at temperatures from 0 to 40°C for samples prepared from natural waters. It is estimated that the uncertainty introduced by the use of this provisional relation is about 1×10^{-3} kg m^{-3}. This error can be reduced by using samples of water having an isotopic composition as close as possible to that of SMOW.

Preparation of water of known density

Sea water has a very stable isotopic composition and as a result density changes of samples of mean ocean water resulting solely from differences in isotopic composition do not exceed 1×10^{-3} kg m^{-3}. Cox, McCartney and Culkin[13] have proposed a triple distillation method for the purification of sea water and natural waters which, if followed rigorously, does not alter the deuterium or oxygen isotopic concentration. This fact has been verified by Menaché[14] employing the mass spectrometric determinations of the D/H and ^{18}O/^{16}O ratios by the methods described by Nief et al.[15,16]

For density determinations of high precision it may be necessary to make a fourth distillation under reduced pressure to degas the water sample. To ensure that the method of triple distillation and degassing has been carried out adequately and that no risk of errors remain, the exact isotopic composition of the resultant water must be determined by mass spectrometric analysis. It is advantageous to use purified sea water to minimise the isotopic corrections.

The difference in absolute density of the sample from that of SMOW can be calculated using equations (1) and (2). The absolute density of the sample can then be calculated at the required temperature once the absolute density of SMOW is known at that temperature.

The absolute density of SMOW as a function of temperature

Since the beginning of this century a large number of tabulations of the relative and absolute densities of water in the temperature range 0–40°C have been published which give appreciably different values for any particular temperature. These tables are often given without reference to their origin, without adequate definition of the particular temperature scale to which they refer and, for absolute values, without reference to the isotopic composition of the water used. This leads to considerable confusion and doubt in the assessment of precise density data as scientists may use a particular, but unspecified, tabulation in the belief that its contents are both unique and accurate. This unfortunate situation has been reviewed recently by Menaché and Girard.[17]

Relative density of water

All the published tables of relative density ($d_t = \rho_t/\rho_{\text{max}}$) are based on the direct observations of the thermal expansion of water made by Thiesen et al.[18] published in 1900 and values published by Chappuis[19] in 1907. More recently Steckel and Szapiro[20] have made new determinations which have yielded values closer to those reported by Thiesen et al. than to those recorded by Chappuis. The tables published by Mendeleev,[21] Tilton and Taylor,[22] Kell,[23] Bigg,[24] Aleksandrov and Trakhtengerts[25] and

Wagenbreth and Blanke[26] which can be designated "derived tables" are all based on reassessments of the basic measurements made by Thiesen et al. and by Chappuis.

Menaché and Girard[17] have emphasised that the values of relative density, d, shown in these basic and derived tables are independent of the isotopic composition of the water used, as both t_{max} and the thermal expansion coefficient show negligible variation within the range of isotopic concentrations found for natural waters.

At the present time, our knowledge of the values of the relative density of water as a function of temperature in the range 0 to 40°C is, unfortunately, subject to appreciable uncertainties.

The values given in the two basic tables by Thiesen and Chappuis show deviations that increase in absolute value with the temperature, Thiesen's values being generally lower than those reported by Chappuis. Above 16°C these deviations exceed 1×10^{-3} kg m^{-3} and rapidly reach an unacceptable level of 6×10^{-3} kg m^{-3} at 25° rising to 9×10^{-3} kg m^3 at 40°C.

In addition to this, there are problems due to the definitions of temperature scales. The data reported by Thiesen et al. and by Chappuis related to the "Echelle Normale" of the hydrogen thermometer. There are two schools of thought;[17] one which believes this temperature scale to coincide practically (in the range 0–40°C) with the International Practical Temperature Scale of 1968 (IPTS-68) and another which believes it to coincide practically with the International Practical Temperature Scale of 1948 (IPTS-48). In spite of the thorough investigations made by Hall,[27] this difference of opinion cannot be resolved until new precise density determinations relative to IPTS-68 have been made. At 40°C the difference between IPTS-68 and IPTS-48 is 0·01 K. The measurements made by Steckel and Szapiro[20] were related to IPTS-48.

Absolute density of SMOW

To calculate the absolute density of SMOW as a function of temperature from values of relative density we require a value of ρ_{max}(SMOW). Absolute determinations of ρ_{max} for water made at the beginning of the century[28] led to the mean value $\rho_{max} = 999\cdot972$ kg m^{-3}, but we do not know the isotopic composition of the water corresponding to this value. Girard and Menaché[7,17] have proposed to take for the maximum absolute density of SMOW, which occurs at a temperature close to 4°C under a pressure of one standard atmosphere (101 325 Pa) in the absence of dissolved atmospheric gases, the value:

$$\rho_{max}(\text{SMOW}) = 999\cdot975 \text{ kg m}^{-3}.$$

Recommended table of the absolute density of SMOW for the temperature range 0–40°C

To reduce confusion and to promote uniformity in the determination of liquid densities, it is felt by this IUPAC Commission that a single table of provisional values of the absolute density of SMOW, a water of known isotopic composition, be recommended pending new precise determinations of the density of water. The table of recommended values attached to this report uses ρ_{max}(SMOW) equal to 999·975 kg m^{-3} and is based on the table given by Bigg[24] in which the figures are the weighted means of the values presented by Thiesen et al. and by Chappuis. It has been assumed that the Echelle Normale coincides with IPTS-68 and therefore that the

temperatures in reference 24 refer to the currently used scale. Account has been taken of the possible effects of the uncertaintities in the temperature scale of the original measurements in the estimates now given of the maximum uncertainties in the tabulated values of density.

Maximum uncertainty in tabulated density values—units of 10^{-3} kg m^{-3}

Source	15°C	25°C	40°C
Uncertainty in ρ_{max}(SMOW)	±3	±3	±3
Differences between basic d_t tables of Thiesen and Chappuis	±1	±2	±5
Uncertainty in temperature scale	−1	−2	−4
Total maximum uncertainty	±5	±7	±12

These uncertainties can only be reduced by precise redeterminations of the absolute density, relative to IPTS-68, of samples of water of known isotopic composition. Measurements have already been commenced in Australia and in Japan and it is hoped that other countries will also contribute.

Problems due to the effect of pressure and dissolved gases on the density of water

The effect of these two factors on the density of water has been discussed by Menaché.[29] A change in pressure of 1 mmHg (133·3 Pa) changes the density of water by approximately $0\cdot066 \times 10^{-3}$ kg m^{-3}. Values of the compressibility of water from −20 to 110°C are also given by Kell.[23]

The effect of dissolved gases is not known with adequate accuracy and may introduce some uncertainty in density measurements. At 0°C air-saturated water is about $2-3 \times 10^{-3}$ kg m^{-3} less dense than air-free water; from 5 to 8°C, this difference is about 3×10^{-3} kg m^{-3} and above 20°C it is less than 1×10^{-3} kg m^{-3}.

MERCURY AS A REFERENCE MATERIAL

The density of mercury at 20°C has been measured with great accuracy by Cook,[30,31] its thermal expansion is known over a wide range of temperature probably more exactly than that of any other liquid,[32,33] and a table of values of the density of mercury in the range −20 to +300°C (International Practical Temperature Scale of 1948) based on these measurements has been published.[34] Nevertheless, it is questionable whether mercury will often be the most suitable calibration or test material for use in pycnometric measurement of densities because it suffers from the following disadvantages.

(i) As the density of mercury is so much greater than the density of most other liquids, difficulties may arise because of the relatively large mass that must be determined when the pycnometer contains mercury.

(ii) The interpretation of measurements may be difficult because the contact angle of mercury with the walls of the vessel (ca. 140° when the vessel is glass) differs greatly from that of other liquids and is affected by the cleanliness of the apparatus and the purity of the mercury.

However the density of mercury is particularly important because of the use of mercury as a manometric fluid. The following paragraph is extracted from the report on the International Practical Temperature Scale of 1968 (IPTS-68).[35]

"In practice pressures are usually determined by means of a mercury column. The mean density of pure mercury at the temperature t_{68} in a barometric column supported by the pressure p being measured is given, with sufficient accuracy over the temperature range from 0 to 40°C and for the pressures relevant to these measurements, by the relation

$$\rho\left(t_{68}, \frac{p}{2}\right) = \frac{\rho(20°C, p_0)}{[1 + A(t_{68} - 20°C) + B(t_{68} - 20°C)^2] \times \left[1 - \chi\left(\frac{p}{2} - p_0\right)\right]}$$

where $A = 18\ 115 \times 10^{-8}\ °C^{-1}$, $B = 0\cdot8 \times 10^{-8}\ °C^{-2}$,

$\chi = 4 \times 10^{-11} N^{-1}\ m^2$,

$\rho(20°C,\ p_0) = 13\ 545\cdot87\ kg\ m^{-3}$ is the density of pure mercury at $t_{68} = 20°C$ under a pressure $p_0 = 1$ standard atmosphere (101 325 Pa)." A sufficiently accurate value of the local gravity may be obtained by using the Réseau Gravimétrique International Unifié 1971 (IGSN-71) de l'Union Géodésique et Géophysique Internationale.

A simple relationship between density and the compressibility has been assumed in the above relation. Mercury is also used for confining the sample and transmitting the pressure in volumetric measurements on fluids at high pressures, and under these conditions a more complex equation for the compressibility may be required.[36] When mercury is used as a manometric fluid, the effect of capillary depression must also be taken into account.[37-40]

Mercury is also frequently used for the determination by weighing of the volumes of vessels. For this purpose the large mass involved may not always be a disadvantage, and mercury may in many instances be the most suitable substance because of its low volatility and non-wetting character.

Preparation of a suitable sample of mercury

The most widely used method of purifying mercury, after it has been filtered to remove gross contamination, is treatment by dilute nitric acid (say, 1 part by volume of concentrated acid in 20 parts of the solution) to remove base metals, followed by washing with water, and by distillation to remove the higher-boiling metals.[30,41,42] It has been shown that the nitric acid treatment is more effective if the mercury is shaken for a few minutes with the acid rather than for the mercury to fall in drops through a column of the acid (although the latter procedure has often been used, and commercial apparatus for carrying it out conveniently is available); and that distillation is most effective if carried out in the presence of clean air at a pressure of about 3 kPa.

The purified mercury is best stored in soft glass or polythene bottles (it may be more difficult to pour cleanly from the latter because of the development of electrostatic charges)[43] and the bottles, their interior surfaces free of scratches, should be cleaned with nitric acid before use. If base metals, such as zinc or copper, are present in mercury a film quickly forms on the bright surface, but slight surface contamination of even the purest samples is often observed after prolonged storage in air, and it is therefore preferable for air to be displaced from the bottles by an inert gas or for the mercury to be stored *in vacuo*. Small amounts of impurity on the surface of mercury may be removed by filtration, or a pure sample

may be drawn off through a tube dipping below the surface.

Effect of impurities and isotopic composition on the density of mercury

The following table[30] shows the amounts of impurities by weight which might produce a change in the density of mercury of $1 \times 10^{-2}\ kg\ m^{-3}$.

Metal	ppm	Metal	ppm
platinum	2·7	tin	1·1
gold	3·4	iron	1·4
zinc	1·5	sodium	0·13
copper	1·9	calcium	0·13
lead	4·3	aluminium	0·25

Furthermore, mercury is composed of isotopes of mass numbers 196, 198, 199, 200, 201, 202 and 204 and variations of 0·005% in the abundances of one or two isotopes would change the density of a sample of mercury by $1 \times 10^{-2}\ kg\ m^{-3}$. The sensitivities of analysis of impurities or of the determination of isotopic abundances available at the time of the investigation by Cook and Stone[30,31] were not adequate to ensure the absence of impurities or of isotopic constancy to a degree sufficient for the density to be specified more closely than $10 \times 10^{-2}\ kg\ m^{-3}$. Nevertheless, four samples of mercury of different origins were purified by at least two successive shakings with nitric acid and at least two distillations in the presence of air, and the values obtained for their densities agreed within $1 \times 10^{-2}\ kg\ m^{-3}$. It therefore appears probable that mercury can be prepared with a lower concentration of impurities than could then be assayed and that the methods of purification do not have a significant effect on the isotopic composition.

Absolute density of mercury

A table of the absolute density of mercury from −20 to +300°C, based on the table given by Bigg,[34] is attached. In this table due allowance has been made for the change in the temperature scale to IPTS-1968. The likely errors in the values are also shown.

OTHER REFERENCE MATERIALS

Samples of a number of hydrocarbons with certified values of density are available from National Laboratories.[44] Samples of 2,2,4-trimethylpentane are available from suppliers (A), (B) and (C). Samples of hexane, octane, nonane, cyclohexane, methylcyclohexane, *trans*-decahydronaphthalene and toluene are also available from supplier (A) with values of density certified to $\pm 0\cdot005\ kg\ m^{-3}$ at temperatures at 5 K intervals from 20 to 50°C. Samples of methylcyclohexane and toluene are available from supplier (C) with densities to $\pm 0\cdot05\ kg\ m^{-3}$ at 20°, 25° and 30°C and samples of hexadecane, *trans*-decahydronaphthalene and 1-methylnaphthalene with densities to $\pm 0\cdot08\ kg\ m^{-3}$ at the same temperatures are also available from supplier (C).

Three of these Certified Reference Materials have been chosen as suitable examples. Data sheets are attached for 2,2,4-trimethylpentane, cyclohexane and *trans*-bicyclo[4,4,0]decane (*trans*-decahydronaphthalene).

The following provisos apply to the information on sources of supply: (a) the recommended materials, in most instances, have not been checked independently by

the IUPAC; (b) the quality of material may change with time; (c) the quoted sources of supply may not be exclusive sources because no attempt has been made to seek out 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 improvement and extension of the Recommendations to the Secretary of Commission I.4.

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1

Physical property: Density, ρ
Unit: $kg\,m^{-3}$
Recommended reference material: Water (H_2O)
Range of variables: 0–40°C
Physical state within the range: Liquid
Class: Calibration and Test Material
Contributors: D. Ambrose, G. T. Armstrong, H. A. Bowman, I. Brown, J. P. Cali, G. Girard, E. F. G. Herington, J. E. Lane, M. Menaché, T. Plebanski, J. Terrien

Intended usage. Water can be used for the determination by weighing of the volume of apparatus such as that used for the measurement of density. A good general description of methods is given by Bauer and Lewin[1] and by Bowman and Schoonover[2].

Sources of supply and/or methods of preparation. Suitable samples can be prepared from natural waters, preferably from sea water by the method described by Cox *et al.*[3] with the deuterium and oxygen isotopic composition of the specimen determined by mass spectrometry after the sample has been degassed.

Pertinent physicochemical data. The following table of recommended values for the absolute density of Standard Mean Ocean Water was calculated from the table presented by Bigg[4] (see also Wagenbreth and Blanke[5]). Values calculated by the relation

$$\rho(SMOW)/kg\,m^{-3} = [\rho(Bigg)/kg\,m^{-3}] \times 999{\cdot}975/999{\cdot}972$$

were fitted within $10^{-4}\,kg\,m^{-3}$ by the following equation from which the table was generated:

$$\rho(SMOW)/kg\,m^{-3} = a_0 + a_1 t + a_2 t^2 + a_3 t^3 + a_4 t^4 + a_5 t^5$$

where

$$a_0 = 999{\cdot}842\,594; \qquad a_1 = 6{\cdot}793\,952 \times 10^{-2}$$
$$a_2 = -9{\cdot}095\,290 \times 10^{-3}; \quad a_3 = 1{\cdot}001\,685 \times 10^{-4}$$
$$a_4 = -1{\cdot}120\,083 \times 10^{-6}; \quad a_5 = 6{\cdot}536\,332 \times 10^{-9}.$$

If the absolute density, ρ(sample), of a given specimen of degassed water is required at a temperature, t, it is first necessary to determine the isotopic composition of the sample. The quantities δ_{18} and δ_D are then calculated by means of equation (1) (see page 2) and the resulting quantities are substituted into equation (2) (see page 2) to obtain the isotopic density correction to the appropriate

value of ρ(SMOW) taken from the table of recommended values. The table preserves the format of that from which it was derived but if the estimates of maximum uncertainties (page 3) are correct the last digit of each value is not significant. Samples of water purified in accordance with the method described by Cox et al.[3] from natural waters of undetermined isotopic concentration can be used with the attached table for absolute density determinations if an accuracy of only 20×10^{-3} kg m^{-3} is required.

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Absolute Density of Standard Mean Ocean Water (SMOW)

ρ/kg m^{-3}

Free from dissolved atmospheric gases, at a pressure of 101 325 Pa for temperatures t/°C on the International Practical Temperature Scale of 1968

	·0	·1	·2	·3	·4	·5	·6	·7	·8	·9
0	999·8426	8493	8558	8622	8683	8743	8801	8857	8912	8964
1	999·9015	9065	9112	9158	9202	9244	9284	9323	9360	9395
2	999·9429	9461	9491	9519	9546	9571	9595	9616	9636	9655
3	999·9672	9687	9700	9712	9722	9731	9738	9743	9747	9749
4	999·9750	9748	9746	9742	9736	9728	9719	9709	9696	9683
5	999·9668	9651	9632	9612	9591	9568	9544	9518	9490	9461
6	999·9430	9398	9365	9330	9293	9255	9216	9175	9132	9088
7	999·9043	8996	8948	8898	8847	8794	8740	8684	8627	8569
8	999·8509	8448	8385	8321	8256	8189	8121	8051	7980	7908
9	999·7834	7759	7682	7604	7525	7444	7362	7279	7194	7108
10	999·7021	6932	6842	6751	6658	6564	6468	6372	6274	6174
11	999·6074	5972	5869	5764	5658	5551	5443	5333	5222	5110
12	999·4996	4882	4766	4648	4530	4410	4289	4167	4043	3918
13	999·3792	3665	3536	3407	3276	3143	3010	2875	2740	2602
14	999·2464	2325	2184	2042	1899	1755	1609	1463	1315	1166
15	999·1016	0864	0712	0558	0403	0247	0090	9932†	9772†	9612†
16	998·9450	9287	9123	8957	8791	8623	8455	8285	8114	7942
17	998·7769	7595	7419	7243	7065	6886	6706	6525	6343	6160
18	998·5976	5790	5604	5416	5228	5038	4847	4655	4462	4268
19	998·4073	3877	3680	3481	3282	3081	2880	2677	2474	2269
20	998·2063	1856	1649	1440	1230	1019	0807	0594	0380	0164
21	997·9948	9731	9513	9294	9073	8852	8630	8406	8182	7957
22	997·7730	7503	7275	7045	6815	6584	6351	6118	5883	5648
23	997·5412	5174	4936	4697	4456	4215	3973	3730	3485	3240
24	997·2994	2747	2499	2250	2000	1749	1497	1244	0990	0735
25	997·0480	0223	9965†	9707†	9447†	9186†	8925†	8663†	8399†	8135†
26	996·7870	7604	7337	7069	6800	6530	6259	5987	5714	5441
27	996·5166	4891	4615	4337	4059	3780	3500	3219	2938	2655
28	996·2371	2087	1801	1515	1228	0940	0651	0361	0070	9778†
29	995·9486	9192	8898	8603	8306	8009	7712	7413	7113	6813
30	995·6511	6209	5906	5602	5297	4991	4685	4377	4069	3760
31	995·3450	3139	2827	2514	2201	1887	1572	1255	0939	0621
32	995·0302	9983†	9663†	9342†	9020†	8697†	8373†	8049†	7724†	7397†
33	994·7071	6743	6414	6085	5755	5423	5092	4759	4425	4091
34	994·3756	3420	3083	2745	2407	2068	1728	1387	1045	0703
35	994·0359	0015	9671†	9325†	8978†	8631†	8283†	7934†	7585†	7234†
36	993·6883	6531	6178	5825	5470	5115	4759	4403	4045	3687
37	993·3328	2968	2607	2246	1884	1521	1157	0793	0428	0062
38	992·9695	9328	8960	8591	8221	7850	7479	7107	6735	6361
39	992·5987	5612	5236	4860	4483	4105	3726	3347	2966	2586
40	992·2204									

†The leading figure decreases by 1·0.

Any future revision of the above table will be done in co-operation with the International Association for the Properties of Steam which is currently engaged in a comprehensive review of the properties of water.

2

Physical property: Density ρ

Unit: kg m^{-3}

Recommended reference material: Mercury (Hg)

Range of variables: −20 to +300°C

Physical state within the range: Liquid

Class: Calibration and Test Material

Contributors: D. Ambrose, I. Brown, E. F. G. Herington.

Intended usage. Mercury can be used for the determination by weighing of the volume of apparatus such as pycnometers and other equipment used for density determinations. A good general description of methods is given by Bauer and Lewin.[1]

Source of supply and/or methods of preparation. Samples of mercury can be purified by treatment with

dilute nitric acid (1:20) followed by washing with water and by distillation at reduced pressure (about 3 kPa) in the presence of clean air. For further details see earlier in this report.

Pertinent physicochemical data. Values for the absolute density of mercury are given in the attached table which is based on data presented by Bigg[2] corrected to bring the values to the International Practical Temperature Scale of 1968.

REFERENCES

[1] N. Bauer and S. Z. Lewin, *Technique of Organic Chemistry* (editor A. Weissberger) Vol. 1. Part 1, 3rd Edn, p. 131. Interscience, New York (1963).

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Absolute Density of Mercury

$\rho/\text{kg m}^{-3}$

at a pressure of 101 325 Pa for temperatures $t/°C$ on the International Practical Temperature Scale of 1968

t/°C											Mean diff. per kelvin kg m⁻³ K⁻¹	Error in density likely to be within ± kg m⁻³
t/°C	−20	−19	−18	−17	−16	−15	−14	−13	−12	−11		
	13 644·59†	642·11	639·62	637·14	634·66	632·18	629·70	627·22	624·75	622·27	2·48	0·3
t/°C	−10	−9	−8	−7	−6	−5	−4	−3	−2	−1		
	13 619·79	617·32	614·85	612·37	609·90	607·43	604·96	602·49	600·02	597·55	2·47	0·04
t/°C	0	1	2	3	4	5	6	7	8	9		
0	13 595·08	592·62	590·15	587·68	585·22	582·76	580·29	577·83	575·36	572·91	2·46	0·02
10	13 570·44	567·98	565·52	563·07	560·60	558·15	555·69	553·24	550·78	548·33	2·46	0·01
20	13 545·87	543·42	540·97	538·52	536·06	533·62	531·17	528·71	526·26	523·82	2·45	0·01
30	13 521·37	518·92	516·47	514·03	511·58	509·14	506·70	504·26	501·82	499·37	2·44	0·02
40	13 496·93	494·49	492·05	489·62	487·18	484·73	482·29	479·86	477·42	474·99	2·44	
50	13 472·55	470·11	467·68	465·25	462·82	460·38	457·96	455·52	453·09	450·67	2·43	0·04
60	13 448·23	445·81	443·37	440·95	438·52	436·10	433·67	431·24	428·82	426·39	2·43	
70	13 423·97	421·55	419·13	416·70	414·28	411·86	409·43	407·01	404·60	402·18	2·42	0·06
80	13 399·77	397·34	394·92	392·50	390·09	387·67	385·26	382·85	380·42	378·01	2·42	
90	13 375·60	373·18	370·77	368·36	365·94	363·54	361·12	358·72	356·30	353·89	2·41	0·08
t/°C	100	110	120	130	140	150	160	170	180	190		
	13 351·5	327·4	303·4	279·4	255·4	231·5	207·6	183·7	159·8	136·0	2·40	0·1
t/°C	200	210	220	230	240	250	260	270	280	290		
	13 112·1	088·3	064·5	040·7	016·9	993·0‡	969·2‡	945·4‡	921·5‡	897·6‡	2·38	0·2
t/°C	300											
	12 873·7											

†Leading figures are 13 except where otherwise indicated.
‡Leading figures are 12 in each instance.

3

Physical Property: Density ρ
Unit: kg m⁻³
Recommended reference material: 2,2,4-trimethylpentane
(C₈H₁₈)
Range of variables: 20 to 50°C
Physical state within the range: Liquid
Class: Certified Reference Material
Contributors: I. Brown, J. P. Cali, E. F. G. Herington, T. Plebanski.

Intended usage. Samples of 2,2,4-trimethylpentane can be used for the determination by weighing of the volume of apparatus such as is used for density determinations. A good general description of methods is given by Bauer and Lewin[1] and by Bowman and Schoonover.[2]

Sources of supply and/or methods of preparation. Samples with certified values of density are available from suppliers (A), (B) and (C).

Pertinent physicochemical data. The following values of density, which apply to air-saturated material available from supplier (A), were determined using precise pycnometric and flotation methods;[3] the pycnometers were calibrated with water,[4-6] and mercury.[7] Supplier (A) sample 99·75 mole % pure, air saturated

Temperature relative to IPTS-68

t/°C	ρ/kg m⁻³	t/°C	ρ/kg m⁻³
20	691·959	40	675·348
25	687·849	45	671·124
30	683·711	50	666·871
35	679·543		

Uncertainty limit at 99% confidence level = $\pm 5 \times 10^{-3}$ kg m⁻³. The density values were calculated from the equation

$$\rho/\text{kg m}^{-3} = \sum_{i=0}^{3} c_i t^i$$

where

$c_0 = +708·113$, $c_1 = -7·962 \times 10^{-1}$, $c_2 = -5·77 \times 10^{-4}$, $c_3 = +6·7 \times 10^{-8}$.

The following values of density apply to air-free material available from supplier (B)

2,2,4-trimethylpentane   Sample 217-b   99·993 ± 0·003 mol % pure

t/°C	ρ/kg m⁻³
20	691·83 ± 0·02
25	687·72 ± 0·02
30	683·62 ± 0·02

The following values of density determined at the U.S. National Bureau of Standards, Washington, D.C., apply to air-saturated material available from supplier (C).

2,2,4-trimethylpentane	Sample 217-x 99.968 ± 0.006 mol % pure
$t/°C$	$\rho/\text{kg m}^{-3}$
20	691.93 ± 0.05
25	687.81 ± 0.05
30	683.66 ± 0.05

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4

Physical Property: Density ρ
Unit: kg m^{-3}
Recommended reference material: Cyclohexane (C_6H_{12})
Range of variables: 20 to 50°C,
Physical state within the range: Liquid
Class: Certified Reference Material
Contributor: T. Plebanski

Intended usage. Samples of cyclohexane can be used for the determination by weighing of the volume of apparatus such as that used for density measurement. A good general description of methods is given by Bauer and Lewin[1] and by Bowman and Schoonover.[2]

Sources of supply and/or method of preparation. Samples with certified values of density are available from supplier (A).

Pertinent physicochemical data. The following values of density, which apply to air-saturated material available from supplier (A) were determined using precise pycnometric and flotation methods;[3] the pycnometers were calibrated with water[4-6] and mercury.[7]
Supplier (A) Sample 99.98 mol % pure, air-saturated. Temperatures relative to IPTS-68

$t/°C$	$\rho/\text{kg m}^{-3}$	$t/°C$	$\rho/\text{kg m}^{-3}$
20	778.583	40	759.624
25	773.896	45	754.805
30	769.172	50	749.960
35	764.414		

Uncertainty limit at 99% confidence level = $\pm 5 \times 10^{-3} \text{ kg m}^{-3}$. These density values were calculated from the equation

$$\rho/\text{kg m}^{-3} = \sum_{i=0}^{3} c_i t^i$$

where

$c_0 = +796.922$, $c_1 = -8.989 \times 10^{-1}$, $c_2 = -9.67 \times 10^{-4}$, $c_3 = +3.19 \times 10^{-6}$.

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5

Physical property: Density ρ
Unit: kg m^{-3}
Recommended reference material:
    trans-bicyclo[4,4,0]decane ($C_{10}H_{18}$)
    (*trans*-decahydronaphthalene)
Range of variables: 20 to 50°C
Physical state within the range: Liquid
Class: Certified Reference Material
Contributors: I. Brown, J. P. Cali, E. F. G. Herington, T. Plebanski.

Intended usage. Samples of *trans*-bicyclo(4,4,0)decane can be used for the determination by weighing of the volume of apparatus such as that used for density measurement. A good general description of methods is given by Bauer and Lewin[1] and by Bowman and Schoonover.[2]

Sources of supply and/or method of preparation. Samples with certified values of density are available from suppliers (A) and (C).

Pertinent physicochemical data. The following values of density, which apply to air-saturated material available from supplier (A) were determined using precise pycnometric and flotation methods;[3] the pycnometers were calibrated with water[4-6] and mercury.[7]
Supplier (A) sample 97.00 mol % pure, air-saturated. Temperatures relative to IPTS-68.

$t/°C$	$\rho/\text{kg m}^{-3}$	$t/°C$	$\rho/\text{kg m}^{-3}$
20	869.623	40	854.693
25	865.895	45	850.945
30	862.165	50	847.185
35	858.432		

Uncertainty limit at 99% confidence level = $\pm 5 \times 10^{-3} \text{ kg m}^{-3}$.

These density values were calculated from the equation

$$\rho/\text{kg m}^{-3} = \sum_{i=0}^{3} c_i t^i$$

where

$c_0 = +884.579$, $c_1 = -7.513 \times 10^{-1}$, $c_2 = +2.440 \times 10^{-4}$, $c_3 = -3.519 \times 10^{-6}$.

The following values of density apply to air-saturated material available from supplier (C). The density values were determined by the American Petroleum Institute Research Project 6 at the Carnegie-Mellon University.

trans-bicyclo[4,4,0]decane (*trans*-decahydronaphthalene)

Sample 561-x	$99 \cdot 98 \pm 0 \cdot 02$
$t/°C$	mol % pure
20	$\rho/\mathrm{kg\,m}^{-3}$
25	$869 \cdot 71 \pm 0 \cdot 08$
30	$865 \cdot 92 \pm 0 \cdot 08$
	$862 \cdot 22 \pm 0 \cdot 08$

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