

**NIST Special Publication 260-186**

***Standard Reference Materials***<sup>®</sup>

**Certification Report for SRM 2214:  
Density of Iso-octane for Extended  
Ranges of Temperature and Pressure**

Mark O. McLinden  
Jolene Splett

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<https://doi.org/10.6028/NIST.SP.260-186>

**NIST**  
**National Institute of  
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October 2016



U.S. Department of Commerce  
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National Institute of Standards and Technology  
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**National Institute of Standards and Technology Special Publication 260-186**  
**Natl. Inst. Stand. Technol. Spec. Publ. 260-186, 38 pages (October 2016)**  
**CODEN: NSPUE2**

**This publication is available free of charge from: <https://doi.org/10.6028/NIST.SP.260-186>**

## Abstract

This report of analysis documents procedures used to obtain certified values and associated uncertainties of the density of iso-octane SRM 2214 over an extended range of temperatures and pressures. This SRM is certified over the temperature range  $-50^{\circ}\text{C}$  to  $160^{\circ}\text{C}$  and pressure range of 0.1 MPa to 30 MPa; an interpolation model is provided to calculate the density within these ranges. This SRM has a density of  $691.853\text{ kg}\cdot\text{m}^{-3}$  at  $t = 20^{\circ}\text{C}$  and  $p = 0.1\text{ MPa}$ . The certification measurements were carried out in a two-sinker magnetic-suspension densimeter. The SRM material is commercial, high-purity iso-octane (2,2,4-trimethylpentane, CAS 540-84-1). Measurements were made on both degassed material and material saturated with nitrogen, and an estimated correction surface (valid over the range  $-50^{\circ}\text{C} \leq t \leq 100^{\circ}\text{C}$  and  $0.1\text{ MPa} \leq p \leq 20\text{ MPa}$ ) gives the density difference between the nitrogen-saturated and degassed materials. A thorough analysis of the uncertainties is presented; this includes effects resulting from the experimental density determination, possible degradation of the sample due to time and exposure to high temperatures, dissolved air, uncertainties in the empirical density model, and the sample-to-sample variations in the SRM vials. Also considered is the effect of uncertainties in the user's temperature and pressure measurements. This SRM is intended for the calibration of industrial densimeters.

## Keywords

Standard reference material; iso-octane; density; measurement

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## 1. Introduction

This document describes the measurement procedures and analyses used to characterize the uncertainty associated with the density of liquid iso-octane (SRM 2214) for a wide range of temperatures and pressures.

The property of fluid density is a vital parameter in a multitude of industrial processes. These include the control of chemical processes and the metering of fuels and other commodity chemicals. Often, the process stream is sampled through an industrial densimeter for continuous, real-time determination of the density. Such densimeters are not absolute instruments—they must be regularly calibrated at the conditions of use with fluids of known density. The work presented here utilizes an absolute fluid densimeter to establish the density of iso-octane as a function of temperature and pressure for use as a calibration standard.

Iso-octane (formal IUPAC name 2,2,4-trimethylpentane, with CAS registry number 540-84-1) has a number of advantages as a density standard: it is a stable chemical of relatively low toxicity; its density of  $692 \text{ kg}\cdot\text{m}^{-3}$  at ambient conditions is well matched to many applications, particularly liquid hydrocarbon fuels; its freezing point of  $-107^\circ\text{C}$  and boiling point of  $99^\circ\text{C}$  cover the range of many industrial processes. Iso-octane has low surface tension compared to that of water, and it is relatively inexpensive. The National Institute of Standards and Technology (NIST) has sold a density Standard Reference Material (SRM®) based on iso-octane since 2001, but the previous SRM was certified only at ambient conditions:  $15^\circ\text{C}$  to  $25^\circ\text{C}$  and normal atmospheric pressure.

This SRM certifies the density of a particular batch of iso-octane. This approach is preferred for high-accuracy calibrations over the alternative approach of measuring the density of “very pure” iso-octane for at least two reasons. First, a batch certification is directly traceable to NIST, and this is often a requirement for high-level calibration laboratories. Second, iso-octane in very high purities is difficult to obtain. Impurities, such as closely related organic compounds, are often present. The use of “pure” iso-octane would greatly complicate the traceability of density and shift the problem to one of determining purity and/or the effects of impurities on the density.

In section 2, we briefly summarize the experimental methodology used to generate density measurements. Section 3 describes an empirical model used to estimate fluid density for various temperatures and pressures, and section 4 provides details regarding the uncertainty evaluation for the density values. Combined standard uncertainties and expanded uncertainties are summarized in section 5. Finally, a brief discussion and conclusions are given in section 6.

## 2. Experimental Methodology

### 2.1 Densimeter

The two-sinker densimeter used in this work is described in detail by McLinden and Lösch-Will [1] and McLinden and Splett [2], and this general type of instrument is described by Wagner and Kleinrahm [3]. In the present densimeter, two sinkers of nearly the same mass, surface area, and surface material, but very different volumes, are weighed separately with a high-precision balance while immersed in a fluid of unknown density. The fluid density  $\rho$  is given by

$$\rho = \frac{(m_1 - m_2) - (W_1 - W_2)}{(V_1 - V_2)}, \quad (1)$$

where  $m$  and  $V$  are the sinker mass and volume,  $W$  is the balance reading, and the subscripts refer to the two sinkers. The main advantage of the two-sinker method is that adsorption onto the surface of the sinkers, systematic errors in the weighing, and other effects that reduce the accuracy of most buoyancy techniques cancel. Equation (1) must be corrected for magnetic effects; this is considered in Section 4 and described in detail by McLinden *et al.* [4].

A magnetic suspension coupling transmits the gravity and buoyancy forces on the sinkers to the balance, thus isolating the fluid sample (which may be at high pressure and/or extremes of temperature) from the balance. The central elements of the coupling are two magnets, one on each side of a nonmagnetic pressure separating wall. The top magnet, which is an electromagnet with a ferrite core, is hung from the balance. The bottom (permanent) magnet is held in stable suspension with respect to the top magnet by means of a feedback control circuit making fine adjustments in the electromagnet current. The permanent magnet is linked with a lifting device to pick up a sinker for weighing. A mass comparator with a resolution of 1  $\mu\text{g}$  and a capacity of 111 g is used for the weighings. Each sinker has a mass of 60 g; one is made of tantalum and the other is titanium.

In addition to the sinkers, suspension coupling, and balance that comprise the density measuring system, the apparatus included a thermostat, pressure instrumentation, and a sample handling system. The temperature was measured with a standard-reference-quality platinum resistance thermometer (SPRT) and resistance bridge referenced to a thermostatted standard resistor. The signal from the SPRT was used directly in a digital control circuit to maintain the cell temperature constant within  $\pm 0.001$  K. The pressures were measured with state-of-the-art transducers combined with careful calibration. The transducers (as well as the pressure manifold) were thermostatted to minimize the effects of variations in laboratory temperature.

The thermostat served to isolate the measuring cell from ambient conditions. It was a vacuum-insulated, cryostat-type design. The measuring cell was surrounded by an isothermal shield, which thermally isolated it from variations in ambient temperature; this shield was maintained at a constant ( $\pm 0.01$  K) temperature 1 K below the cell temperature. Electric heaters compensated for the small heat flow from the cell to the shield and allowed millikelvin-level control of the cell

temperature. Operation at sub-ambient temperatures was effected by circulating ethanol from an external chiller through channels in the shield.

## 2.2 Experimental material

The material used is identical to the previous SRM, which was obtained from a commercial source.[5] The SRM is provided in 5 mL flame-sealed glass ampoules. At the same time the 5 mL ampoules were prepared, several large 1.5 L flame-sealed ampoules were also prepared containing the same iso-octane. We worked with material from one of the 1.5 L ampoules, except for some of the chemical analysis, which used the 5 mL ampoules. We transferred the iso-octane from the 1.5 L ampoule to a stainless-steel sample cylinder for convenience in sample handling.

The sample was degassed by freezing the stainless-steel cylinder in liquid nitrogen, evacuating the vapor space, and thawing. This freeze/pump/thaw process was repeated a total of eleven times. The residual pressure over the frozen sample on the final cycle was 0.001 Pa. The SRM as supplied by NIST contains some amount of dissolved air. The sample was degassed to obtain a well characterized state for the measurements. Also, we were concerned that dissolved air could react with the iso-octane at the elevated temperatures measured in this work. We felt that the uncertainties introduced by “purifying” the SRM material in this way would be offset by a reduction in possible effects resulting from reaction with air.

To quantify the effect of dissolved air on the density, additional measurements were made on a sample that was saturated with nitrogen at a temperature of 20 °C and pressure of 0.10 MPa. A quantity of the degassed iso-octane was transferred to an evacuated 500 mL stainless steel sample cylinder. Ultra-high-purity nitrogen (99.9995 %) was admitted to the cylinder to a pressure of 0.10 MPa; additional nitrogen was admitted periodically over the course of five days to maintain the pressure at 0.10 MPa. The cylinder was periodically mixed to promote equilibrium. This point is discussed further in Section 4.2.

A chemical analysis by gas chromatography-mass spectrometry yielded an overall purity of 99.72 %. The major impurities, totaling 0.20 %, were isomers of dimethylpentane. In addition, 2,3-dimethylbutane was present at 0.058 % and 2-methylbutane was present at 0.017 %. Two additional peaks at the level of 0.001 % could not be identified.

## 2.3 Density measurement procedures

Each density determination involved weighings in the order: tantalum (Ta) sinker, titanium (Ti) sinker, balance calibration weight, balance tare weight, balance tare weight (again), balance calibration weight, Ti sinker, and Ta sinker, for a total of eight weighings—two for each object. For each weighing, the balance was read six times over the course of ten seconds. For each object, the 12 balance readings were averaged for the calculation of density. Between each of the object weighings, and also before the first weighing and following the final weighing, the temperature and pressure were recorded, for a total of nine readings of  $t$  and  $p$ ; these were also averaged. A complete density determination required 12 minutes. The weighing design was

symmetrical with respect to time, and this tended to cancel the effects of any drift in the temperature or pressure.

The sample was loaded at a low temperature and pressure. Higher pressures were generated by heating the liquid-filled cell; thus avoiding the need for any type of compressor, which could have been a source of contamination. Starting at the lowest temperature and pressure for a given filling, measurements were made at increasing temperatures (and nearly constant density) until the maximum desired pressure was reached. The sample was then vented to a lower pressure along an isotherm.

The densimeter control program monitored the system temperatures and pressures once every 60 seconds. A running average and standard deviation of the temperatures and pressures were computed for the preceding eight readings. When these were within preset tolerances of the set point conditions, a weighing sequence was triggered. Once the specified number of replicate density determinations were made at a given  $(t, p)$  state point, the control program then moved to the next temperature or automatically vented the sample to the next pressure on an isotherm.

A total of three separate fillings of the densimeter were carried out with the degassed sample. The first two covered the entire range of temperature and pressure. Following the measurements at high temperatures and high pressures with the first two fillings, the densimeter was cooled to 30°C and a small quantity of fresh sample was added to refill the cell; replicate measurements were performed to check for possible degradation. These tests are discussed in Section 4.4. The third filling extended over the temperature range of -59°C to 62°C. A fourth filling was carried out with the nitrogen-saturated sample; it extended over the full range of temperature and pressure.

Between each filling, and also before the first filling and following the last filling, the system was evacuated and the density recorded multiple times. The indicated density was used to determine the apparatus zero  $\rho_0$ . The value of  $\rho_0$  used in the density calculation is the time-weighted average of  $\rho_0$  values measured before and after a given density determination (see Section 4.6.3).

### 3. Results for Fluid Density

The density of iso-octane was measured over the temperature range  $-59^{\circ}\text{C}$  to  $160^{\circ}\text{C}$ , with pressures ranging from 0.5 MPa to 30 MPa. The measured values are tabulated in the Appendix, and a plot of the densities measured on the degassed sample is shown in Figure 1.

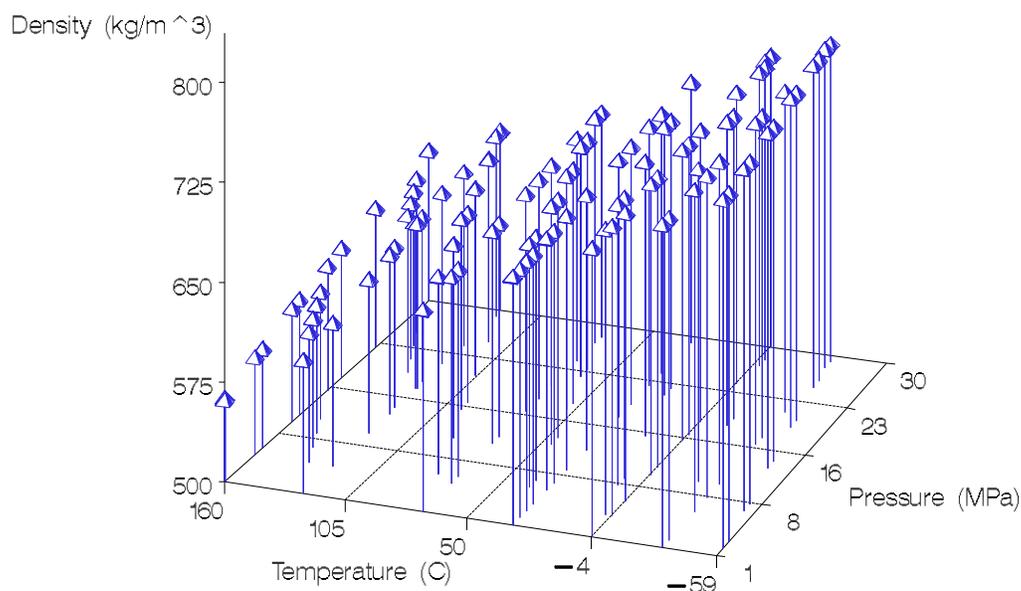


Figure 1. Degassed density measurements versus temperature and pressure.

An empirical model for interpolation was fit to the degassed density data

$$\rho = f(T, p) = \frac{\hat{a} + \hat{c} \cdot \ln(T) + \hat{e} \cdot p + \hat{g} \cdot [\ln(T)]^2 + \hat{i} \cdot p^2 + \hat{k} \cdot p \cdot \ln(T)}{1 + \hat{b} \cdot \ln(T) + \hat{d} \cdot p + \hat{f} \cdot [\ln(T)]^2 + \hat{h} \cdot p^2 + \hat{j} \cdot p \cdot \ln(T)} + \varepsilon, \quad (2)$$

where  $T$  is temperature in kelvins ( $T/\text{K} = t/^{\circ}\text{C} + 273.15$ ) and  $p$  is pressure in MPa. The estimated model parameters are listed in Table 1. Table 2 gives estimated fluid density values calculated with Eq. 2 at even temperature and pressure increments.

Table 1. Estimated parameters for the density model given in Eq. 2.

$\hat{a}$	$1.022794253 \cdot 10^3$
$\hat{b}$	$-2.832862261 \cdot 10^{-1}$
$\hat{c}$	$-3.049340500 \cdot 10^2$
$\hat{d}$	$2.565415217 \cdot 10^{-3}$
$\hat{e}$	$2.724090192 \cdot 10^0$
$\hat{f}$	$1.985515546 \cdot 10^{-2}$
$\hat{g}$	$2.265907341 \cdot 10^1$
$\hat{h}$	$1.768055678 \cdot 10^{-6}$
$\hat{i}$	$1.685280491 \cdot 10^{-3}$
$\hat{j}$	$-3.255136085 \cdot 10^{-4}$
$\hat{k}$	$-3.866274772 \cdot 10^{-1}$

Table 2. Estimated fluid density  $\rho$  in  $\text{kg}\cdot\text{m}^{-3}$  for degassed samples ( $\Delta = g = 0 \text{ kg}\cdot\text{m}^{-3}$ ) from Eq. 2.

$t$ (°C)	Pressure (MPa)								
	0.1	1	2	5	10	15	20	25	30
-50	747.992	748.564	749.194	751.049	754.033	756.895	759.647	762.299	764.859
-40	740.081	740.690	741.360	743.330	746.494	749.522	752.428	755.225	757.923
-30	732.159	732.807	733.520	735.616	738.972	742.177	745.248	748.198	751.039
-20	724.213	724.905	725.666	727.896	731.460	734.854	738.098	741.209	744.200
-10	716.232	716.972	717.784	720.162	723.949	727.545	730.973	734.253	737.402
0	708.204	708.996	709.865	712.403	716.432	720.243	723.866	727.325	730.638
10	700.116	700.966	701.896	704.610	708.900	712.942	716.773	720.420	723.905
20	691.956	692.869	693.868	696.774	701.347	705.637	709.687	713.532	717.199
30	683.709	684.693	685.767	688.884	693.765	698.320	702.604	706.659	710.515
40	675.361	676.423	677.582	680.930	686.146	690.987	695.520	699.796	703.850
50	666.896	668.046	669.298	672.902	678.484	683.632	688.431	692.939	697.202
60	658.297	659.545	660.900	664.789	670.770	676.250	681.331	686.086	690.567
70	649.543	650.902	652.374	656.578	662.997	668.835	674.218	679.233	683.942
80	640.614	642.097	643.700	648.257	655.156	661.381	667.086	672.377	677.326
90	631.484	633.109	634.860	639.810	647.239	653.884	659.934	665.515	670.716
100		623.911	625.830	631.223	639.237	646.337	652.756	658.645	664.111
110		614.476	616.586	622.478	631.140	638.735	645.549	651.765	657.507
120		604.768	607.098	613.556	622.937	631.072	638.309	644.872	650.905
130		594.749	597.332	604.433	614.617	623.341	631.034	637.963	644.302
140		584.372	587.248	595.086	606.168	615.535	623.718	631.037	637.696
150		573.582	576.799	585.484	597.575	607.649	616.359	624.091	631.087
160		562.310	565.929	575.594	588.823	599.674	608.953	617.124	624.474

## 4. Uncertainty Evaluation

The overall uncertainty in the fluid density arises from several distinct sources. The first source is the empirical model (*i.e.*, Eq. 2) used to represent the density and allow interpolation at a desired temperature and pressure. A second category relates to the material itself; these include uncertainties associated with the degree of air saturation of the iso-octane and possible degradation resulting from exposure to high temperatures. Since the SRM is provided in 5 mL ampoules (vials), the variation in density from vial to vial must also be considered. The third, and most complex, source arises from the experimental measurement of the density. Finally, when using the SRM for the calibration of a densimeter, the uncertainty in the *user's* temperature and pressure measurement must be included.

The uncertainty evaluation described in this document closely follows the procedures outlined in [2]; please refer to that document for further details. The measurement equation used to estimate the density of iso-octane,  $\rho_c$ , is

$$\rho_c = \rho + \Delta + V + x + e + tp, \quad (3)$$

where

$\rho$  is the estimated fluid density based on an empirical model (Eq. 2),  
 $\Delta$  is the effect due to air saturation,  
 $V$  is the effect due to differences between vials,  
 $x$  is the effect due to material degradation over time,  
 $e$  is the effect due to the apparatus (*i.e.*, experimental uncertainty), and  
 $tp$  is the effect due to the user's temperature and pressure measurements.

The combined standard uncertainty of  $\rho_c$  is

$$u(\rho_c) = \left[ u^2(\rho) + u^2(\Delta) + u^2(V) + u^2(x) + u^2(e) + u^2(tp) \right]^{0.5}. \quad (4)$$

The degrees of freedom associated with  $u(\rho_c)$  are computed using the Welch-Satterthwaite approximation.

The remainder of section 4 is devoted to defining and describing each individual uncertainty component.

### 4.1 Fluid density, $\rho$ , and its uncertainty, $u(\rho)$

Fluid density values are computed using Eq. 2. The residuals of Eq. 2 from the measured data are shown in Figure 2. The root-mean-square-error (RMSE) of the fit was  $0.010 \text{ kg}\cdot\text{m}^{-3}$ . For any given temperature and pressure combination within the range of data, the value of  $u(\rho)$  is conservatively estimated to be  $0.020 \text{ kg}\cdot\text{m}^{-3}$  based on  $495 - 11 = 484$  degrees of freedom

( $df_p = 484$ ). Four points at  $T = 397.13$  K and  $p = 0.98$  MPa were removed from the analysis, as were data measured on the thermally-degraded sample (test numbers c8\_1201a and c8\_1202a).

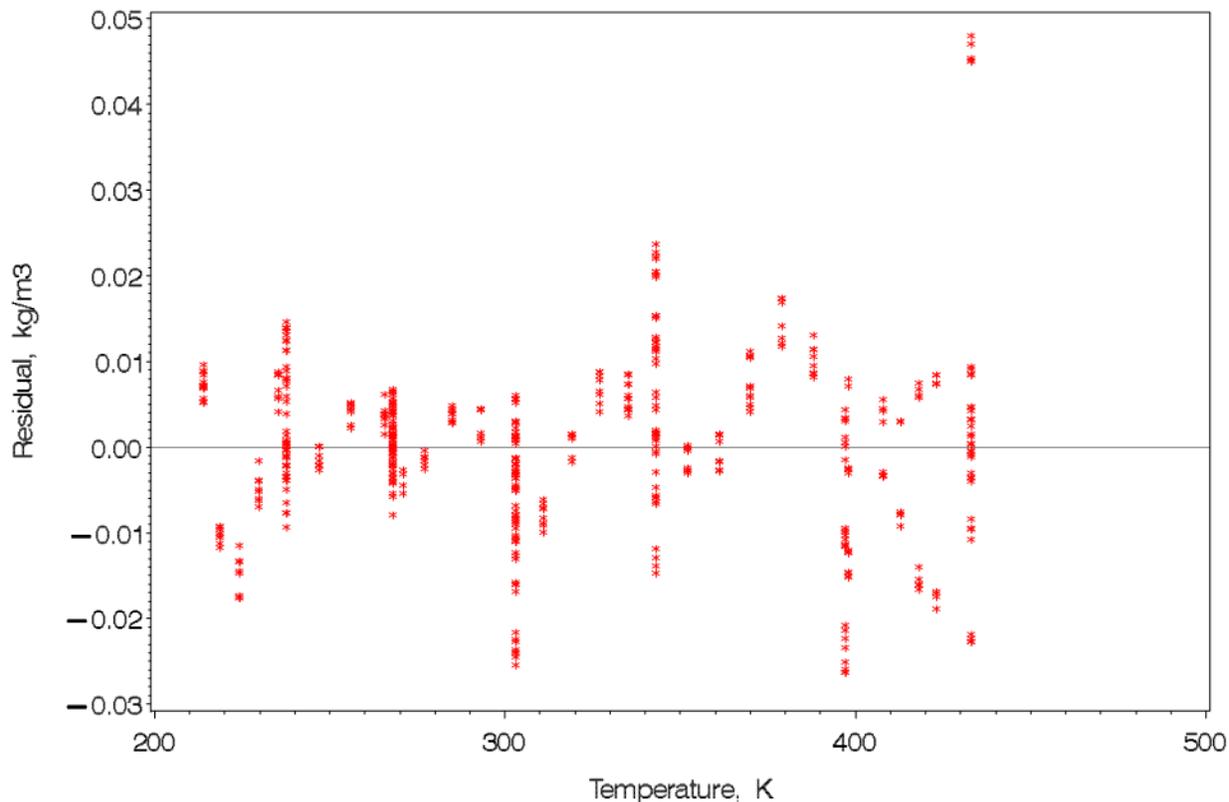


Figure 2. Residuals of the density interpolation model (Eq. 2) from the measured data versus temperature.

#### 4.2 Air-saturation, $\Delta$ , and its uncertainty, $u(\Delta)$

The correction for air saturation is

$$\Delta = F_{\text{air}} \cdot g, \quad (5)$$

where  $F_{\text{air}}$  is the fraction of air contained in the sample relative to a fully saturated sample, and  $g$  is the difference between density measurements of air-saturated and degassed samples (Figure 3). We assume here that nitrogen (which was measured) and air have the same effect on density. The proportion of air contained in the SRM is estimated to be between 0.57 and 0.77. Thus the uncertainty of  $F_{\text{air}}$ , based on a uniform distribution, is  $u(F_{\text{air}}) = 0.058$  ( $df_{F_{\text{air}}} = 8$ ).

To estimate  $g$ , we first fitted rational functions to density measurements of the air-saturated and degassed samples separately. Temperatures higher than 390 K were not fitted.

$$\rho_{\text{saturated}} = \frac{a_1 + a_2 \ln(t) + a_3 p + a_4 [\ln(t)]^2 + a_6 p^2 + a_7 p \ln(t)}{1 + a_8 \ln(t) + a_9 p + a_{10} [\ln(t)]^2 + a_{11} p^2 + a_{12} p \ln(t)} \quad (6)$$

$$\rho_{\text{degassed}} = \frac{b_1 + b_2 \ln(t) + b_3 p + b_4 [\ln(t)]^2 + b_6 p^2 + b_7 p \ln(t)}{1 + b_8 \ln(t) + b_9 p + b_{10} [\ln(t)]^2 + b_{11} p^2 + b_{12} p \ln(t)} \quad (7)$$

Next, we computed  $g = \hat{\rho}_{\text{saturated}} - \hat{\rho}_{\text{degassed}}$  and fit a planar model based on temperature and pressure to the computed  $g$  values (as shown in Figure 4):

$$g = -0.1323697352 - 0.0004029095 \cdot t + 0.0039491677 \cdot p - 0.0000356174 \cdot t \cdot p, \quad (8)$$

where the limits are  $t = -50$  °C to 100 °C, and  $p = 0.1$  MPa to 20 MPa.

The uncertainty of  $g$  is estimated as the worst-case prediction error associated with the planar model,  $u(g) = 0.020 \text{ kg}\cdot\text{m}^{-3}$  ( $df_g = 563 - 4 = 559$ ). The uncertainty of the correction for air-saturation,  $\Delta$ , is

$$u(\Delta) = \left[ g^2 \cdot u^2(F_{\text{air}}) + F_{\text{air}}^2 \cdot u^2(g) \right]^{0.5}. \quad (9)$$

For example,  $u(\Delta) = 0.0156 \text{ kg}\cdot\text{m}^{-3}$  for the SRM sample at  $t = 20$ °C and  $p = 0.1$  MPa with  $F_{\text{air}} = 0.67$  (with  $u(F_{\text{air}})$  defined above) and  $u(g) = 0.020 \text{ kg}\cdot\text{m}^{-3}$ .

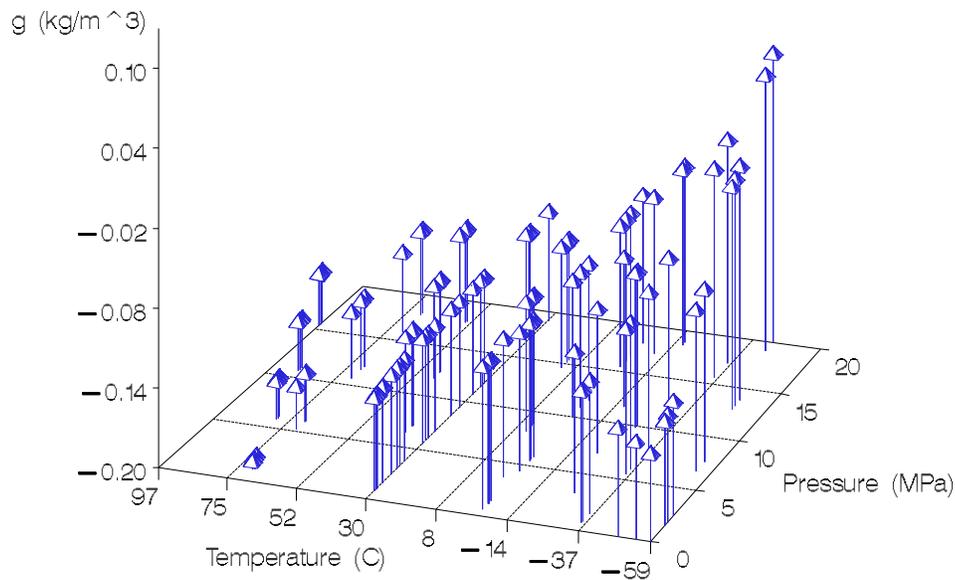


Figure 3. Density correction for air-saturated versus degassed iso-octane based on experimentally measured points.

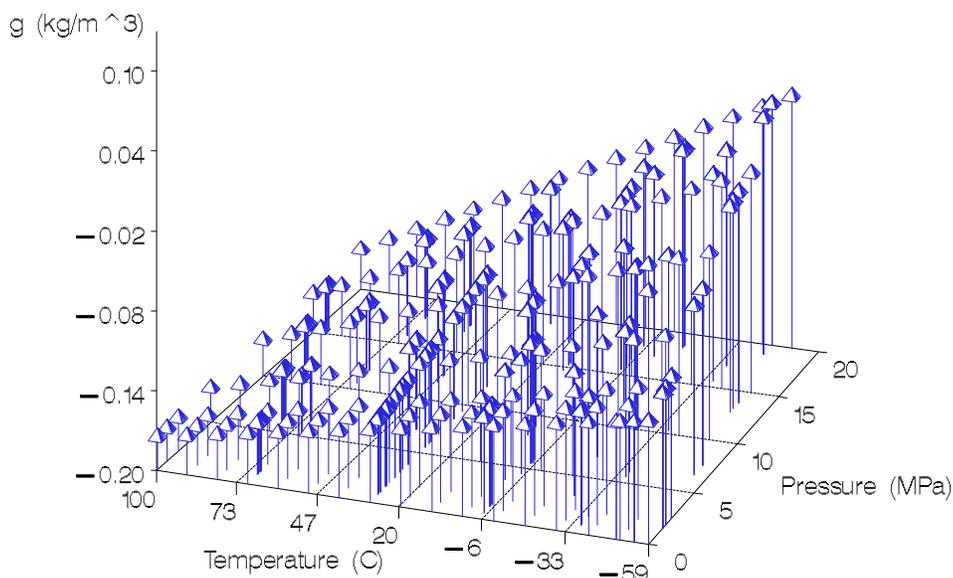


Figure 4. Estimated correction surface for air-saturated versus degassed iso-octane (Eq. 8).

### 4.3 Vial-to-vial uncertainty, $u(V)$

The uncertainty due to differences among vials was obtained from Bean and Houser [5] as summarized in Table 3.

Table 3. Vial-to-vial uncertainty.

Source	Uncertainty ( $\text{kg}\cdot\text{m}^{-3}$ )	Degrees of Freedom	Type
Apparatus*	$u(A) = 0.003$	$\infty$	B
Day-to-Day	$u(D) = 0.010$	4	A
Ampoule-to-Ampoule	$u(v) = 0.012$	10	A
Combined Standard Uncertainty	$u(V) = 0.016$	13	B

\*The apparatus used for these tests was a vibrating-tube densimeter.

### 4.4 Uncertainty due to material degradation, $u(x)$

For the first two fillings of the densimeter, a sample of iso-octane was loaded into the densimeter and measured at continuously increasing temperatures and decreasing densities over the course of (16 to 22) days. At the end of the sequence, the densimeter was cooled; a quantity of additional (fresh) sample was added to refill the cell; and densities were re-measured along the 30 °C isotherm. Figure 5 displays data for two samples that were not thermally degraded (tests c8\_1112fg and c8\_1201i) and for two samples that were thermally degraded (tests c8\_1201a and c8\_1202a).

To quantify material degradation, we fit a 4<sup>th</sup> order polynomial to the 30°C isotherm for samples that were not thermally degraded and examined residuals for the thermally degraded samples (see Figure 6). The largest absolute residual (0.024 kg·m<sup>-3</sup>) represents the worst-case error that might be observed. Thus, residuals from the fit are bounded by 0 and 0.024 kg·m<sup>-3</sup>. Assuming that these bounds represent limits to a uniform distribution, then  $u(x) = 0.007 \text{ kg}\cdot\text{m}^{-3}$  ( $df_x = 42$ ).

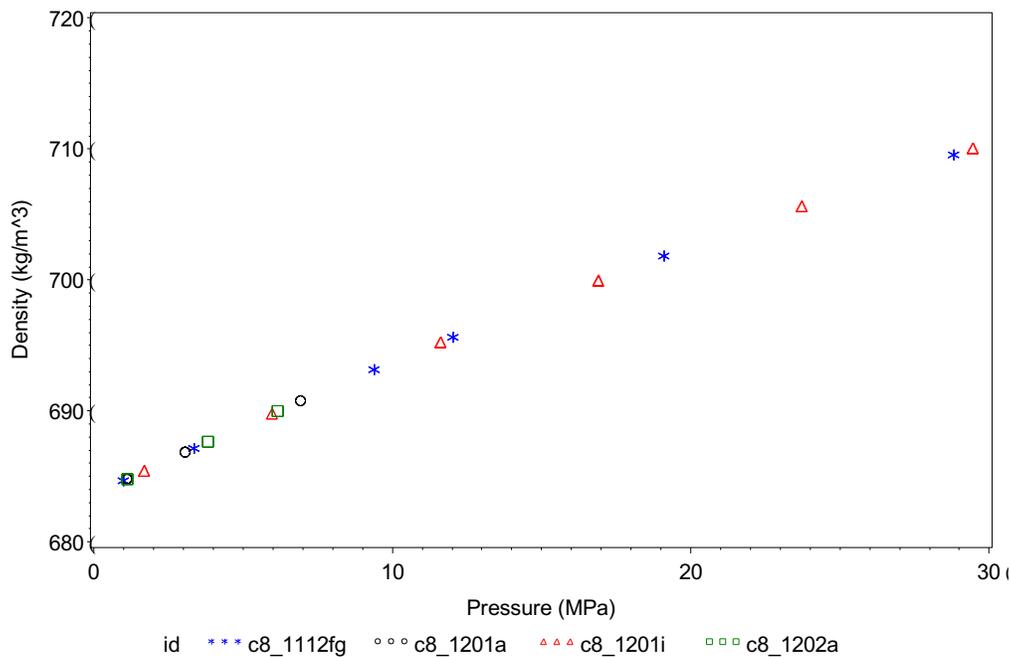


Figure 5. Replicate measurements at 30 °C for various samples of iso-octane. Samples measured for tests c8\_1112fg and c8\_1201i were not thermally degraded; samples measured for tests c8\_1201a and c8\_1202a were thermally degraded.

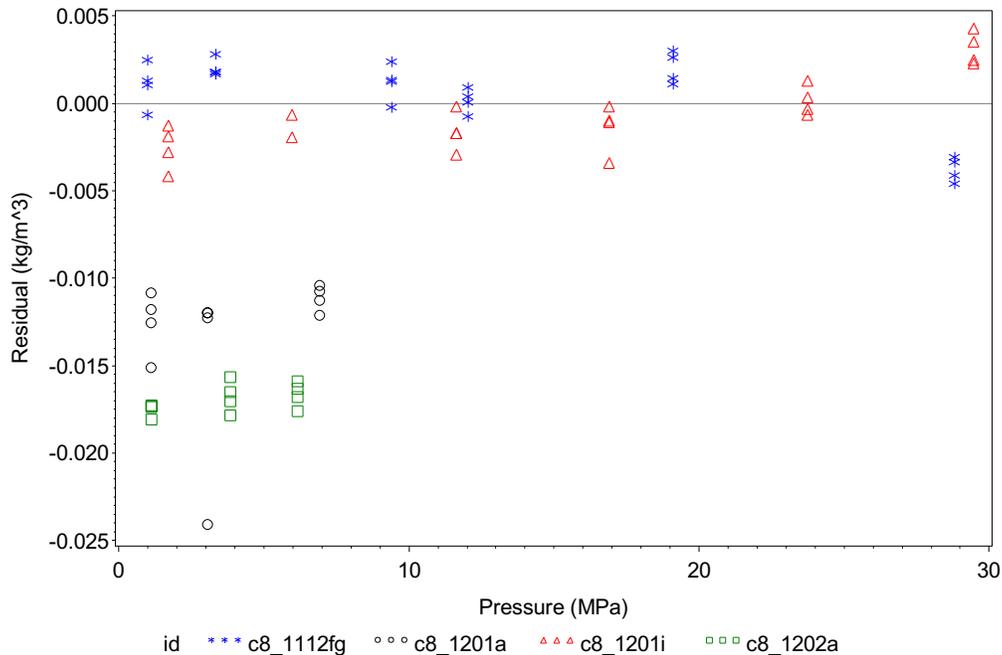


Figure 6. Residuals from the polynomial fit of data at  $T = 30\text{ }^{\circ}\text{C}$ ; the data from tests 8\_1112fg and c8\_1201i were fitted; tests c8\_1201a and c8\_1202a were on the thermally degraded material.

#### 4.5 Uncertainty due to user’s temperature and pressure errors, $u(tp)$

We estimated the uncertainty due to a user’s temperature and pressure errors by randomly perturbing the temperature and pressure values input into Eq. 2. The uncertainty of the density values based on the random perturbations is  $u(tp)$ . The results generated for low, medium, and high levels of error are displayed in Table 4.

Table 4. Estimated uncertainty due to user’s temperature and pressure uncertainties.

Limit to Temperature Error ( $^{\circ}\text{C}$ )	Limit to Pressure Error (MPa)	$u(tp)$ ( $\text{kg}\cdot\text{m}^{-3}$ )
$\pm 0.001$	$\pm 0.001$	0.001
	$\pm 0.01$	0.006
	$\pm 0.1$	0.069
$\pm 0.01$	$\pm 0.001$	0.004
	$\pm 0.01$	0.008
	$\pm 0.1$	0.070
$\pm 0.1$	$\pm 0.001$	0.046
	$\pm 0.01$	0.047
	$\pm 0.1$	0.085

The uncertainty values in the table are based on density surface boundaries of  $t = (-50 \text{ to } 160) \text{ }^\circ\text{C}$  and  $p = (0.1 \text{ to } 30) \text{ MPa}$ . For our measurement system,  $u(tp) = 0.003 \text{ kg}\cdot\text{m}^{-3}$ , based on  $u(t) = 0.002 \text{ }^\circ\text{C}$  and  $u(p) = 0.0025 \text{ kPa}$ . We assume eight degrees of freedom ( $df_{tp} = 8$ ). These errors represent modeling errors and apply to the predicted  $\rho$  calculated using the rational function model (Eq. 2); they describe how the predicted  $\rho$  might be different for different levels of errors in temperature and pressure.

#### 4.6 Uncertainty due to the apparatus, $u(e)$

The uncertainty due to the measurement apparatus is the uncertainty predicted using a polynomial equation fitted to the uncertainty in the fluid density. The equation for  $u(e)$  listed below was based on both saturated and degassed measurements.

$$u(e) = u(\hat{\rho}_{\text{fluid}}) = f(t, p) = \hat{c}_1 + \hat{c}_2 t + \hat{c}_3 t^2 + \hat{c}_4 t^3 + \hat{c}_5 t^3 + \hat{c}_6 p + \hat{c}_7 p^2 \quad (10)$$

$$u(e) = 4.249057 \times 10^{-3} - 6.942 \times 10^{-6} \cdot t - 2.0376 \times 10^{-8} \cdot t^2 + 8.0679 \times 10^{-11} \cdot t^3 \\ + 1.2451 \times 10^{-13} \cdot t^4 + 1.64787 \times 10^{-4} \cdot p + 5.345 \times 10^{-6} \cdot p^2 \quad (11)$$

The measurement equation for  $\rho_{\text{fluid}}$  is

$$\alpha = \frac{W_{\text{cal}} - W_{\text{tare}}}{(m_{\text{cal}} - m_{\text{tare}}) - \rho_{\text{N}_2} (V_{\text{cal}} - V_{\text{tare}})} \quad (12)$$

$$\beta = \frac{W_{\text{cal}}}{\alpha} - (m_{\text{cal}} - \rho_{\text{N}_2} V_{\text{cal}}) \quad (13)$$

$$\rho_{\text{fluid}} = \left[ (m_1 - m_2) - \frac{m_1(W_1 - W_2)}{W_1 - \alpha\beta} \right] / \left[ (V_1 - V_2) - \frac{V_1(W_1 - W_2)}{W_1 - \alpha\beta} \right] - \rho_0 \quad (14)$$

The uncertainty of  $\rho_{\text{fluid}}$  is estimated using propagation of errors and the degrees of freedom are estimated using the Welch-Satterthwaite approximation. The remainder of section 4.6 describes the uncertainties required to compute  $u(\rho_{\text{fluid}})$ .

##### 4.6.1 Weighings $W_1$ , $W_2$ , $W_{\text{cal}}$ , $W_{\text{tare}}$

The recorded values of the sinker weighings  $W_1$ ,  $W_2$ ,  $W_{\text{cal}}$ ,  $W_{\text{tare}}$  are averages of 12 measurements, so the uncertainty of a weighing,  $u(W_x)$  is the standard deviation of the 12 readings divided by  $\sqrt{12}$  ( $df_{W_1} = df_{W_2} = df_{W_{\text{cal}}} = df_{W_{\text{tare}}} = 11$ ). Typical values of  $u(W_1)$ ,  $u(W_2)$ ,  $u(W_3)$ , and  $u(W_4)$  are  $1.48 \cdot 10^{-6} \text{ g}$ ,  $1.07 \cdot 10^{-6} \text{ g}$ ,  $2.65 \cdot 10^{-6} \text{ g}$ , and  $2.51 \cdot 10^{-6} \text{ g}$ , respectively.

#### 4.6.2 Density of Nitrogen, $\rho_{N_2}$

We use the equation of state from [6] to estimate the density of nitrogen, which is used as a purge gas surrounding the balance, as a function of temperature and pressure. Propagation of errors is used to estimate the uncertainty of  $\rho_{N_2}$ .

The uncertainties of temperature and pressure are comprised of uncertainties due to systematic and random effects that are added in quadrature. The values of the standard deviation in  $T$  and  $p$ ,  $S_T$  and  $S_p$ , are computed from nine repeat measurements.

Table 5. Uncertainties due to systematic and random effects for the density of nitrogen.

Source	Uncertainty Due to Systematic Effects	Uncertainty due to Random Effects
Temperature	0.2 K ( $df_T = 8$ )	$S_T / \sqrt{9}$ K ( $df_T = 8$ )
Pressure	$p \cdot 0.0001$ kPa ( $df_p = 8$ )	$S_p / \sqrt{9}$ kPa ( $df_p = 8$ )

#### 4.6.3 Drift Correction, $\rho_0$

The drift correction,  $\rho_0$ , is estimated from “vacuum” data that was collected between fillings. Table 6 displays the sequence in which vacuum and iso-octane measurements were taken and Figure 7 shows the vacuum measurements.

Table 6. Sequence of vacuum and iso-octane measurements.

Dates	Vacuum Measurements	Iso-octane Filling
8 November 2011 – 16 November 2011	A	
		1
5 January 2012 – 8 January 2012	B	
		2
2 February 2012 – 3 February 2012	C	
		3
16 February 2012 – 17 February 2012	D	
		4
10 March 2012 – 12 March 2012	E	

The drift correction was estimated by fitting a straight line to the vacuum data before and after an iso-octane filling. For example, a straight line was fit to vacuum data sets B and C to estimate  $\rho_0$  for the second iso-octane filling. To ensure data stability of the measurement system, we used the last 20 points in each measurement series for the analysis.

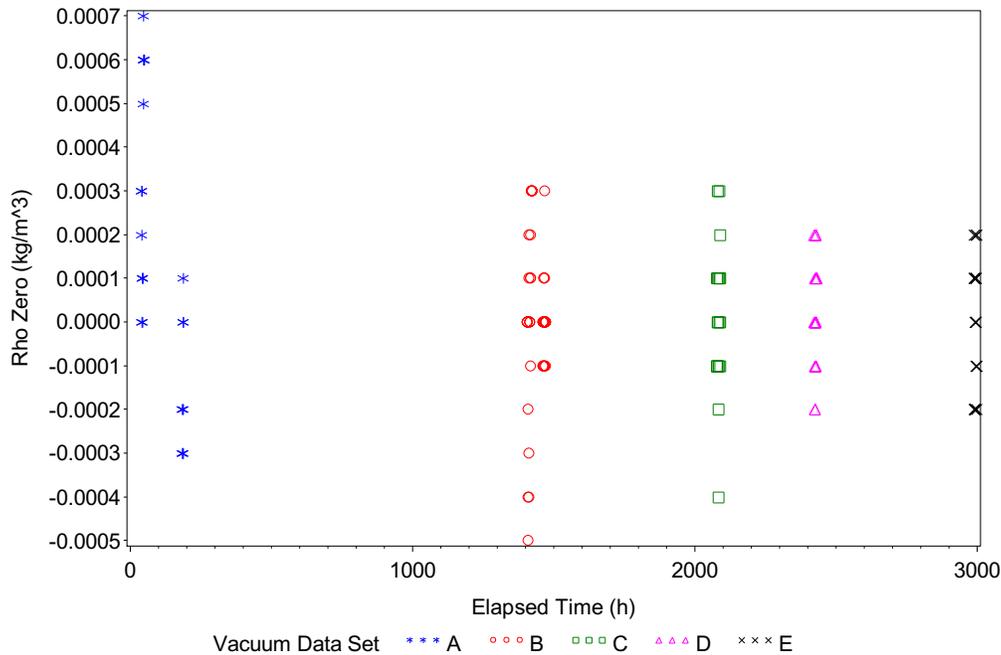


Figure 7. Values of  $\rho_0$  for five vacuum data sets over time.

Thus, the drift correction,  $\rho_0$ , for a straight line fit to adjacent pairs of vacuum data sets, is a function of the elapsed time,  $\tau_0$ ,

$$\rho_0 = \hat{d}_0 + \hat{d}_1 \tau_0, \quad (15)$$

where  $\hat{d}_0$  and  $\hat{d}_1$  are fitting parameters. The uncertainty of  $\rho_0$  is

$$u(\rho_0) = s \left[ \frac{1}{n} + (\tau_0 - \bar{\tau})^2 / \sum_{i=1}^n (\tau_i - \bar{\tau})^2 \right], \quad (16)$$

where  $n$  is the number of observations used to estimate the regression parameters and  $s$  is the standard deviation of the fit. The degrees of freedom associated with the uncertainty estimate is  $n - 2$ . Values of  $\rho_0$  ranged from  $2.12 \cdot 10^{-5} \text{ kg} \cdot \text{m}^{-3}$  to  $3.90 \cdot 10^{-5} \text{ kg} \cdot \text{m}^{-3}$ .

#### 4.6.4 Mass of Sinkers, $m_x$

The mass of the density sinkers ( $m_1$  and  $m_2$ ) and calibration masses ( $m_{\text{cal}}$  and  $m_{\text{tare}}$ ) were determined by a double-substitution weighing design as described by Harris and Torres [7]. A mass determination involved weighings of the unknown object  $m_x$  (*i.e.*, a sinker) and a standard mass  $m_s$ , with each being weighed alone and together with a small “sensitivity mass”  $m_{\text{sw}}$ . Propagation of errors was used to estimate the uncertainty of a single mass determination using the measurement equation

$$m_x = \left\{ m_s \left( 1 - \frac{\rho_{\text{air}}}{\rho_s} \right) + \left[ \frac{(O_2 - O_1) + (O_3 - O_4)}{2(O_3 - O_2)} \right] \left[ m_{\text{sw}} \left( 1 - \frac{\rho_{\text{air}}}{\rho_{\text{sw}}} \right) \right] \right\} / \left( 1 - \frac{\rho_{\text{air}}}{\rho_x} \right), \quad (17)$$

where

$O_1$ ,  $O_2$ ,  $O_3$ , and  $O_4$  represent balance readings,  
 $\rho_{\text{air}}$  is the density of ambient air during the mass determination,  
 $m_s$  and  $m_{\text{sw}}$  are the standard masses,  
 $\rho_s$  and  $\rho_{\text{sw}}$  are the densities of the standard masses, and  
 $\rho_x$  is the density of the object (*e.g.*, sinker).

#### 4.6.4.1 Balance Readings, $O_1$ , $O_2$ , $O_3$ , $O_4$

The uncertainty of the balance reading was derived from the expanded uncertainty provided in the manufacturer's instrument specifications:

$$u(O_1) = u(O_2) = u(O_3) = u(O_4) = \frac{0.00003}{2} = 0.000015 \text{ g} . \quad (18)$$

#### 4.6.4.2 Calibration Data for Standard Masses

Calibration data for the standard masses are listed in Table 7 as reported by the manufacturer of the standard masses.

Table 7. Calibration data for standard masses.

Nominal Mass (g)	Certified Mass (g)	Uncertainty (g)	Density ( $\text{g}\cdot\text{cm}^{-3}$ )	Uncertainty ( $\text{g}\cdot\text{cm}^{-3}$ )
50	50.000006	0.0000080	8.00	0.01545
20	20.000012	0.0000065	8.00	0.01545
20*	20.000009	0.0000065	8.00	0.01545
10	10.000010	0.0000050	8.00	0.01545
5	5.0000077	0.0000041	8.00	0.01545
2	2.0000050	0.00000305	8.00	0.01545

\*one of the 20 g masses was distinguished by a small dimple

Nominal masses of  $(50 + 10) = 60$  g and  $(20 + 20^* + 5) = 45$  g were used for  $m_s$ , and nominal masses of 5 g or 2 g were used for  $m_{\text{sw}}$ . The nominal masses and their associated uncertainties were calculated as follows.

$$m_s(60) = 50.000006 + 10.000010 = 60.000016\text{g}$$

$$u(m_s(60)) = \left[ (0.000008)^2 + (0.000005)^2 \right]^{0.5} = 0.0000094\text{g}$$

$$m_s(45) = 20.000012 + 20.000009 + 5.0000077 = 45.0000287\text{g}$$

$$u(m_s(45)) = \left[ 2 \cdot (0.0000065)^2 + (0.0000041)^2 \right]^{0.5} = 0.0000101\text{g}$$

$$m_{sw}(5) = 5.0000077\text{g}$$

$$u(m_{sw}(5)) = 0.0000041\text{g}$$

$$m_{sw}(2) = 2.0000050\text{g}$$

$$u(m_{sw}(2)) = 0.00000305\text{g}$$

$$\rho_s = \rho_{sw} = 8.0\text{g} \cdot \text{cm}^{-3}$$

$$u(\rho_s) = u(\rho_{sw}) = 0.015\text{g} \cdot \text{cm}^{-3}$$

#### 4.6.4.3 Density of air, $\rho_{\text{air}}$

The density of air (in the balance chamber during the mass determinations) was computed with the CIPM 81/91 air density formula [8]:

$$\rho_{\text{air}} = \frac{pM_a}{ZRT} \left[ 1 - x_v \left( 1 - \frac{M_v}{M_a} \right) \right] \quad (19)$$

where

$p$  is pressure,

$T$  is thermodynamic temperature,

$x_v$  is the mole fraction of water,

$M_a$  is the molar mass of dry air,

$M_v$  is the molar mass of water,

$Z$  is the compressibility factor, and

$R$  is the molar gas constant.

Propagation of errors is used to compute the uncertainty of  $\rho_{\text{air}}$  using the following uncertainties for the thermometer, barometer, and hygrometer that were used to measure the atmospheric conditions:

$$u(T) = 0.2\text{ K}$$

$$u(p) = 0.0001p/\text{kPa}$$

$$u(h) = 0.02$$

Although the equation for  $\rho_{\text{air}}$  does not explicitly contain humidity,  $h$ ,  $x_v$  is a function of  $h$ .

#### 4.6.4.4 Density $\rho_x$ , and mass $m_x$ , of sinkers

Sinker densities were computed from repeated measurements of volume and mass using the “hydrostatic comparator” described in [2] (for sinkers 1 and 2) and a simple hydrostatic experiment in water (for the cal and tare sinkers). The uncertainty was generated using the NIST Uncertainty Machine [9]. These values are given in Table 8.

Table 8. Estimated density and the associated uncertainty for each sinker.

Sinker	Density ( $\text{g}\cdot\text{cm}^{-3}$ )	Uncertainty ( $\text{g}\cdot\text{cm}^{-3}$ )
Sinker 1 (Titanium)	4.511732	0.00000691
Sinker 2 (Tantalum)	16.663202	0.0000483
Cal	7.956976	0.0023
Tare	5.923001	0.0017

Between 6 and 12 mass determinations were completed for each sinker. Once the single mass determinations and their uncertainties were computed, they were combined using a random-effects model as described in section H.5.2 of [10]. Degrees of freedom are from the number of mass determinations for each sinker,  $k - 1$ . The final estimates of mass and their uncertainties for the four sinkers are listed in Table 9.

Table 9. Estimated mass and the associated uncertainty,  $u(m_x)$ , for each sinker.

Sinker	Mass (g)	Uncertainty (g)	Degrees of Freedom
Sinker 1 (Titanium)	60.075348	0.0000081	9 - 1 = 8
Sinker 2 (Tantalum)	60.055501	0.0000093	6 - 1 = 5
Cal	59.508634	0.0000067	12 - 1 = 11
Tare	44.296943	0.0000067	11 - 1 = 10

#### 4.6.5 Sinker volumes

The volumes of the sinkers vary with temperature (thermal expansion) and pressure. They were calibrated at reference conditions, and the volume at the temperature and pressure of each density measurement was calculated with the correction terms described in the following sections.

##### 4.6.5.1 Sinker volume, $V_1$ , $V_2$ at reference conditions

The volumes of the sinkers were calibrated at  $t = 20^\circ\text{C}$  and  $p = 82\text{ kPa}$  by comparison to solid density standards of single-crystal silicon by use of a hydrostatic comparator as described by McLinden and Splett [2]. These “reference volumes”  $V_{x,\text{ref}}$  were  $13.315363\text{ cm}^3$  for the titanium sinker (sinker “1”) and  $3.604079\text{ cm}^3$  for the tantalum sinker (sinker “2”). This determination is subject to the systematic errors listed in Table 10, which were added in quadrature. The random

component is derived from a least-squares fit of ratios of sinker data from a designed experiment as described in [11]. The resulting uncertainties are given in Table 11. See [2] for further details.

Table 10. Systematic errors associated with  $V_{1,\text{ref}}$  and  $V_{2,\text{ref}}$ .

Source of Systematic Error	Magnitude of Error	Sinker 1 (Ti) Uncertainty, cm <sup>3</sup>	Sinker 2 (Ta) Uncertainty, cm <sup>3</sup>
Density of Standard	$0.26 \cdot 10^{-6}$ g/cm <sup>3</sup>	$1.49 \cdot 10^{-6}$	$4.03 \cdot 10^{-7}$
Mass of standard	$5.0 \cdot 10^{-5}$ g	$0.29 \cdot 10^{-5}$	$0.803 \cdot 10^{-5}$
Mass of object	$5.0 \cdot 10^{-5}$ g	$3.07 \cdot 10^{-5}$	$3.07 \cdot 10^{-5}$
Weighing of standard	$5.0 \cdot 10^{-5}$ g	$0.96 \cdot 10^{-5}$	$0.26 \cdot 10^{-5}$
Weighing of object	$5.0 \cdot 10^{-5}$ g	$3.07 \cdot 10^{-5}$	$3.07 \cdot 10^{-5}$

Table 11. Uncertainty budgets for  $V_{1,\text{ref}}$  and  $V_{2,\text{ref}}$ .

Source	Sinker 1 (Ti) cm <sup>3</sup>	Sinker 2 (Ta) cm <sup>3</sup>
Systematic Component	$4.46 \cdot 10^{-5}$ cm <sup>3</sup> ( $df_{V1} = 8$ )	$4.42 \cdot 10^{-5}$ cm <sup>3</sup> ( $df_{V2} = 8$ )
Random Component	$1.54 \cdot 10^{-5}$ cm <sup>3</sup> ( $df_{V1} = 6$ )	$4.22 \cdot 10^{-6}$ cm <sup>3</sup> ( $df_{V2} = 6$ )
( $V_{x,\text{ref}}$ )	$4.72 \cdot 10^{-5}$ cm <sup>3</sup> ( $df_{V1} = 9$ )	$4.44 \cdot 10^{-5}$ cm <sup>3</sup> ( $df_{V2} = 8$ )

#### 4.6.5.2 Sinker Volume, $V_1$ , $V_2$ as a $f(t, p)$

The volumes of the density sinkers will vary with the temperature and pressure of the fluid measurement, and thus the sinker volumes used to calculate density by Eq. (2) must be corrected. The volume of the sinkers is computed using

$$V_x = V_{x,\text{ref}} \cdot V_\alpha \cdot V_\kappa \cdot V_T. \quad (20)$$

The correction,  $V_\kappa$ , accounts for the decrease in volume with increased pressure; it is computed as

$$V_\kappa = 1 - \frac{p - p_{\text{ref}}}{\kappa_0}, \quad (21)$$

where  $\kappa_0$  is the bulk modulus of elasticity of the sinker material,  $p$  is the fluid pressure in the densimeter and  $p_{\text{ref}} = 0.082$  MPa. The uncertainty of the correction is

$$u(V_\kappa) = \left[ \left( \frac{p - p_{\text{ref}}}{\kappa_0^2} \right)^2 u^2(\kappa_0) \right]^{0.5}, \quad (22)$$

where  $u(\kappa_0) = \kappa_0 \cdot 0.05$  and the uncertainties in  $p$  and  $p_{\text{ref}}$  are negligible ( $df_{V_\kappa} = 8$ ).

The  $V_\alpha$  term accounts for the change in sinker volume with temperature; it is given by

$$V_\alpha = \frac{(1 + 1.0 \times 10^{-6} \cdot \Lambda_1)^3}{(1 + 1.0 \times 10^{-6} \cdot \Lambda_2)^3}. \quad (23)$$

The value of  $V_\alpha$  for sinker 1 (titanium) is based on literature values for the coefficient of linear expansion reported by Touloukian [12], while the value for sinker 2 (tantalum) is based on data collected by Rubotherm Präzisionsmesstechnik, Germany. For sinker 1 (titanium):

$$\Lambda_1 = 8.6538 \cdot T_1 + 0.0048291 \cdot T_1^2 - 1.4220 \times 10^{-5} \cdot T_1^3 + 2.8263 \times 10^{-8} \cdot T_1^4$$

and

$$\Lambda_2 = 8.6538 \cdot T_2 + 0.0048291 \cdot T_2^2 - 1.4220 \times 10^{-5} \cdot T_2^3 + 2.8263 \times 10^{-8} \cdot T_2^4,$$

where  $T_1 = T - 293.0$  K,  $T_2 = T_{\text{ref}} - 293.0$  K, and  $T_{\text{ref}} = 293.15$  K.

For sinker 2 (tantalum):

$$\Lambda_1 = 0.0020336 + 5.9569 \cdot T_1 - 0.00016957 \cdot T_1^2 + 6.9633 \times 10^{-6} \cdot T_1^3$$

and

$$\Lambda_2 = 0.0020336 + 5.9569 \cdot T_2 - 0.00016957 \cdot T_2^2 + 6.9633 \times 10^{-6} \cdot T_2^3,$$

where  $T_1 = T - 300.738$  K,  $T_2 = T_{\text{ref}} - 300.738$  K, and  $T_{\text{ref}} = 293.15$  K.

The uncertainty of  $V_\alpha$ ,  $u(V_\alpha)$ , is included in  $u(V_T)$  (see below) so uncertainty is not calculated for the  $V_\alpha$  term.

A further correction for temperature effects (which was applied to both sinkers 1 and 2) is given by the  $V_T$  term. This correction was based on argon measurements carried out over a range of pressures along a number of isotherms. The density measured for a temperature  $T$  and pressure  $p$  are ratioed to that measured for a reference temperature  $T_{\text{ref}}$  (here  $T_{\text{ref}} = 20.00$  °C) at the same  $p$ ; these density ratios are extrapolated to zero pressure where the ideal gas law applies. The  $V_T$  term is based on the difference between the extrapolated density ratio and the temperature ratio. See reference [13] for a complete discussion of this method. The  $V_T$  correction is computed using

$$V_T = 1 - \delta, \quad (24)$$

where  $\delta$  is the sinker volume adjustment predicted by

$$\delta = \hat{a}(t - t_{\text{ref}}) + \hat{b}(t - t_{\text{ref}})^2 + \hat{c}(t - t_{\text{ref}})^3. \quad (25)$$

Eq. 25 is shown in Figure 8. The uncertainty of  $V_T$  and its degrees of freedom ( $df_{V_T} = 21 - 3$ ) are derived from a *weighted* fit of calibration data determined from argon measurements as described in [13]. Weights are defined as

$$w = \frac{1}{[u(\delta)]^2}, \quad (26)$$

where  $u(\delta)$  represents the standard deviation of  $\delta$  as predicted by

$$u(\delta) = \hat{d}(t - t_{\text{ref}}) + \hat{f}(t - t_{\text{ref}})^2 \quad (27)$$

for a given temperature. The uncertainty  $u(V_T)$  is the standard error of the predicted  $V_T$ , or equivalently, the predicted value of  $u(\delta)$ . The sinker volume adjustment ranged from  $-0.018\%$  to  $0.041\%$ , and it was zero at  $T_{\text{ref}}$ . The uncertainty of the sinker volume adjustment ranged from  $0.005\%$  to  $0.012\%$ , depending on temperature. Constants for volume correction factors (Eqs. 21–22) are listed in Table 12.

Table 12. Constants for volume correction factors.

Constant	Sinker 1 - Titanium	Sinker 2 - Tantalum
$V_{x, \text{ref}}$	13.315363 cm <sup>3</sup>	3.604079 cm <sup>3</sup>
$t_{\text{ref}}$	293.15 K	293.15 K
$p_{\text{ref}}$	82.0 kPa	82.0 kPa
$\kappa_0$	109.1·10 <sup>6</sup> MPa	196.3·10 <sup>6</sup> MPa

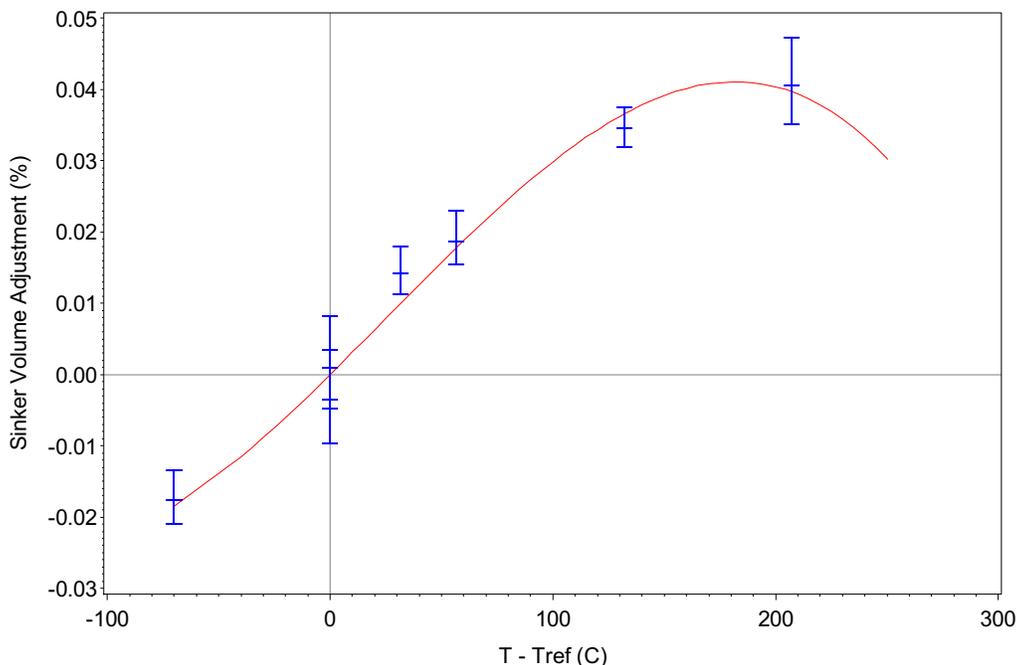


Figure 8. Sinker volume adjustment (eq. 25) as a function of temperature. The reference temperature ( $T_{ref}$ ) is 20.00 °C, and the error bars represent standard uncertainties.

#### 4.6.5.3 Sinker Volume, $V_{cal}$ , $V_{tare}$

The cal and tare masses are housed in the balance chamber, *i.e.*, at nearly constant temperature and pressure. Thus, the corrections needed for the density sinkers are not required. The type B uncertainty evaluations for sinker volume for the cal and tare sinkers are based on uniform distributions bounded by 0.05 % of the nominal sinker volume.

$$u(V_{cal}) = \frac{0.0005 \cdot V_{cal}}{\sqrt{3}} \quad \text{and} \quad u(V_{tare}) = \frac{0.0005 \cdot V_{tare}}{\sqrt{3}} \quad (28)$$

$V_{cal} = V_{tare} = 7.4788 \text{ cm}^3$ , and the uncertainties are  $u(V_{cal}) = u(V_{tare}) = 0.002159 \text{ cm}^3$  ( $df_{V_{cal}} = df_{V_{tare}} = 8$ ).

#### 4.6.6 Summary of $u(\rho_{fluid})$

Uncertainty budgets for  $\rho_{fluid}$ , based on Eqs. 12–14, are shown in Tables 13 and 14 for two combinations of temperature and pressure. Table 15 gives the relative (percentage) contribution to the overall uncertainty in  $\rho_{fluid}$  from the different sources.

Table 13. Uncertainty budget for  $\rho_{\text{fluid}}$  at 30 °C and 1 MPa. For this case,  
 $u(\rho_{\text{fluid}}) = 0.004 \text{ kg}\cdot\text{m}^{-3}$  and  $df_{\text{eff}} = 21$ .

Source	$(x_i)$	$c_i$	$c_i \cdot (x_i)$ ( $\text{kg}\cdot\text{m}^{-3}$ )	Degrees of Freedom
$W_{\text{cal}}$	$2.10\cdot 10^{-6} \text{ g}$	33.1	$6.94\cdot 10^{-5}$	11
$W_{\text{tare}}$	$1.66\cdot 10^{-6} \text{ g}$	44.47	$7.38\cdot 10^{-5}$	11
$m_{\text{cal}}$	$6.74\cdot 10^{-6} \text{ g}$	33.1	$2.23\cdot 10^{-4}$	11
$m_{\text{tare}}$	$6.75\cdot 10^{-6} \text{ g}$	44.47	$3.00\cdot 10^{-4}$	10
$V_{\text{cal}}$	$2.16\cdot 10^{-3} \text{ cm}^3$	0.03	$6.78\cdot 10^{-5}$	8
$V_{\text{tare}}$	$2.16\cdot 10^{-3} \text{ cm}^3$	0.04	$9.11\cdot 10^{-5}$	8
$\rho_{\text{air}}$	$6.47\cdot 10^{-7} \text{ g/cm}^3$	85.03	$5.50\cdot 10^{-5}$	8
$m_1$	$8.13\cdot 10^{-6} \text{ g}$	98.73	$8.02\cdot 10^{-4}$	8
$m_2$	$9.35\cdot 10^{-6} \text{ g}$	87.36	$8.17\cdot 10^{-4}$	5
$V_1$	$4.76\cdot 10^{-5} \text{ cm}^3$	67.6	$3.22\cdot 10^{-3}$	10
$V_2$	$4.44\cdot 10^{-5} \text{ cm}^3$	59.82	$2.66\cdot 10^{-3}$	8
$W_1$	$2.08\cdot 10^{-6} \text{ g}$	98.72	$2.05\cdot 10^{-4}$	11
$W_2$	$7.82\cdot 10^{-7} \text{ g}$	87.35	$6.83\cdot 10^{-5}$	11
$\rho_0$	$3.47\cdot 10^{-8} \text{ g/cm}^3$	1000	$3.47\cdot 10^{-5}$	55

Table 14. Uncertainty budget for  $\rho_{\text{fluid}}$  at 160 °C and 30 MPa. For this case,  $u(\rho_{\text{fluid}}) = 0.012 \text{ kg}\cdot\text{m}^{-3}$  and  $df_{\text{eff}} = 10$ .

Source	$(x_i)$	$c_i$	$c_i \cdot (x_i)$ ( $\text{kg}\cdot\text{m}^{-3}$ )	Degrees of Freedom
$W_{\text{cal}}$	$1.73\cdot 10^{-6} \text{ g}$	30.15	$5.22\cdot 10^{-5}$	11
$W_{\text{tare}}$	$1.87\cdot 10^{-6} \text{ g}$	40.51	$7.57\cdot 10^{-5}$	11
$m_{\text{cal}}$	$6.74\cdot 10^{-6} \text{ g}$	30.16	$2.03\cdot 10^{-4}$	11
$m_{\text{tare}}$	$6.75\cdot 10^{-6} \text{ g}$	40.51	$2.73\cdot 10^{-4}$	10
$V_{\text{cal}}$	$2.16\cdot 10^{-3} \text{ cm}^3$	0.03	$6.15\cdot 10^{-5}$	8
$V_{\text{tare}}$	$2.16\cdot 10^{-3} \text{ cm}^3$	0.04	$8.26\cdot 10^{-5}$	8
$\rho_{\text{air}}$	$6.41\cdot 10^{-7} \text{ g/cm}^3$	77.46	$4.97\cdot 10^{-5}$	8
$m_1$	$8.13\cdot 10^{-6} \text{ g}$	98.76	$8.03\cdot 10^{-4}$	8
$m_2$	$9.35\cdot 10^{-6} \text{ g}$	88.41	$8.26\cdot 10^{-4}$	5
$V_1$	$1.87\cdot 10^{-4} \text{ cm}^3$	61.62	$1.15\cdot 10^{-2}$	9
$V_2$	$5.21\cdot 10^{-5} \text{ cm}^3$	55.16	$2.88\cdot 10^{-3}$	13
$W_1$	$1.74\cdot 10^{-6} \text{ g}$	98.76	$1.72\cdot 10^{-4}$	11
$W_2$	$2.44\cdot 10^{-6} \text{ g}$	88.4	$2.15\cdot 10^{-4}$	11
$\rho_0$	$3.06\cdot 10^{-8} \text{ g/cm}^3$	1000	$3.06\cdot 10^{-5}$	60

Table 15. Percentages of total variation in  $u(\rho_{\text{fluid}})$  for six sources of uncertainty at various temperatures and pressures. The column labeled “all others” contains the combined percentage of total variation for the remaining eight sources. The value of  $u(\rho_{\text{fluid}})$  is also listed. The quantities in the table represent average values for the given temperatures and pressures.

$t$ (°C)	$p$ (MPa)	Percent of Total Variation							$(\rho_{\text{fluid}})$ ( $\text{kg}\cdot\text{m}^{-3}$ )
		$V_1$	$V_2$	$m_{\text{cal}}$	$m_{\text{tare}}$	$m_1$	$m_2$	all others	
-5	1	55.2	37.1	0.3	0.5	3.2	3.2	0.5	0.005
-5	15	84.8	12.8	0.1	0.2	1	1	0.1	0.008
-5	30	93.7	5.5	0	0.1	0.3	0.3	0.1	0.014
30	1	54.6	37.3	0.3	0.5	3.4	3.5	0.4	0.004
30	30	93.5	5.6	0	0.1	0.4	0.4	0	0.014
160	1	52.0	36.7	0.2	0.4	4.7	5.1	0.8	0.004
160	15	82.2	14.3	0.1	0.2	1.5	1.6	0.1	0.007
160	30	93.1	5.8	0	0.1	0.5	0.5	0.1	0.012

## 5. Summary of Uncertainties

### 5.1 Combined Standard Uncertainty

Combined standard uncertainty, computed using Eq. 4 for degassed samples and excluding uncertainties due to the effects of the user's temperature and pressure measurements, is listed in Table 16 for various combinations of temperature and pressure. (The value of  $u(\Delta)$  is zero for degassed samples.)

When the SRM is used to calibrate a user's densimeter, the uncertainties listed in Table 16 can be utilized in conjunction with uncertainties in the user's temperature and pressure measurements,  $u(tp)$  (Table 4), and their level of fluid saturation,  $u(\Delta)$ .

### 5.2 Expanded Uncertainty and Degrees of Freedom

The average expanded uncertainty for degassed measurements reported in this document is  $0.054 \text{ kg}\cdot\text{m}^{-3}$ . The coverage factor,  $k$ , is approximately 2 based on a Student's  $t$  distribution with 63 effective degrees of freedom. The effective degrees of freedom were computed using the Welch-Satterthwaite approximation. To obtain a conservative estimate of combined standard uncertainty, we used the largest value of  $u(e)$  ( $0.014 \text{ kg}\cdot\text{m}^{-3}$ ) and the smallest degrees of freedom associated with  $\rho_{\text{fluid}}$  ( $df_e = 10$ ) across all temperatures and pressures.

Table 16. Combined standard uncertainty in  $\rho_c$  ( $\text{kg}\cdot\text{m}^{-3}$ ) including the effects of  $u(\rho)$ ,  $u(V)$ ,  $u(x)$ , and  $u(e)$  for degassed samples.

$t$ ( $^{\circ}\text{C}$ )	Pressure (MPa)								
	0.1	1	2	5	10	15	20	25	30
-50	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
-40	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
-30	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
-20	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
-10	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
0	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
10	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
20	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
30	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
40	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
50	0.025	0.025	0.025	0.025	0.025	0.026	0.026	0.027	0.028
60	0.025	0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
70	0.025	0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
80	0.025	0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
90	0.025	0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
100		0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
110		0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
120		0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
130		0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
140		0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
150		0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028
160		0.025	0.025	0.025	0.025	0.025	0.026	0.027	0.028

## 6. Discussion and Conclusions

We report values for the density of liquid iso-octane that form the basis of NIST Standard Reference Material<sup>®</sup> 2214 “Iso-octane Liquid Density—Extended Range.” This work extends the range of this SRM, which was previously limited to 15 °C to 25 °C and normal atmospheric pressure, to the temperature range –50 °C to 160 °C and pressure range 0.1 MPa to 30 MPa. This SRM will be useful in the calibration of industrial densimeters.

The uncertainties for the density values were obtained by a thorough statistical analysis of multiple sources of uncertainty. In many cases, a measured quantity depended on other underlying measurands, and the uncertainties at each level were considered.

The measurements reported here are directly traceable to SI quantities. The density was determined by weighing sinkers immersed in the fluid. The volume (or, equivalently, density) of the sinkers was determined by comparison to solid density standards that are directly traceable to the meter and kilogram. The balance that carried out the weighings was calibrated for each density determination using calibration weights, which were, in turn, calibrated against standard masses. The temperature of the fluid was measured with a standard platinum resistance thermometer calibrated with ITS-90 fixed points. The pressure transducer was calibrated against a piston gage pressure standard.

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## APPENDIX—Measured Values of Iso-octane Fluid Density

Table A1. Experimentally measured temperatures  $t$ , pressures  $p$ , and densities  $\rho_{\text{exp}}$ , for degassed SRM iso-octane with standard uncertainties of the experimental measurement,  $u(\rho_{\text{exp}}) = [u^2(\rho_{\text{fluid}}) + u^2(x)]^{0.5}$ , where  $u(\rho_{\text{exp}})$  includes uncertainties due to apparatus and material degradation.

$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )	$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )
Filling 1				Filling 1 (continued)			
-59.001	2.5415	756.580	0.009	-26.148	9.8819	735.999	0.010
-59.000	2.5429	756.579	0.009	-17.147	18.4805	735.082	0.012
-58.999	2.5436	756.579	0.009	-17.146	18.4806	735.079	0.012
-58.999	2.5424	756.579	0.009	-17.145	18.4801	735.077	0.012
-54.450	7.6396	756.029	0.009	-17.144	18.4786	735.078	0.012
-54.449	7.6408	756.028	0.009	-7.498	27.2048	733.943	0.015
-54.448	7.6412	756.029	0.009	-7.496	27.2052	733.942	0.015
-54.448	7.6423	756.027	0.009	-7.495	27.2039	733.941	0.015
-48.897	13.8450	755.412	0.011	-7.496	27.2026	733.941	0.015
-48.897	13.8444	755.413	0.011	-5.006	29.4331	733.662	0.015
-48.898	13.8444	755.412	0.011	-5.006	29.4322	733.661	0.015
-48.898	13.8441	755.411	0.011	-5.006	29.4311	733.660	0.015
-43.348	19.9644	754.816	0.012	-5.006	29.4299	733.660	0.015
-43.345	19.9663	754.816	0.012	-5.000	24.3084	730.335	0.013
-43.344	19.9688	754.819	0.012	-5.000	24.3028	730.331	0.013
-43.344	19.9682	754.816	0.012	-5.001	24.2970	730.327	0.013
-37.843	25.9640	754.248	0.014	-5.002	24.2916	730.325	0.013
-37.843	25.9638	754.248	0.014	-5.001	15.4809	724.245	0.011
-37.843	25.9642	754.248	0.014	-5.000	15.4813	724.245	0.011
-37.842	25.9657	754.248	0.014	-5.000	15.4805	724.244	0.011
-35.491	28.5027	754.009	0.015	-5.001	15.4787	724.246	0.011
-35.492	28.5019	754.010	0.015	-5.001	10.1263	720.290	0.010
-35.492	28.5015	754.010	0.015	-5.000	10.1273	720.290	0.010
-35.491	20.6112	749.543	0.012	-5.000	10.1264	720.290	0.010
-35.490	20.6096	749.542	0.012	-5.001	10.1257	720.289	0.010
-35.493	15.6813	746.618	0.011	-5.001	4.4550	715.846	0.009
-35.493	15.6792	746.617	0.011	-5.000	4.4568	715.847	0.009
-35.491	15.6779	746.615	0.011	-5.000	4.4573	715.848	0.009
-35.491	6.0516	740.548	0.009	-5.000	4.4567	715.848	0.009
-35.490	6.0514	740.547	0.009	-5.001	0.6652	712.710	0.008
-35.490	6.0504	740.547	0.009	-5.000	0.6656	712.709	0.008
-35.491	6.0462	740.543	0.009	-5.000	0.6656	712.709	0.008
-35.491	0.7846	737.001	0.008	-5.001	0.6651	712.709	0.008
-35.490	0.7853	737.001	0.008	4.000	8.0802	711.863	0.009
-35.490	0.7845	737.002	0.008	4.001	8.0806	711.863	0.009
-35.491	0.7830	737.001	0.008	4.000	8.0795	711.864	0.009
-26.150	9.8816	735.999	0.010	12.003	14.5767	711.147	0.010
-26.149	9.8826	735.998	0.010	12.005	14.5785	711.146	0.010
-26.148	9.8825	735.998	0.010	12.004	14.5784	711.148	0.010

Table A1 (continued)

$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )	$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )
Filling 1 (continued)				Filling 1 (continued)			
4.001	8.0807	711.863	0.009	70.002	20.1915	674.430	0.012
12.003	14.5779	711.147	0.010	70.001	27.4311	681.551	0.014
20.006	20.9783	710.455	0.012	69.998	20.1894	674.428	0.012
20.007	20.9796	710.455	0.012	70.002	20.1912	674.430	0.012
20.008	20.9797	710.454	0.012	69.998	15.9224	669.873	0.010
30.013	28.8184	709.596	0.015	70.001	15.9239	669.872	0.010
30.013	28.8184	709.595	0.015	70.001	15.9237	669.871	0.010
30.013	28.8190	709.595	0.015	69.998	15.9218	669.871	0.010
30.015	28.8197	709.595	0.015	70.001	10.6528	663.789	0.009
29.999	19.1125	701.869	0.012	69.999	10.6516	663.789	0.009
30.001	19.1126	701.867	0.012	69.997	10.6505	663.790	0.009
30.000	19.1116	701.866	0.012	69.999	10.6515	663.789	0.009
29.999	19.1106	701.867	0.012	70.001	5.2028	656.851	0.008
30.000	12.0436	695.664	0.010	69.998	5.2007	656.848	0.008
30.001	12.0447	695.664	0.010	69.998	5.2014	656.851	0.008
30.001	12.0444	695.664	0.010	70.000	5.2027	656.851	0.008
29.999	12.0430	695.664	0.010	70.001	1.2131	651.240	0.008
29.997	9.4033	693.200	0.009	69.998	1.2122	651.242	0.008
29.999	9.4042	693.200	0.009	70.001	1.2126	651.241	0.008
30.001	9.4054	693.199	0.009	70.001	1.2110	651.237	0.008
30.000	9.4039	693.199	0.009	78.996	6.0371	650.582	0.008
30.000	3.3476	687.178	0.008	78.998	6.0380	650.582	0.008
30.000	3.3471	687.178	0.008	79.000	6.0388	650.582	0.008
29.998	3.3461	687.177	0.008	78.998	6.0371	650.581	0.008
29.998	3.3461	687.178	0.008	87.998	10.8197	649.954	0.009
29.998	0.9986	684.688	0.008	87.997	10.8199	649.954	0.009
29.997	0.9982	684.689	0.008	87.999	10.8207	649.954	0.009
29.998	0.9996	684.689	0.008	88.002	10.8227	649.954	0.009
30.000	1.0003	684.688	0.008	97.006	15.5545	649.342	0.010
38.005	6.4264	684.026	0.009	97.008	15.5552	649.341	0.010
38.005	6.4258	684.026	0.009	97.005	15.5537	649.341	0.010
38.003	6.4256	684.026	0.009	97.008	15.5556	649.341	0.010
38.002	6.4251	684.027	0.009	106.004	20.2275	648.738	0.011
46.020	11.7886	683.380	0.010	106.007	20.2290	648.738	0.011
46.022	11.7902	683.380	0.010	106.006	20.2285	648.737	0.011
46.024	11.7908	683.379	0.010	115.001	24.8332	648.126	0.013
46.022	11.7898	683.380	0.010	115.005	24.8348	648.127	0.013
54.037	17.0838	682.752	0.011	115.004	24.8333	648.124	0.013
54.036	17.0831	682.751	0.011	115.000	24.8300	648.122	0.013
54.036	17.0837	682.752	0.011	124.994	29.8462	647.412	0.015
54.037	17.0847	682.752	0.011	124.995	29.8441	647.409	0.015
62.050	22.3140	682.145	0.012	124.998	29.8444	647.407	0.015
62.049	22.3133	682.144	0.012	124.998	29.8401	647.402	0.015
62.048	22.3131	682.145	0.012	124.997	21.4278	636.676	0.012
62.049	22.3136	682.145	0.012	124.995	21.4269	636.677	0.012
70.000	27.4320	681.552	0.014	124.997	17.5044	631.054	0.010
70.002	27.4307	681.550	0.014	124.995	17.4976	631.046	0.010
69.999	27.4293	681.550	0.014	124.993	17.4919	631.039	0.010
70.002	20.1926	674.431	0.012	124.996	14.3307	626.138	0.010

Table A1 (continued)

$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )	$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )
Filling 1 (continued)				Filling 1b (continued)			
124.993	14.3295	626.139	0.010	29.995	3.0531	686.858	0.008
124.994	14.3300	626.138	0.010	29.994	3.0531	686.857	0.008
124.997	17.4953	631.041	0.010	29.993	1.1100	684.795	0.008
124.997	14.3317	626.139	0.010	29.992	1.1077	684.794	0.008
134.979	18.7561	625.505	0.011	29.994	1.1084	684.793	0.008
134.983	18.7573	625.504	0.011	29.996	1.1087	684.790	0.008
134.983	18.7566	625.503	0.011	29.995	3.0530	686.857	0.008
134.979	18.7548	625.503	0.011				
139.955	20.9461	625.198	0.011	Filling 2			
139.958	20.9474	625.198	0.011	-58.996	1.6038	756.019	0.009
144.936	23.1192	624.880	0.012	-58.997	1.5999	756.019	0.009
144.936	23.1181	624.879	0.012	-58.998	1.5982	756.020	0.009
144.938	23.1190	624.878	0.012	-58.998	1.5973	756.018	0.009
144.941	23.1190	624.878	0.012	-58.999	1.5960	756.018	0.009
149.930	25.2859	624.565	0.013	-54.452	6.6806	755.472	0.009
149.929	25.2848	624.565	0.013	-54.451	6.6820	755.472	0.009
149.930	25.2855	624.565	0.013	-54.450	6.6836	755.471	0.009
149.933	25.2881	624.568	0.013	-54.449	6.6836	755.471	0.009
159.904	29.5738	623.938	0.014	-48.898	12.8810	754.860	0.010
159.903	29.5744	623.939	0.014	-43.346	18.9905	754.265	0.012
159.906	29.5765	623.940	0.014	-43.345	18.9917	754.265	0.012
159.907	29.5778	623.942	0.014	-43.345	18.9908	754.265	0.012
159.906	22.1354	612.635	0.012	-43.346	18.9900	754.266	0.012
159.907	22.1359	612.636	0.012	-37.845	24.9723	753.698	0.014
159.905	22.1354	612.636	0.012	-37.845	24.9722	753.698	0.014
159.904	22.1346	612.636	0.012	-37.844	24.9737	753.699	0.014
159.906	16.9606	603.539	0.010	-37.843	24.9746	753.696	0.014
159.905	16.9602	603.538	0.010	-35.493	27.5180	753.467	0.015
159.903	16.9603	603.540	0.010	-35.492	27.5170	753.466	0.015
159.903	16.9605	603.540	0.010	-35.491	27.5170	753.461	0.015
159.905	10.9573	591.135	0.009	-35.490	27.5171	753.462	0.015
159.907	10.9579	591.136	0.009	-35.491	20.7885	749.643	0.012
159.905	10.9576	591.136	0.009	-35.490	20.7881	749.647	0.012
159.903	10.9571	591.138	0.009	-35.490	20.7864	749.642	0.012
159.905	5.5680	577.397	0.008	-35.491	20.7858	749.645	0.012
159.905	5.5676	577.394	0.008	-35.493	17.2838	747.581	0.011
159.903	5.5668	577.393	0.008	-35.493	17.2837	747.582	0.011
159.901	5.5663	577.394	0.008	-35.492	17.2853	747.577	0.011
159.905	1.4130	563.945	0.008	-35.490	17.2882	747.584	0.011
159.906	1.4119	563.938	0.008	-35.491	10.3697	743.330	0.010
159.904	1.4108	563.938	0.008	-35.490	10.3714	743.326	0.010
159.902	1.4098	563.934	0.008	-35.489	10.3720	743.334	0.010
				-35.490	10.3712	743.331	0.010
				-35.492	5.5763	740.236	0.009
Filling 1b (addition of additional, fresh sample)				-35.490	5.5778	740.234	0.009
29.992	6.9293	690.791	0.009	-35.490	5.5786	740.235	0.009
29.992	6.9295	690.792	0.009	-35.491	5.5782	740.236	0.009
29.992	6.9298	690.793	0.009	-35.492	0.9248	737.098	0.008
29.993	6.9312	690.792	0.009	-26.151	10.0586	736.117	0.010
29.994	3.0523	686.845	0.008				

Table A1 (continued)

$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )	$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )
Filling 2 (continued)				Filling 2 (continued)			
-26.150	10.0595	736.120	0.010	29.998	29.4657	710.089	0.015
-26.151	10.0591	736.120	0.010	29.999	29.4660	710.090	0.015
-17.149	18.7207	735.239	0.012	30.000	23.7405	705.654	0.013
-17.148	18.7224	735.241	0.012	30.001	23.7400	705.653	0.013
-17.146	18.7244	735.241	0.012	29.999	23.7385	705.652	0.013
-26.150	10.0593	736.117	0.010	29.999	16.9100	699.990	0.011
-17.145	18.7253	735.240	0.012	29.999	23.7398	705.655	0.013
-7.493	27.8096	734.323	0.015	30.000	16.9099	699.987	0.011
-7.494	27.8088	734.328	0.015	29.999	16.9088	699.989	0.011
-7.495	27.8085	734.325	0.015	29.998	16.9073	699.988	0.011
-7.495	27.8095	734.326	0.015	30.000	11.6312	695.281	0.010
-5.004	30.1191	734.092	0.016	29.999	11.6299	695.281	0.010
-5.002	30.1202	734.091	0.016	29.998	11.6293	695.282	0.010
-5.002	30.1222	734.093	0.016	29.997	11.6288	695.280	0.010
-5.002	30.1209	734.094	0.016	29.999	5.9632	689.843	0.009
-5.001	23.5681	729.841	0.013	30.000	5.9648	689.844	0.009
-5.001	23.5680	729.841	0.013	29.999	1.6966	685.435	0.008
-5.001	23.5681	729.842	0.013	30.000	1.6974	685.435	0.008
-5.002	23.5671	729.842	0.013	30.000	1.6983	685.434	0.008
-5.001	16.0740	724.670	0.011	29.999	1.6978	685.435	0.008
-5.000	16.0747	724.669	0.011	38.003	7.1418	684.770	0.009
-5.000	16.0752	724.670	0.011	38.002	7.1408	684.769	0.009
-5.001	16.0743	724.672	0.011	38.001	7.1391	684.769	0.009
-5.002	11.0045	720.955	0.010	38.000	7.1379	684.767	0.009
-5.001	11.0054	720.953	0.010	46.021	12.5319	684.126	0.010
-5.001	11.0060	720.953	0.010	46.018	12.5307	684.128	0.010
-5.001	11.0047	720.952	0.010	54.030	17.8464	683.501	0.011
-5.002	5.9046	717.010	0.009	54.029	17.8458	683.502	0.011
-5.003	5.8972	717.005	0.009	54.031	17.8460	683.502	0.011
-5.004	1.2557	713.208	0.008	54.033	17.8426	683.497	0.011
-5.002	1.2566	713.208	0.008	62.043	23.0904	682.891	0.013
-5.000	1.2584	713.208	0.008	62.042	23.0887	682.888	0.013
-5.001	1.2568	713.206	0.008	62.042	23.0872	682.889	0.013
-2.000	3.7472	712.917	0.009	62.043	23.0866	682.887	0.013
-2.001	3.7470	712.921	0.009	70.054	28.2552	682.282	0.014
-2.003	3.7461	712.921	0.009	70.052	28.2534	682.281	0.014
-2.003	3.7466	712.920	0.009	70.053	28.2541	682.280	0.014
3.999	8.6983	712.368	0.009	70.055	28.2551	682.279	0.014
4.000	8.6991	712.368	0.009	70.056	23.8998	678.125	0.013
12.005	15.2226	711.658	0.011	70.056	23.8977	678.122	0.013
12.004	15.2188	711.657	0.011	70.053	23.8959	678.121	0.013
12.002	15.2152	711.654	0.011	70.052	23.8945	678.121	0.013
12.002	15.2137	711.653	0.011	70.055	17.8442	671.919	0.011
20.005	21.6182	710.950	0.012	70.051	17.8375	671.912	0.011
20.007	21.6191	710.949	0.012	70.054	17.8386	671.912	0.011
20.008	21.6189	710.949	0.012	70.054	17.8376	671.912	0.011
20.008	21.6179	710.948	0.012	70.051	17.8352	671.911	0.011
29.998	29.4663	710.092	0.015	70.054	11.9717	665.321	0.010
29.998	29.4655	710.090	0.015	70.051	11.9700	665.321	0.010

Table A1 (continued)

$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )	$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )
Filling 2 (continued)				Filling 2 (continued)			
70.051	11.9702	665.321	0.010	123.981	9.9462	619.517	0.009
70.053	11.9717	665.321	0.010	123.985	9.9477	619.518	0.009
70.053	6.0564	657.943	0.009	123.982	9.9467	619.517	0.009
70.055	1.0920	651.011	0.008	123.983	4.8952	609.725	0.008
70.053	1.0908	651.011	0.008	123.981	4.8943	609.726	0.008
70.051	1.0900	651.012	0.008	123.985	4.8956	609.726	0.008
70.054	1.0918	651.011	0.008	123.984	0.9856	600.846	0.008
70.050	6.0557	657.943	0.009	123.981	0.9839	600.844	0.008
78.998	5.8876	650.367	0.008	123.979	4.8932	609.726	0.008
78.998	5.8864	650.365	0.008	123.980	0.9833	600.842	0.008
79.001	5.8877	650.364	0.008	123.983	0.9835	600.839	0.008
79.002	5.8874	650.362	0.008	134.979	5.1657	600.196	0.008
87.998	10.6675	649.744	0.009	134.983	5.1673	600.199	0.008
87.996	10.6668	649.743	0.009	134.983	5.1679	600.199	0.008
87.998	10.6679	649.743	0.009	134.978	5.1663	600.200	0.008
88.001	10.6695	649.744	0.009	139.951	7.0485	599.918	0.008
97.005	15.3919	649.126	0.010	139.952	7.0475	599.914	0.008
97.005	15.3921	649.126	0.010	139.955	7.0479	599.912	0.008
97.002	15.3920	649.128	0.010	139.955	7.0468	599.908	0.008
97.004	15.3928	649.125	0.010	144.929	8.9218	599.624	0.009
97.002	15.3906	649.125	0.010	144.931	8.9221	599.626	0.009
97.000	15.3905	649.125	0.010	144.930	8.9219	599.624	0.009
96.999	15.3921	649.127	0.010	144.932	8.9226	599.624	0.009
97.003	15.3940	649.129	0.010	144.933	8.9229	599.625	0.009
105.998	20.0584	648.523	0.011	149.922	10.7951	599.339	0.009
105.998	20.0580	648.523	0.011	149.925	10.7960	599.339	0.009
106.000	20.0593	648.525	0.011	149.927	10.7961	599.338	0.009
106.002	20.0610	648.523	0.011	149.924	10.7952	599.336	0.009
115.000	24.6644	647.918	0.013	159.902	14.5196	598.779	0.010
115.002	24.6639	647.915	0.013	159.903	14.5201	598.779	0.010
114.999	24.6633	647.916	0.013	159.901	14.5193	598.777	0.010
115.001	24.6641	647.916	0.013	159.901	14.5187	598.779	0.010
123.984	29.2015	647.312	0.014	159.903	9.9731	588.848	0.009
123.984	29.1999	647.311	0.014	159.902	9.9724	588.848	0.009
123.987	29.2013	647.310	0.014	159.903	4.9171	575.494	0.008
123.987	29.2008	647.310	0.014	159.901	1.0295	562.511	0.008
123.982	23.6679	640.399	0.012	159.902	1.0296	562.511	0.008
123.986	23.6689	640.397	0.012	159.902	1.0298	562.512	0.008
123.986	23.6676	640.395	0.012	159.901	1.0294	562.511	0.008
123.982	23.6654	640.397	0.012				
123.985	16.7747	630.716	0.010	Filling 2b (addition of additional, fresh sample)			
123.983	16.7742	630.716	0.010	29.993	6.1726	690.037	0.009
123.981	16.7742	630.718	0.010	29.992	6.1726	690.037	0.009
123.983	16.7753	630.717	0.010	29.993	6.1735	690.037	0.009
123.984	12.8134	624.455	0.009	29.994	6.1741	690.037	0.009
123.981	12.8120	624.456	0.009	29.996	3.8451	687.674	0.008
123.985	12.8138	624.457	0.009	29.994	3.8435	687.674	0.008
123.985	12.8135	624.453	0.009	29.992	3.8422	687.673	0.008
123.984	9.9473	619.516	0.009	29.992	3.8420	687.673	0.008

Table A1 (continued)

$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )	$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )
Filling 2b (continued)				Filling 3 (continued)			
29.993	1.1283	684.809	0.008	-5.003	18.1353	726.126	0.011
29.992	1.1281	684.809	0.008	-5.002	5.5103	716.691	0.009
29.993	1.1286	684.810	0.008	-5.002	5.5107	716.694	0.009
29.994	1.1300	684.810	0.008	-5.003	5.5092	716.689	0.009
62.017	22.4431	682.276	0.012	-5.004	5.5088	716.693	0.009
62.018	22.4439	682.276	0.012	-5.003	1.2422	713.193	0.008
62.020	22.4447	682.275	0.012	-5.002	1.2441	713.195	0.008
62.020	22.4438	682.273	0.012	-5.002	1.2445	713.195	0.008
Filling 3				-5.003	1.2441	713.195	0.008
-58.996	1.9346	756.216	0.009	29.998	29.4661	710.089	0.015
-58.997	1.9321	756.214	0.009	29.999	29.4674	710.088	0.015
-58.998	1.9275	756.211	0.009	30.000	29.4665	710.088	0.015
-58.998	1.9267	756.211	0.009	30.000	29.4676	710.089	0.015
-48.899	13.2465	755.068	0.010	29.997	22.4838	704.644	0.013
-48.899	13.2488	755.069	0.010	30.000	22.4847	704.645	0.013
-48.897	13.2505	755.068	0.010	29.998	22.4830	704.645	0.013
-35.493	27.8960	753.672	0.015	29.997	22.4814	704.643	0.013
-35.492	27.8972	753.672	0.015	29.998	17.0552	700.113	0.011
-35.493	27.8981	753.674	0.015	29.999	17.0560	700.114	0.011
-35.492	8.1206	741.890	0.009	29.998	17.0550	700.115	0.011
-35.491	8.1206	741.891	0.009	29.997	17.0552	700.114	0.011
-35.493	1.6483	737.596	0.008	29.997	5.5912	689.472	0.009
-35.492	1.6481	737.591	0.008	29.999	5.5930	689.470	0.009
-35.492	1.6500	737.592	0.008	29.999	5.5936	689.471	0.009
-35.492	1.6506	737.591	0.008	29.998	5.5930	689.470	0.009
-5.007	29.7592	733.864	0.016	29.998	0.8371	684.510	0.008
-5.005	29.7613	733.864	0.016	30.000	0.8375	684.510	0.008
-5.005	29.7616	733.864	0.016	29.999	0.8368	684.508	0.008
-5.006	29.7623	733.864	0.016	62.036	22.1299	681.975	0.012
-5.004	18.1349	726.127	0.011	62.033	22.1288	681.974	0.012
-5.002	18.1368	726.125	0.011	62.031	22.1281	681.976	0.012
-5.002	18.1363	726.127	0.011	62.033	22.1290	681.975	0.012

Table A2. Experimentally measured temperatures  $t$ , pressures  $p$ , and densities  $\rho_{\text{exp}}$ , for nitrogen-saturated SRM iso-octane with standard uncertainties of the experimental measurement,  $u(\rho_{\text{exp}}) = [u^2(\rho_{\text{fluid}}) + u^2(x)]^{0.5}$ , where  $u(\rho_{\text{exp}})$  includes uncertainties due to apparatus and material degradation.

$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )	$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )
Filling 4				Filling 4 (continued)			
-58.997	0.0767	754.994	0.008	-5.002	1.4824	713.297	0.008
-58.997	0.0768	754.995	0.008	-5.002	1.4825	713.294	0.008
-58.997	0.0768	754.993	0.008	-5.002	1.4821	713.295	0.008
-58.997	0.0768	754.994	0.008	3.998	8.9156	712.447	0.009
-54.450	0.0734	751.403	0.008	3.999	8.9163	712.449	0.009
-54.448	0.0735	751.403	0.008	3.999	8.9160	712.448	0.009
-54.447	0.0734	751.401	0.008	3.999	8.9157	712.446	0.009
-54.447	0.0735	751.400	0.008	12.002	15.4319	711.730	0.011
-48.897	0.0734	746.994	0.008	12.003	15.4333	711.730	0.011
-48.897	0.0733	746.994	0.008	12.003	15.4341	711.731	0.011
-26.149	3.2609	731.330	0.009	12.003	15.4337	711.729	0.011
-26.149	3.2620	731.328	0.009	20.000	21.8483	711.040	0.012
-26.148	3.2630	731.328	0.009	20.002	21.8501	711.036	0.012
-26.147	3.2636	731.330	0.009	20.002	21.8494	711.040	0.012
-22.148	7.0257	730.918	0.009	20.001	21.8487	711.036	0.012
-22.147	7.0262	730.918	0.009	29.997	29.7243	710.198	0.015
-22.147	7.0264	730.917	0.009	29.998	29.7249	710.198	0.015
-22.147	7.0264	730.918	0.009	29.999	29.7265	710.197	0.015
-17.147	11.6962	730.426	0.010	30.001	29.7282	710.197	0.015
-17.148	11.6966	730.423	0.010	29.999	21.4993	703.744	0.012
-17.148	11.6977	730.429	0.010	30.001	21.4999	703.746	0.012
-17.147	11.6992	730.429	0.010	30.001	21.5000	703.745	0.012
-11.156	17.2289	729.853	0.011	30.000	21.4992	703.745	0.012
-11.155	17.2307	729.852	0.011	29.999	16.6350	699.646	0.011
-11.154	17.2303	729.851	0.011	30.001	16.6352	699.647	0.011
-11.155	17.2303	729.851	0.011	30.001	16.6351	699.646	0.011
-5.003	22.8324	729.275	0.013	30.000	16.6340	699.646	0.011
-5.003	22.8336	729.274	0.013	30.000	10.7984	694.394	0.010
-5.002	22.8360	729.275	0.013	30.001	10.7996	694.395	0.010
-5.003	22.8391	729.280	0.013	30.001	10.7988	694.394	0.010
-5.002	16.6301	724.984	0.011	30.000	10.7987	694.395	0.010
-5.001	16.6293	724.981	0.011	29.998	8.5286	692.241	0.009
-5.001	16.6294	724.981	0.011	29.998	8.5288	692.243	0.009
-5.002	16.6271	724.981	0.011	29.999	8.5289	692.240	0.009
-5.002	11.8625	721.506	0.010	30.000	8.5296	692.239	0.009
-5.002	11.8634	721.508	0.010	30.000	2.5120	686.167	0.008
-5.002	11.8638	721.510	0.010	30.001	2.5140	686.168	0.008
-5.003	11.8623	721.507	0.010	29.999	2.5140	686.170	0.008
-5.000	5.6603	716.714	0.009	29.999	1.6219	685.221	0.008
-5.002	5.6590	716.713	0.009	29.997	1.6176	685.218	0.008
-5.002	5.6582	716.715	0.009	29.999	1.6175	685.217	0.008
-5.001	5.6590	716.716	0.009	30.001	1.6176	685.216	0.008
-5.003	1.4820	713.294	0.008	38.004	7.0645	684.562	0.009

Table A2 (continued)

$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )	$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )
Filling 4 (continued)				Filling 4 (continued)			
38.005	7.0634	684.559	0.009	97.003	15.7114	649.388	0.010
38.004	7.0590	684.555	0.009	106.007	20.3773	648.769	0.011
38.002	7.0556	684.551	0.009	106.004	20.3740	648.767	0.011
46.001	12.4222	683.908	0.010	106.008	20.3760	648.768	0.011
45.999	12.4172	683.904	0.010	106.008	20.3755	648.767	0.011
46.001	12.4154	683.902	0.010	114.995	24.9765	648.159	0.013
46.004	12.4162	683.900	0.010	114.991	24.9789	648.164	0.013
54.004	17.7096	683.268	0.011	114.995	24.9810	648.162	0.013
54.003	17.7079	683.268	0.011	114.994	24.9806	648.164	0.013
54.003	17.7069	683.267	0.011	124.978	30.0198	647.484	0.015
54.004	17.7069	683.267	0.011	124.981	30.0202	647.483	0.015
61.996	22.9366	682.661	0.012	124.982	30.0158	647.476	0.015
61.998	22.9387	682.660	0.012	124.979	30.0125	647.474	0.015
62.000	22.9397	682.661	0.012	124.982	24.5355	640.683	0.013
61.996	22.9379	682.662	0.012	124.981	24.5351	640.679	0.013
70.001	28.0849	682.047	0.014	124.980	19.2825	633.498	0.011
70.000	28.0830	682.045	0.014	124.980	19.2812	633.496	0.011
70.001	28.0825	682.045	0.014	124.978	19.2798	633.496	0.011
70.002	28.0826	682.044	0.014	124.976	19.2785	633.494	0.011
70.004	22.6867	676.838	0.012	124.980	10.4804	619.437	0.009
70.001	22.6854	676.844	0.012	124.978	10.4801	619.437	0.009
70.000	22.6884	676.840	0.012	124.976	10.4800	619.438	0.009
70.003	22.6905	676.843	0.012	124.980	10.4814	619.437	0.009
70.003	18.0811	672.078	0.011	135.001	14.7590	618.821	0.010
70.000	18.0779	672.078	0.011	135.001	14.7582	618.819	0.010
69.999	18.0735	672.073	0.011	134.998	14.7569	618.819	0.010
70.002	18.0745	672.070	0.011	134.997	14.7566	618.821	0.010
70.003	11.6303	664.811	0.009	139.988	16.8712	618.520	0.010
70.003	11.6312	664.810	0.009	139.986	16.8687	618.514	0.010
70.000	11.6297	664.812	0.009	139.987	16.8679	618.513	0.010
70.002	6.1395	657.933	0.009	139.988	16.8672	618.511	0.010
70.003	6.1380	657.929	0.009	144.991	18.9718	618.201	0.011
70.001	6.1363	657.929	0.009	144.990	18.9702	618.200	0.011
69.998	6.1347	657.928	0.009	144.992	18.9707	618.202	0.011
70.001	1.3811	651.305	0.008	144.994	18.9706	618.199	0.011
70.002	1.3798	651.302	0.008	149.997	21.0656	617.894	0.011
69.998	1.3763	651.300	0.008	149.997	21.0639	617.893	0.011
70.001	1.3780	651.299	0.008	149.998	21.0638	617.892	0.011
79.003	6.2097	650.644	0.009	149.999	21.0627	617.890	0.011
79.003	6.2099	650.645	0.009	159.996	25.2179	617.289	0.013
79.006	6.2113	650.647	0.009	159.994	25.2180	617.293	0.013
79.006	6.2112	650.645	0.009	159.995	25.2183	617.292	0.013
88.004	10.9881	650.010	0.009	159.998	23.7821	615.043	0.012
88.007	10.9906	650.011	0.009	159.997	23.7815	615.044	0.012
88.007	10.9911	650.011	0.009	159.997	23.7812	615.043	0.012
88.003	10.9900	650.014	0.009	159.997	23.7800	615.042	0.012
97.002	15.7108	649.387	0.010	159.997	17.9722	605.132	0.010
97.005	15.7121	649.388	0.010	159.996	17.9712	605.132	0.010
97.006	15.7130	649.387	0.010	159.994	17.9702	605.130	0.010

Table A2 (continued)

$t$ (°C)	$p$ (MPa)	$\rho_{\text{exp}}$ (kg·m <sup>-3</sup> )	$u(\rho_{\text{exp}})$ (kg·m <sup>-3</sup> )
Filling 4 (continued)			
159.994	17.9697	605.131	0.010
159.998	12.0608	593.278	0.009
159.996	12.0604	593.278	0.009
159.994	12.0599	593.277	0.009
159.994	12.0599	593.280	0.009
159.995	6.0465	578.362	0.008
159.997	6.0468	578.362	0.008
159.995	6.0460	578.361	0.008
159.994	6.0457	578.362	0.008
159.996	1.4547	563.615	0.008
159.997	1.4542	563.611	0.008
159.995	1.4534	563.610	0.008
159.994	1.4524	563.607	0.008