UNITED STATES DEPARTMENT OF COMMERCE
WASHINGTON 25, D.C.

National Bureau of Standards
Certificate

Standard Sample 217 b

2,2,4-Trimethylpentane

Material

This lot of 2,2,4-trimethylpentane was prepared at this Bureau by purification[1] of commercial material of original high purity. The amount of impurity in the final product was determined from measurements of freezing points to be 0.007±0.003 mole percent.[1]

Density

The density of a sample of this material was measured in a picnometer of special design having a volume of approximately 50 ml. The temperature of the bath was maintained constant to ±0.002 °C. It is believed that the uncertainties in the values of density, which are given in the following table, are less than ±0.00002 g/ml.

Temperature	20 °C	25 °C	30 °C
Density,[a] in g/ml (for air-saturated material)	0.69183	0.68772	0.68362

[a] These measurements were made by the NBS Section on Volumetry and Densimetry.

The values of density are on the basis of weights in vacuum, with the sample at a pressure of 1 atmosphere and saturated with air.

Refractive Index

The indices of refraction of a sample of this material were measured by the minimum deviation method, by the use of a water-jacketed hollow prism mounted on the table of a precision spectrometer. A calibrated thermometer was immersed in the liquid during the measurements. All index measurements were carried out in a temperature controlled laboratory where the room temperature varied not more than ±0.5 °C from the listed temperatures. The values of refractive index are corrected to refer to air at the listed temperatures and at a pressure of 76 cm Hg. It is believed that the uncertainties in the values of refractive index, which are given in the following table, are less than ±0.00002.

Wavelength in Angstrom units	Spectral source	Index of refraction		
		20.0 °C	25.0 °C	30.0 °C
6678.1	Helium	1.38918	1.38672	1.38426
6562.8	Hydrogen, *C*	1.38947	1.38700	1.38454
5892.6 [a]	Sodium, D_1, D_2	1.39147	1.38900	1.38652
5460.7	Mercury, *e*	1.39318	1.39070	1.38822
5015.7	Helium	1.39546	1.39296	1.39046
4861.3	Hydrogen, *F*	1.39641	1.39391	1.39140
4358.3	Mercury, *g*	1.40031	1.39778	1.39525

[a] Intensity-weighted mean of doublet, D_1, D_2.

As measured on a spectrometer in air, values of refractive index decrease by 0.000005 for each 1 cm Hg increase in pressure of the air. See J. Research NBS **14**, 400 (1935) RP776. When determined by the use of refractometers, such as those of the Abbe and Pulfrich types, the refractive index is, in general, largely independent of the condition of the air at the emergence face of the refractometer block. This is especially true when a strictly comparison procedure is followed. Consequently, the refractive indices of "unknown" samples thus observed are referred to conditions essentially the same as those for the standard samples with which the instrument is adjusted. See J. Research NBS **30**, 320 (1943) RP1535.

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[1] The purification and determination of purity were performed by the NBS Section on Pure Substances.

Calorimetric Heat of Combustion

The quantity of heat evolved by combustion of a sample of this material in a closed bomb calorimeter has been found to be 47.713 absolute kilojoules per gram mass (weight in vacuo) with an estimated uncertainty of about 0.02 percent, when the sample is used under the following conditions.[2]

A. The sample before combustion is all in the liquid phase and the combustion reaction is referred to 25 °C.[3]
B. The sample is burned in a bomb of constant volume in pure oxygen at an initial pressure of 30 atmospheres at 25 °C.
C. The number of grams of sample burned is equal to three times the volume of the bomb in liters.
D. The number of grams of water placed in the bomb before combustion is equal to three times the volume of the bomb in liters.

When the sample is burned under conditions differing from those given under A, B, C, and D above, the value given for the heat evolved should be multiplied by the following factor, if this factor is found to differ from unity to a significant extent:

$$1+10^{-6}\left[4(p-30)+45.5\left(\frac{m_s}{v}-3\right)+21\left(\frac{m_w}{v}-3\right)-81(t-25)\right]$$

where p=initial absolute pressure of oxygen, in atmospheres, at the temperature t.
m_s=mass of sample burned in grams.
m_w=mass, in grams, of water placed in bomb before combustion.
v=volume of bomb in liters.
t=temperature to which the reaction is referred, in degrees.

In using the standard sample for calibrating a bomb calorimeter for determining the heats of combustion of gasolines or other volatile liquids, the procedure followed should be the same as that followed in the measurement of heats of combustion, especially with respect to the kind of capsule used to enclose the liquids, the weighing of the samples, and the method of correcting for heat of combustion of the capsules, if these are combustible. If gelatin capsules are used to enclose the liquid, the method should take account of the effect of the variation of water content of the gelatin with varying relative humidity. For procedures involving sealed glass ampoules, reference is made to the following publications: J. Am. Chem. Soc. **37**, 993 (1915); Precise Measurement of Heat of Combustion with a Bomb Calorimeter, NBS Monograph 7, 1960.[4]

The charge should be fired by passing electric current through a short length of iron or chromel wire (about No. 34 AWG) or a fine platinum wire. Correction should be made for the heat of combustion of the wire (6.63 kilojoules per gram of iron or 5.98 kilojoules per gram of chromel) and for the electric energy used in igniting the wire. The energy used to fire the charge (heat of combustion of iron or chromel wire plus electric energy) may be determined by blank calorimetric experiments on the fuse alone. A battery of 4 to 7 storage cells or 6 to 10 dry cells in series or a small transformer with a secondary voltage of about 10 can be used for ignition.

The charge should be burned in pure oxygen, or in commercially pure oxygen containing not more than 1 percent nitrogen and no combustible gases. The effect of combustible constituents (probably mostly hydrogen) in some samples of commercial electrolytic oxygen has been found to be of the order of 1 percent of the total heat produced by combustion in a bomb of about 0.37 liter capacity.

The amount of nitric acid formed in combustion may be determined by titration with a 0.1 normal solution of sodium hydroxide, using methyl orange as indicator. The correction for the formation of nitric acid is 59 kilojoules per mole, or 0.94 kilojoules per gram of HNO_3.

If the heat of combustion of the sample in calories per gram is desired, the following conversion factor may be used:

1 calorie=0.0041840 absolute kilojoules

The calorie thus defined is being used in connection with practically all of the thermochemical work done in the United States. See Am. J. Phys. **12**, 1 (1944).

The International Steam Tables calorie (I.T. cal.) and the corresponding Btu which are used in most modern tables of engineering data are defined by the relations

1 I.T. cal=0.0041868 absolute kilojoules
1 I.T. cal/gram=1.8 Btu/lb.

In the ordinary use of the bomb calorimeter where an accuracy of not better than 0.1 percent is required, the factor given above for correcting for departures from the standard conditions of oxygen pressure, temperature, etc. may be omitted and the heat evolved expressed as 47.78_8 absolute kilojoules (kilowatt-seconds) per gram weight against brass weights in air (11,422 calories per gram weight in air, or 11,414 I.T. calories per gram weight in air, or 20,545 Btu per pound weight in air). In determining the heating values of fuels, it is desirable to follow a standardized procedure such as that specified by the American Society for Testing Materials in their standard D-240-57T for liquid hydrocarbon fuels, or as given in NBS Monograph 7, Precise Measurement of Heat of Combustion with a Bomb Calorimeter.

WASHINGTON 25, D.C., September 28, 1962. A. V. ASTIN, *Director.*

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[2] The measurements of heat of combustion were made by the NBS Section on Heat Measurements.

[3] Methods of reducing bomb caloric data to a common temperature are described in BS J. Research **10**, 525 (1933) RP546. This paper also describes the calculation of heats of reaction at a constant pressure from bomb calorimetric data.

[4] For sale by Superintendent of Documents, U.S. Government Printing Office, Washington 25, D.C., price 25 cents.

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