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Natural gas — Calculation of calorific values, density, relative density and Wobbe indices from composition (ISO 6976:2016)

National foreword

This British Standard is the UK implementation of EN ISO 6976:2016. It supersedes BS EN ISO 6976:2005 which is withdrawn.

The UK participation in its preparation was entrusted to Technical Committee PTI/15, Natural Gas and Gas Analysis.

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Natural gas - Calculation of calorific values, density, relative density and Wobbe indices from composition (ISO 6976:2016)

Gaz naturel - Calcul des pouvoirs calorifiques, de la masse volumique, de la densité relative et des indices de Wobbe à partir de la composition (ISO 6976:2016)

Erdgas - Berechnung von Brenn- und Heizwert, Dichte, relativer Dichte und Wobbeindex aus der Zusammensetzung (ISO 6976:2016)

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European foreword

This document (EN ISO 6976:2016) has been prepared by Technical Committee ISO/TC 193 "Natural gas" in collaboration with Technical Committee CEN/TC 278 "Test gases, test pressures, appliance categories and gas appliance types" the secretariat of which is held by AFNOR.

This European Standard shall be given the status of a national standard, either by publication of an identical text or by endorsement, at the latest by February 2017, and conflicting national standards shall be withdrawn at the latest by February 2017.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. CEN [and/or CENELEC] shall not be held responsible for identifying any or all such patent rights.

This document supersedes EN ISO 6976:2005.

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Endorsement notice

The text of ISO 6976:2016 has been approved by CEN as EN ISO 6976:2016 without any modification.

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation on the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT) see the following URL: www.iso.org/iso/foreword.html.

The committee responsible for this document is ISO/TC 193, *Natural gas*, Subcommittee SC 1, *Analysis of natural gas*.

This third edition cancels and replaces the second edition (ISO 6976:1995), which has been technically revised.

Introduction

Both international and intra-national custody transfer of natural gas usually require precise determination of both the quantity and the quality of the gas to be traded. This document specifies methods for the calculation of key properties that describe gas quality, namely gross and net calorific value, density, relative density, and gross and net Wobbe index. The methods provide the means of calculating these properties and their uncertainties for any natural gas, natural gas substitute or similar combustible gaseous fuel of known composition at commonly used reference conditions.

Values of the various properties calculated in accordance with this document will, in general, differ only by very small amounts from those calculated using the second (1995) edition of this document. In this context, it is recognized that:

a) adoption of the revisions detailed in this document will not be without cost, since instrumental software will need updating;

b) recorded energy content and hence billed energy will, in consequence of these revisions, change by small amounts;

c) unintended impacts could occur if the revisions are implemented uncritically; for instance, if the revisions are implemented at input points to a pipeline system but not at exit points, then a costly accountancy imbalance may result;

d) commercial, contractual, regulatory and legislative obligations will need to be taken into account.

For these reasons, and depending upon the user’s application, it may be appropriate to undertake an impact assessment in order to determine an agreed timing and procedure for implementation of the provisions of this document.

Natural gas — Calculation of calorific values, density, relative density and Wobbe indices from composition

1 Scope

This document specifies methods for the calculation of gross calorific value, net calorific value, density, relative density, gross Wobbe index and net Wobbe index of natural gases, natural gas substitutes and other combustible gaseous fuels, when the composition of the gas by mole fraction is known. The methods specified provide the means of calculating the properties of the gas mixture at commonly used reference conditions.

Mole fractions by definition sum to unity. Guidance on the achievement of this requirement by chromatographic analysis is available in ISO 6974-1 and ISO 6974-2.

The methods of calculation require values for various physical properties of the pure components; these values, together with associated uncertainties, are provided in tables and their sources are identified.

Methods are given for estimating the standard uncertainties of calculated properties.

The methods of calculation of the values of properties on either a molar, mass or volume basis are applicable to any natural gas, natural gas substitute or other combustible fuel that is normally gaseous, except that for properties on the volume basis the method is restricted to mixtures for which the compression factor at reference conditions is greater than 0,9.

Example calculations are given in Annex D for the recommended methods of calculation.

NOTE 1 The qualifiers “superior”, “higher”, “upper” and “total” are, for the purposes of this document, synonymous with “gross”; likewise, “inferior” and “lower” are synonymous with “net”. The term “heating value” is synonymous with “calorific value”; “mass density” and “specific density” are synonymous with “density”; “specific gravity” is synonymous with “relative density”; “Wobbe number” is synonymous with “Wobbe index”; “compressibility factor” is synonymous with “compression factor”. The dimensionless quantity molecular weight is numerically equal to the molar mass in $\text{kg}\cdot\text{kmol}^{-1}$.

NOTE 2 There are no explicit limits of composition to which the methods described in this document are applicable. However, the restriction of volume-basis calculations to mixtures with a compression factor greater than 0,9 at reference conditions sets implicit limits on composition.

NOTE 3 Because the mole fraction of any water present is not normally available from chromatographic analysis, it is common practice to calculate the physical properties on a dry gas basis and to allow for the effects of water vapour in a separate procedure. However, if the mole fraction of water vapour is known then the property calculations can be carried out completely in accordance with the procedures described herein. The effects of water vapour on calorific value, whether the latter is directly measured or calculated, are discussed in ISO/TR 29922.

NOTE 4 For aliphatic hydrocarbons of carbon number 7 or above, any isomer present is included with the normal isomer of the same carbon number.

NOTE 5 If the user’s requirement includes the replacement of, for example, a C6+ or C7+ grouping of analytically unresolved components by a single pseudo-component, then it is the user’s own task to set the mole fraction composition, and hence properties, of this pseudo-component so as to be fit for purpose in the particular application. Any so-called “spectator water” and “non-combustible hydrogen sulfide” are treated as pseudo-components by setting the appropriate enthalpy of combustion values to zero.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 6974-1, *Natural gas — Determination of composition and associated uncertainty by gas chromatography — Part 1: General guidelines and calculation of composition*

ISO 6974-2, *Natural gas — Determination of composition and associated uncertainty by gas chromatography — Part 2: Uncertainty calculations*

ISO 14912:2003, *Gas analysis — Conversion of gas mixture composition data*

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

- IEC Electropedia: available at http://www.electropedia.org/
- ISO Online browsing platform: available at http://www.iso.org/obp

3.1
gross calorific value
amount of heat that would be released by the complete combustion with oxygen of a specified quantity of gas, in such a way that the pressure, p_1, at which the reaction takes place remains constant, and all the products of combustion are returned to the same specified temperature, t_1, as that of the reactants, all of these products being in the gaseous state except for water, which is condensed to the liquid state at t_1

Note 1 to entry: Where the quantity of gas is specified on a molar basis, the gross calorific value is designated as $(Hc)_G(t_1,p_1)$; on a mass basis, the gross calorific value is designated as $(Hm)_G(t_1,p_1)$. Where the quantity of gas is specified on a volume basis, the gross calorific value is designated as $(Hv)_G(t_1,p_1;t_2,p_2)$, where t_2 and p_2 are the gas volume (metering) reference conditions (see Figure 1).

3.2
net calorific value
amount of heat that would be released by the complete combustion with oxygen of a specified quantity of gas, in such a way that the pressure, p_1, at which the reaction takes place remains constant, and all the products of combustion are returned to the same specified temperature, t_1, as that of the reactants, all of these products being in the gaseous state

Note 1 to entry: On molar, mass and volume bases, the net calorific value is designated respectively as $(Hc)_N(t_1,p_1)$, $(Hm)_N(t_1,p_1)$ and $(Hv)_N(t_1,p_1;t_2,p_2)$.

3.3
density
mass of a gas sample divided by its volume at specified conditions of pressure and temperature

3.4
relative density
density of a gas divided by the density of dry air of reference composition at the same specified conditions of pressure and temperature

Note 1 to entry: The term ideal relative density applies when both gas and air are considered as gases that obey the *ideal gas* law (3.8). The term real relative density applies when both gas and air are considered as real fluids (3.9). For the fixed reference composition of dry air, see ISO/TR 29922.

3.5

gross Wobbe index

volume-basis gross calorific value, at specified reference conditions, divided by the square root of the relative density at the same specified metering reference conditions

Note 1 to entry: In common usage, and in the absence of any other qualifier, the term Wobbe index is taken to mean the quantity that is here identified as gross Wobbe index.

3.6

net Wobbe index

volume-basis net calorific value, at specified reference conditions, divided by the square root of the relative density at the same specified metering reference conditions

3.7

enthalpy of transformation

amount of heat release that accompanies the change in condition (transformation) of a substance or system from one (initial) condition to another (final) condition

Note 1 to entry: A *positive* heat release is represented by thermodynamic convention as a numerically equal *negative* increment of enthalpy.

Note 2 to entry: In the context of this document, the following can be identified:

- **enthalpy of combustion:** the initial condition is that of an unburned stoichiometric mixture of reactants and the final condition is that of the products of combustion at the same pressure and temperature;
- **standard enthalpy of vaporization:** the initial condition is that of a substance in the liquid state at saturation and the final condition is that of the same substance in the hypothetical state of the ideal gas at the same temperature;
- **enthalpy (or enthalpic) difference:** the initial condition is that of a gas or gas mixture at temperature T_1 and the final condition is that of the same gas or gas mixture at the same pressure but at a different temperature T_2;
- **enthalpy (or enthalpic) correction (residual enthalpy):** the initial condition is that of a gas or gas mixture in the hypothetical state of an ideal gas and the final condition is that of the same gas or gas mixture at the same pressure and temperature in the state of the real gas.

3.8

ideal gas

gas that obeys the ideal gas law

Note 1 to entry: The ideal gas law can be expressed as

$$p \cdot V^o = R \cdot T$$

where

p is the absolute pressure;

T is the thermodynamic temperature;

V^o is the volume occupied by one mole of ideal gas (ideal molar volume);

R is the gas constant in coherent units.

3.9

real gas

gas that deviates from volumetric ideality

Note 1 to entry: No real gas obeys the ideal gas law. Deviations from volumetric ideality can be written in terms of the equation of state

$$p \cdot V = Z(p,T) \cdot R \cdot T$$

where

V is the volume occupied by one mole of the real gas (real molar volume);

$Z(p,T)$ is a variable, often close to unity, and is known as the *compression factor* (3.10).

3.10
compression factor

actual (real) volume of a given amount of gas at a specified pressure and temperature divided by its volume under the same conditions as calculated from the ideal gas law

3.11
combustion reference conditions

specified temperature, t_1, and pressure, p_1, at which the fuel is notionally burned

3.12
metering reference conditions

specified temperature, t_2, and pressure, p_2, at which the volume of fuel to be burned is notionally determined

Note 1 to entry: There is no *a priori* reason for the metering reference conditions to be the same as the combustion reference conditions (see Figure 1).

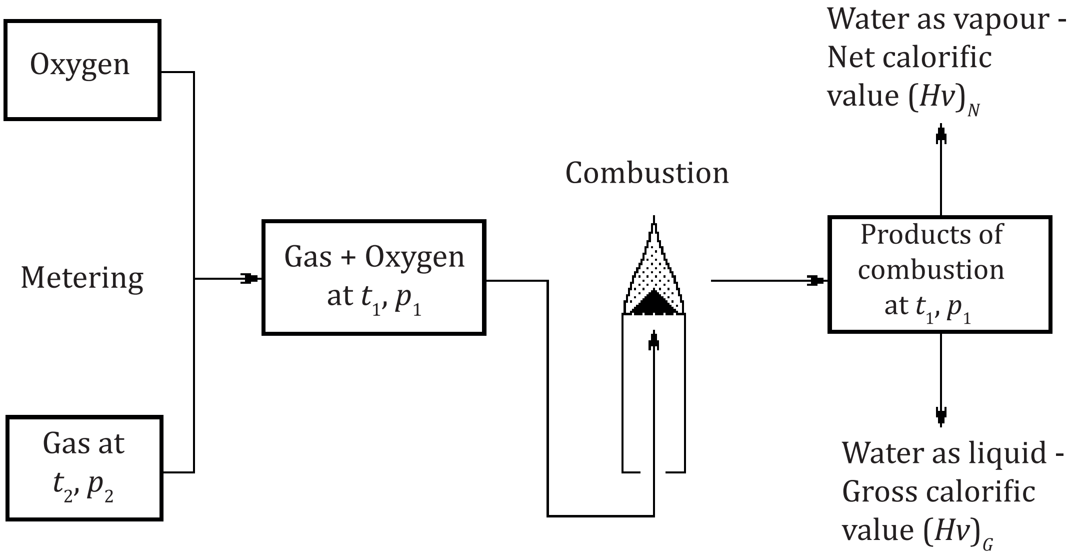
Note 2 to entry: A range of reference conditions is in use throughout the world.

Note 3 to entry: Throughout this document, the use of 15,55 °C is intended as shorthand for the exact Celsius equivalent of 60 °F, i.e. $15^{5/9}$ or 15,55 (recurring) °C.

Note 4 to entry: The exact equivalent of 101,325 kPa in psi can be calculated from

$(101\ 325) \cdot (0{,}304\ 8/12)^2 \ / \ (0{,}453\ 592\ 37) \cdot (9{,}806\ 65) = 14,\ 695\ 949\ \ldots.$

This value is, in practice, normally rounded to 14,696 psi and the rounded value deemed equal to 101,325 kPa.



$$\frac{\text{Heat released}}{\text{Metered volume of gas}} = \text{Calorific value } Hv$$

Figure 1 — Calorific value on a volume basis — Metering and combustion reference conditions

4 Symbols and units

4.1 Quantities

Symbol	Meaning	Unit
A	atomic mass	kg·kmol^{-1}
a	atomic index for carbon in the generalized molecular species $C_aH_bN_cO_dS_e$	—
b	atomic index for hydrogen in the generalized molecular species $C_aH_bN_cO_dS_e$	—
c	atomic index for nitrogen in the generalized molecular species $C_aH_bN_cO_dS_e$	—
D	density	kg·m^{-3}
d	atomic index for oxygen in the generalized molecular species $C_aH_bN_cO_dS_e$	—
e	atomic index for sulfur in the generalized molecular species $C_aH_bN_cO_dS_e$	—
F	function that generates property Y	—
G	relative density	—
Hc	molar-basis calorific value	kJ·mol^{-1}
Hm	mass-basis calorific value	MJ·kg^{-1}
Hv	volume-basis calorific value	MJ·m^{-3}
k	coverage factor	—
L	molar enthalpy of vaporization of water	kJ·mol^{-1}
M	molar mass	kg·kmol^{-1}
N	number of components in a mixture	—
n	number of determinations in a set of values	—
p	pressure (absolute)	kPa
q	exact input quantity for calculation of Y	(varies)
R	molar gas constant	J·mol^{-1}·K^{-1}
r	correlation coefficient	—
s	summation factor	—
T	thermodynamic (absolute) temperature	K
t	Celsius temperature	°C
$U(Y)$	expanded uncertainty of Y	(varies)

$u(Y)$	standard uncertainty of Y	(varies)
V	molar volume	$m^3 \cdot mol^{-1}$
W	Wobbe index	$MJ \cdot m^{-3}$
x	mole fraction	—
Y	general (unspecified) physical property	(varies)
y	inexact input quantity for calculation of Y	(varies)
Z	compression factor	—

4.2 Subscripts

Symbol	**Meaning**
G	gross (calorific value or Wobbe index)
i	serial counter component identifier
j	serial counter component identifier
k	serial counter
m	serial counter
N	net (calorific value or Wobbe index)
n	serial counter
air	for air
0	reference (base) value (of pressure)
1	combustion reference state
2	metering reference state

4.3 Superscript

Symbol	**Meaning**
o	for the ideal gas state

5 Principles

Methods are provided for the calculation of the calorific values (gross and net), density, relative density and Wobbe indices (gross and net) of any natural gas, natural gas substitute or other combustible gaseous fuel from a known molar composition.

For calorific values, these methods use formulae in which, for all individual molecular species of the gas mixture, the tabulated ideal-gas molar-basis gross calorific value is weighted in accordance with its mole fraction, all terms then being added together to obtain the mole fraction average of this quantity for the ideal gas mixture on a molar basis. Further formulae are given that convert this quantity into the ideal-gas net calorific value, and then into the ideal-gas gross and net calorific values on either a mass basis or a volume basis.

Likewise, for density and relative density, the methods use formulae in which, for all individual molecular species of the gas mixture, the tabulated value of molar mass is weighted in accordance with its mole fraction, all terms then being added together to obtain the mole fraction average of this quantity. Formulae are given that convert this mole fraction average molar mass into the ideal-gas density or relative density.

Values of the density and relative density for the real gas are then obtained by the application of a volumetric correction factor (compression factor), a prescription for the calculation of which is given.

For calorific values, conversion from the ideal-gas state to the real-gas state is in principle slightly less simple. The application should first be made of a small enthalpic correction (residual enthalpy) to the calorific value (gross or net) of the ideal gas on the molar basis, so as to obtain the calorific value of the real gas on the molar basis. For the purposes of this document, however, this enthalpic correction has been estimated as so small as to be justifiably negligible (see ISO/TR 29922).

In consequence of neglecting the enthalpic correction, the real-gas calorific values on the molar and mass bases are in effect set as equal to the corresponding ideal-gas values. To obtain the values of the real-gas calorific values (gross or net) on the volume basis from the corresponding ideal-gas values, however, the volumetric correction factor (compression factor) mentioned above is applied.

Finally, formulae are given for the calculation of Wobbe indices, for either the ideal gas or real gas, from the other properties considered herein.

For each of the natural gas properties for which formulae are provided as described above, the methods prescribed in GUM[5] have been applied so as to provide further formulae that enable an estimate of associated uncertainty.

The derivation of each such uncertainty formula is presented fully in ISO/TR 29922. In essence, each results from the analytical derivation of sensitivity coefficients, by means of partial differentiation of the relevant mixture-property formula with respect to each of the input quantities (namely the pure-component physical properties and component mole fractions) with which an uncertainty may be associated. The derivations also take into account the unavoidable correlations between the component mole fractions and the likewise unavoidable, but less obvious, correlations between the component molar masses (see also Clause 11).

For each property, the total variance (squared uncertainty) is obtained by addition of the independent contributions to the variance from each source of uncertainty and the overall uncertainty result is taken as the square root of this quantity. The formulae to be used are given in Annex B.

In Clause 12, tabulated values are given for the relevant physical properties and their associated uncertainties of the pure components of natural gas for each of the commonly used reference conditions. Auxiliary data, including uncertainties, are given in Annex A. Example calculations are given in Annex D.

6 Behaviour of ideal and real gases

6.1 Enthalpy of combustion

The most fundamental physical quantities required in the calculation of calorific values from first principles are the ideal-gas (standard) molar enthalpies of combustion (ideal molar-basis calorific values) for the pure component gases. These quantities are complex functions of temperature; thus, the values required depend upon the combustion reference temperature t_1. For practical reasons, it is not intended that the user should carry out calculations that give the appropriate values at any arbitrary combustion reference temperature. Instead, tabulations are given for the temperatures t_1 = 25 °C, 20 °C, 15,55 °C (60 °F, see 3.12, Note 3 to entry), 15 °C (59 °F) and 0 °C. The derivations of the values listed in Table 3 are discussed in ISO/TR 29922; the important point is that all five values for any substance are mutually consistent from a thermodynamic perspective.

6.2 Calculation of compression factor

For any volume-basis calorific value, a real-gas correction is required to account for the deviation of the real gas from volumetric ideality. This correction is not negligible and is also required in the calculation of density, relative density and Wobbe index. ISO/TR 29922 discusses the background to the way in which corrections for volumetric non-ideality shall be applied, the principles involved and justifies the simplifications employed that enable tractable calculations, as detailed in Formula (1), to be made.

This correction for volumetric non-ideality is made through the use of the compression factor Z of the mixture. The formulation to be used for Z at the metering reference conditions, as required for the calculations described in Clauses 9 and 10, is (see ISO/TR 29922)

$$Z(t_2, p_2) = 1 - \left(\frac{p_2}{p_0}\right) \times \left[\sum_{j=1}^{N} x_j \cdot s_j(t_2, p_0)\right]^2 \tag{1}$$

where p_0 = 101,325 kPa (14,696 psi) and the metering reference pressure p_2 is expressed in the same units. The summation is taken over all N components of the mixture and the formula is valid for the range $90 < p_2/\text{kPa} < 110$ ($13{,}05 < p_2/\text{psi} < 15{,}95$). Values of the so-called summation factor $s_j(t_2,p_0)$ are given in Table 2 at the four metering reference temperatures of common interest for all of the components of natural gas and substitute natural gas considered in this document. The derivations of these values are detailed in ISO/TR 29922.

NOTE Formula (1) can also be used to calculate values of compression factor of pure components, but this will not necessarily give the most accurate result possible. In particular, the formula will not provide acceptable values for the compression factors of hydrogen, helium or neon, for which $Z > 1$, nor for any components, such as the higher hydrocarbons, that are not gaseous at the metering reference conditions. The user should consider the fitness-for-purpose of any such calculation before its use outside of the context of this document. Definitive values of compression factor for several pure components, namely the so-called permanent gases, are given in ISO/TR 29922.

7 Calculation of calorific value on a molar basis

7.1 Gross calorific value

The gross calorific value on a molar basis, at a temperature t_1, of a mixture of known composition shall be calculated from

$$(Hc)_G(t_1) = (Hc)_G^o(t_1) = \sum_{j=1}^{N} x_j \cdot [(Hc)_G^o]_j(t_1) \tag{2}$$

where

$(Hc)_G^o(t_1)$ is the ideal-gas gross molar-basis calorific value of the mixture;

$(Hc)_G(t_1)$ is the real-gas gross molar-basis calorific value of the mixture;

$[(Hc)_G^o]_j(t_1)$ is the ideal gross molar-basis calorific value of component j;

x_j is the mole fraction of component j.

NOTE 1 Values of $[(Hc)_G^o]_j$ are independent of pressure; consequently, the combustion reference pressure p_1 is irrelevant and is omitted from the nomenclature adopted.

NOTE 2 The ideal-gas molar-basis calorific value of a gas or gas mixture is defined in this document as a positive quantity. The values given in Table 3 are numerically equal to the standard molar enthalpies of combustion, which are, however, conventionally expressed as negative quantities (see 3.7).

Numerical values of $[(Hc)_G^o]_j(t_1)$ for t_1 = 25 °C are given in Table 3. These values for $[(Hc)_G^o]_j$ (25) are taken from the original literature sources cited in ISO/TR 29922. Values for $[(Hc)_G^o]_j(t_1)$ for other temperatures (t_1 = 20 °C, 15,55 °C, 15 °C and 0 °C) are also given in Table 3. These values have been derived from the 25 °C values in accordance with the methods described in ISO/TR 29922.

7.2 Net calorific value

The net calorific value on a molar basis, at a temperature t_1, of a mixture of known composition shall be calculated from

$$(Hc)_N(t_1) = (Hc)_N^o(t_1) = (Hc)_G^o(t_1) - \sum_{j=1}^{N} x_j \cdot \frac{b_j}{2} \cdot L^o(t_1) \qquad (3)$$

where

$(Hc)_N^o(t_1)$ is the ideal-gas net molar-basis calorific value of the mixture;

$(Hc)_N(t_1)$ is the real-gas net molar-basis calorific value of the mixture;

$L^o(t_1)$ is the standard enthalpy of vaporization of water at t_1;

b_j is the number of hydrogen atoms present in each molecule of component j (hydrogen atomic index).

Values of $L^o(t_1)$ are given in Annex A for 25 °C, 20 °C, 15,55 °C (60 °F), 15 °C and 0 °C. Values of b_j are given in Table 1.

8 Calculation of calorific value on a mass basis

8.1 Gross calorific value

The gross calorific value on a mass basis, at a temperature t_1, of a mixture of known composition shall be calculated from

$$(Hm)_G(t_1) = (Hm)_G^o(t_1) = \frac{(Hc)_G^o(t_1)}{M} \qquad (4)$$

where

$(Hm)_G^o(t_1)$ is the ideal-gas gross mass-basis calorific value of the mixture;

$(Hm)_G(t_1)$ is the real-gas gross mass-basis calorific value of the mixture;

M is the molar mass of the mixture, which shall be calculated from

$$M = \sum_{j=1}^{N} x_j \cdot M_j \qquad (5)$$

where

M_j is the molar mass of component *j*.

The value of molar mass for each component considered in this document is given in Table 1.

8.2 Net calorific value

The net calorific value on a mass basis, at a temperature t_1, of a mixture of known composition shall be calculated from

$$(Hm)_N(t_1) = (Hm)_N^o(t_1) = \frac{(Hc)_N^o(t_1)}{M} \tag{6}$$

where

$(Hm)_N^o(t_1)$ is the ideal-gas net mass-basis calorific value of the mixture;

$(Hm)_N(t_1)$ is the real-gas net mass-basis calorific value of the mixture.

9 Calculation of calorific value on a volume basis

9.1 Ideal-gas gross calorific value

The gross calorific value on an ideal-gas volume basis, for a combustion temperature t_1, of a mixture of known composition, metered at a temperature t_2 and pressure p_2, shall be calculated from

$$(Hv)_G^o(t_1;t_2,p_2) = \frac{(Hc)_G^o(t_1)}{V^o} \tag{7}$$

where

$(Hv)_G^o(t_1;t_2,p_2)$ is the ideal-gas gross volume-basis calorific value of the mixture;

V^o is the ideal molar volume of the mixture, which shall be calculated from

$$V^o = R \cdot T_2/p_2 \tag{8}$$

where

R is the gas constant (see A.1);

T_2 is the absolute temperature.

9.2 Ideal-gas net calorific value

The net calorific value on an ideal-gas volume basis, for a combustion temperature t_1, of a mixture of known composition, metered at a temperature t_2 and pressure p_2, shall be calculated from

$$(Hv)_N^o(t_1;t_2,p_2) = \frac{(Hc)_N^o(t_1)}{V^o} \tag{9}$$

where

$(Hv)_N^o(t_1;t_2,p_2)$ is the ideal-gas net volume-basis calorific value of the mixture.

9.3 Real-gas gross calorific value

The gross calorific value on a real-gas volume basis, for a combustion temperature t_1, of a mixture of known composition, metered at a temperature t_2 and pressure p_2, shall be calculated from

$$(Hv)_G(t_1;t_2,p_2) = \frac{(Hc)_G^o(t_1)}{V} \tag{10}$$

where

$(Hv)_G(t_1;t_2,p_2)$ is the real-gas gross volume-basis calorific value;

V is the real-gas molar volume of the mixture, which shall be calculated from

$$V = Z(t_2,p_2) \cdot R \cdot T_2/p_2 \tag{11}$$

where

$Z(t_2,p_2)$ is the compression factor at the metering reference conditions.

The compression factor $Z(t_2,p_2)$ shall be calculated from Formula (1), using values of $s_j(t_2,p_0)$ given for individual pure substances in Table 2. For the purposes of this document, this calculation is only valid for $Z > 0{,}9$.

9.4 Real-gas net calorific value

The net calorific value on a real-gas volume basis, for a combustion temperature t_1, of a mixture of known composition, metered at a temperature t_2 and pressure p_2, shall be calculated from

$$(Hv)_N(t_1;t_2,p_2) = \frac{(Hc)_N^o(t_1)}{V} \tag{12}$$

where

$(Hv)_N(t_1;t_2,p_2)$ is the real-gas net volume-basis calorific value.

10 Calculation of associated properties

10.1 Ideal-gas relative density

The relative density of an ideal gas is independent of any reference state and shall be calculated from

$$G^o = \frac{M}{M_{\text{air}}} \tag{13}$$

where

G^o is the relative density of the ideal gas;

M is the molar mass of the mixture calculated according to Formula (5);

M_{air} is the molar mass of dry air of reference composition.

The composition of reference air is discussed in ISO/TR 29922, where the value for M_{air} = (28,965 46 ± 0,000 17) kg·kmol^{-1} is derived (see also A.3).

10.2 Ideal-gas density

The density of an ideal gas depends upon its temperature, t, and pressure, p, and shall be calculated from

$$D^o(t_2,p_2) = M / V^o \tag{14}$$

where

$D^o(t_2,p_2)$ is the density of the ideal gas at the metering reference conditions;

M is the molar mass of the mixture calculated according to Formula (5);

V^o is the ideal molar volume of the mixture calculated according to Formula (8).

10.3 Ideal-gas gross Wobbe index

The gross Wobbe index of the ideal gas shall be calculated from

$$W_G^o(t_1;t_2,p_2) = \frac{(Hv)_G^o(t_1;t_2,p_2)}{\sqrt{G^o}} \tag{15}$$

where

$W_G^o(t_1;t_2,p_2)$ is the gross Wobbe index of the ideal gas;

$(Hv)_G^o(t_1;t_2,p_2)$ is calculated as described in 9.1.

10.4 Ideal-gas net Wobbe index

The net Wobbe index of the ideal gas shall be calculated from

$$W_N^o(t_1;t_2,p_2) = \frac{(Hv)_N^o(t_1;t_2,p_2)}{\sqrt{G^o}} \tag{16}$$

where

$W_N^o(t_1;t_2,p_2)$ is the net Wobbe index of the ideal gas;

$(Hv)_N^o(t_1;t_2,p_2)$ is calculated as described in 9.2.

10.5 Real-gas relative density

The relative density of the real gas at the metering reference conditions (t_2,p_2) shall be calculated from

$$G(t_2,p_2)=\frac{G^o\cdot Z_{\mathrm{air}}(t_2,p_2)}{Z(t_2,p_2)} \tag{17}$$

where

$G(t_2,p_2)$ is the relative density of the real gas;

$Z(t_2,p_2)$ is the compression factor of the gas;

$Z_{\mathrm{air}}(t_2,p_2)$ is the compression factor of dry air of reference composition.

The compression factor $Z(t_2,p_2)$ shall be calculated from Formula (1), using values for the summation factor $s_j(t_2,p_0)$ given for individual pure substances in Table 2. The compression factor $Z_{\mathrm{air}}(t_2,p_2)$ shall be calculated from

$$Z_{\mathrm{air}}(t_2,p_2)=1-\frac{p_2}{p_0}\cdot[1-Z_{air}(t_2,p_0)] \tag{18}$$

where p_0 = 101,325 kPa (14,696 psi), the metering reference pressure p_2 is expressed in the same units, and (see A.3)

$Z_{\mathrm{air}}(t_2 = 0\ °\mathrm{C}, p_0) = 0{,}999\ 419$;

$Z_{\mathrm{air}}(t_2 = 15\ °\mathrm{C}, p_0) = 0{,}999\ 595$;

$Z_{\mathrm{air}}(t_2 = 15{,}55\ °\mathrm{C}, p_0) = 0{,}999\ 601$;

$Z_{\mathrm{air}}(t_2 = 20\ °\mathrm{C}, p_0) = 0{,}999\ 645$.

Formula (18) is valid for the range $90 < p_2/\mathrm{kPa} < 110$ ($13{,}05 < p_2/\mathrm{psi} < 15{,}95$).

10.6 Real-gas density

The density of the real gas at metering reference conditions shall be calculated from

$$D(t_2,p_2)=\frac{D^o(t_2,p_2)}{Z(t_2,p_2)} \tag{19}$$

where

$D(t_2,p_2)$ is the density of the real gas.

10.7 Real-gas gross Wobbe index

The gross Wobbe index of the real gas shall be calculated from

$$W_G(t_1;t_2,p_2)=\frac{(Hv)_G(t_1;t_2,p_2)}{\sqrt{G(t_2,p_2)}} \tag{20}$$

where

$W_G(t_1;t_2,p_2)$ is the gross Wobbe index of the real gas;

$(Hv)_G(t_1;t_2,p_2)$ is calculated as described in 9.3.

10.8 Real-gas net Wobbe index

The net Wobbe index of the real gas shall be calculated from

$$W_N(t_1;t_2,p_2)=\frac{(Hv)_N(t_1;t_2,p_2)}{\sqrt{G(t_2,p_2)}} \tag{21}$$

where

$W_N(t_1;t_2,p_2)$ is the net Wobbe index of the real gas;

$(Hv)_N(t_1;t_2,p_2)$ is calculated as described in 9.4.

NOTE Some care in the use of units is required for the calculations described in this clause, particularly for calculations of density, D. With R expressed in units of joules per mole kelvin, p in kilopascals and M in kilograms per kilomole, the value of D is obtained automatically in kilograms per cubic metre.

11 Uncertainty of calculation

11.1 Principles

In accordance with the general principles of metrology, as summarized in GUM,[5] every calculation result shall normally be reported with an attached estimate of uncertainty.

Three distinct techniques are known to be possible for the estimation of the uncertainties in properties that may be calculated by use of this document, namely

a) a technique that uses sensitivity coefficients derived analytically as partial derivatives of the quantity in question with respect to each of the input quantities (this is here termed the analytical method),

b) a technique that likewise uses sensitivity coefficients, but where these are derived using finite difference methods, and

c) a numerical technique based on Monte Carlo methods.

Methods b) and c) may be applicable and acceptable for use with this document but are not considered further in this clause. In general, any method that is compliant with the principles set out in GUM[5] is acceptable, and some of the possible options, including techniques b) and c), are discussed further in ISO/TR 29922.

Methods a) to c) are intended as means to provide an estimate of uncertainty specific to a single independent result. GUM[5] does, however, acknowledge that in many routine operations, it may be impractical or inappropriate to require an independent uncertainty for every result. A good example in the present context might be continual online process gas-chromatographic analysis.

In such cases, GUM suggests that sufficient information for a reasonable general estimate of uncertainty may often be estimated or inferred from relevant calibration, compliance, legal inspection and/or accreditation records etc. (this is here termed the generic method).

11.2 Formulae for the analytical method

The value of any physical property, Y, may be expressed as a function, F, of the relevant input variables y_i and q_k as follows

$$Y = F(y_1, y_2, y_3, ...y_n, q_1, q_2, q_3, ...q_m) \tag{22}$$

where

y_i is an input variable quantity with an associated uncertainty $u(y_i)$;

q_k is an input parameter that is specified without uncertainty (i.e. is deemed to be exact).

The combined standard uncertainty, $u(Y)$, in property, Y, may be calculated according to the general expression given in GUM[5] for correlated input quantities y_i and y_j as follows

$$u^2(Y) = \sum_{i=1}^{n} \sum_{j=1}^{n} \left(\frac{\partial Y}{\partial y_i} \right) \cdot u(y_i) \cdot r(y_i, y_j) \cdot u(y_j) \cdot \left(\frac{\partial Y}{\partial y_j} \right) \tag{23}$$

where

$\left(\frac{\partial Y}{\partial y_i} \right)$ is the partial derivative (sensitivity coefficient) of Y with respect to y_i;

$r(y_i,y_j)$ is the correlation coefficient between y_i and y_j.

Annex B gives the formulae for the calculation of uncertainty that result from the application of Formula (23) to each of the properties that are the subject of this document. The input quantities required are the mixture composition and the pure component (or mixture) physical properties, together with all of their associated uncertainties and the relevant correlation coefficient values.

11.3 Inputs for the analytical method

11.3.1 Composition and compositional uncertainties

For the purpose of estimating the contribution from uncertainties in the molar composition analysis to the overall uncertainty in property calculation, the following assumptions shall normally be made.

a) That a complete molar composition (as required by Clause 1) is available, and that for each component the value of mole fraction has associated with it an estimate of uncertainty, and either

b) that a complete description of the correlations between the known mole fractions is available as a covariance matrix, i.e. as a mole fraction correlation coefficient (normalization) matrix, or

c) that there are no correlations between component mole fractions, i.e. that the component mole fractions are all mutually independent.

The most complete and rigorous estimate of uncertainty results from the application of assumptions a) and b) to the formulae given in Annex B but, in very many instances, the complete mole fraction correlation coefficient matrix $r(x_i,x_j)$ is unavailable. In this case, it is generally acceptable instead to apply assumptions a) and c), but this is not without implications for the status of the final result.

If sufficient raw analytical information is available, then the complete mole fraction correlation coefficient matrix $r(x_i,x_j)$ is calculable by use of ISO 14912:2003, 8.5.2.3, Formula (69), and the use of assumptions a) and b) for the estimation of uncertainty is optimal.

However, in the absence of sufficient information to enable derivation of the complete mole fraction correlation coefficient matrix, then the use of assumptions a) and c) for the estimation of uncertainty is instead acceptable. In this case, the correlation coefficients $r(x_i,x_j)$ shall be taken as the elements of an identity matrix, i.e. a matrix in which all on-diagonal elements have the value of unity and all off-diagonal elements are zero.

NOTE Because of the way in which the composition of a mixture is normally determined, assumption c) cannot ever be strictly valid. The compositions x_i,x_j are always significantly correlated because (in addition to any pre-normalization correlations) the data processing (normalization) required to determine mole fractions from the raw data will introduce correlation. Consequently, the assumption that the $r(x_i,x_j)$ are elements of an identity matrix will in general not hold. However, for a typical natural gas analysis (including uncertainties), the uncertainty in each calculated property obtained by using the assumption of an identity matrix is considered "safe" (i.e. will usually over-estimate the uncertainty in each property, although this is not fully guaranteed).

If the composition of the gas is known by volume fractions, these should first be converted to mole fractions in accordance with ISO 14912:2003, 5.1.2. Note, however, that these derived mole fractions will have uncertainties greater than those of the original volume fractions.

Strategies employed for normalization may vary significantly. Users of this document should be aware that different approaches may lead to different degrees to which the assumption of an identity matrix for the $r(x_i,x_j)$ is invalid. For a discussion of normalization procedures, see ISO 6974-1 and ISO 6974-2.

See Annex D, Example 3 for a guide to the differences that may result from the use of complete knowledge of the elements $r(x_i,x_j)$ of the mole fraction correlation coefficient (normalization) matrix instead of the assumption of an identity matrix.

11.3.2 Non-compositional inputs

Estimates of standard uncertainties for the non-compositional (property) inputs (except for molar masses) are provided in the tables of component-specific data given in Clause 12 and for auxiliary data in Annex A. In the absence of more specific information, all of these data (again except for the molar masses) shall be taken as uncorrelated, i.e. the correlation coefficients $r(y_i,y_j)$ shall be taken as the elements of an identity matrix. The formulae given in Annex B have been derived on the basis of this assumption.

For molar masses, the values listed are inevitably highly correlated because they are evaluated by the summation of common values of the relevant atomic masses. Each element $r(M_i,M_j)$ of the correlation matrix is given by

$$r(M_i,M_j)=\frac{\{[a_i\cdot a_j\cdot u^2(A_\mathrm{C})]+[b_i\cdot b_j\cdot u^2(A_\mathrm{H})]+[c_i\cdot c_j\cdot u^2(A_\mathrm{N})]+[d_i\cdot d_j\cdot u^2(A_\mathrm{O})]+[e_i\cdot e_j\cdot u^2(A_\mathrm{S})]\}}{u(M_i)\cdot u(M_j)} \tag{24}$$

where

a_j, b_j, c_j, d_j and e_j	are the atomic indices of C, H, N, O and S in the j-th molecular species $\mathrm{C}_a\mathrm{H}_b\mathrm{N}_c\mathrm{O}_d\mathrm{S}_e$, values for which are given in Table 1;
$u(A_\mathrm{C})$, $u(A_\mathrm{H})$, $u(A_\mathrm{N})$, $u(A_\mathrm{O})$ and $u(A_\mathrm{S})$	are the standard uncertainties of the atomic masses of C, H, N, O and S, values for which are given in A.2;

$$u(M_j)=\sqrt{\left[a_j\cdot u(A_\mathrm{C})\right]^2+\left[b_j\cdot u(A_\mathrm{H})\right]^2+\left[c_j\cdot u(A_\mathrm{N})\right]^2+\left[d_j\cdot u(A_\mathrm{O})\right]^2+\left[e_j\cdot u(A_\mathrm{S})\right]^2} \tag{25}$$

11.4 Expanded uncertainty

The expanded uncertainty, $U(Y)$, of the calculated property, Y, shall be calculated by multiplying the combined standard uncertainty, $u(Y)$, by an appropriate coverage factor, k, (the value of which shall be stated), as follows

$$U(Y) = k \cdot u(Y) \tag{26}$$

NOTE A coverage factor of $k = 2$ generally provides a level of confidence of approximately 95 %.

11.5 Expression of results

11.5.1 General

Where sufficient data are available, the inclusion of an estimate of uncertainty is strongly recommended as a fundamental part of the full and proper expression of a result. Results shall be expressed according to one of the following schemes, given here in order of preference.

11.5.2 Analytical method

For an estimate of uncertainty made using the analytical method, i.e. using the formulae given in Annex B, the expanded uncertainty shall be rounded to two significant figures, using the normal rules of rounding (i.e. round half-up, see ISO 80000-1:2009, Annex B). The numerical value of Y shall be rounded to the least (second) significant figure in the rounded value of the expanded uncertainty, $U(Y)$.

Report the value of the calculated quantity in the form $Y \pm U(Y)$ (including units).

This scheme represents the proper definitive fully GUM-compliant procedure.

For best practice, reporting of the result should also include a statement of whether the elements $r(x_i,x_j)$ of the mole fraction correlation coefficient (normalization) matrix used in estimating the uncertainty are known or instead are assumed to be those of an identity matrix.

11.5.3 Generic method

When an estimate of uncertainty is made by means of the generic method, the expanded uncertainty shall be rounded to two significant figures, using the normal rules of rounding. The numerical value of Y shall be rounded and reported (including units) to the least significant figure in the rounded value of the inferred expanded uncertainty, $U(Y)$.

It shall be the responsibility of the user to decide whether the application requires the value of $U(Y)$ to be reported explicitly with every result. In many applications, a general statement encompassing many similar results may suffice.

11.5.4 Contingency method

There remain situations where, for example, because of insufficient analytical uncertainty data or inadequate computing arrangements, it is impossible to carry out any proper GUM-compliant estimates of property uncertainties.

In such cases, and in the absence of any evidence to suggest that the analytical input data are of insufficient accuracy for the purpose, the user of this document shall report results for each calculated property rounded as follows.

Calorific value – molar basis	to 0,01 $kJ \cdot mol^{-1}$
Calorific value – mass basis	to 0,01 $MJ \cdot kg^{-1}$
Calorific value – volume basis	to 0,01 $MJ \cdot m^{-3}$
Relative density	to 0,000 1
Density	to 0,000 1 $kg \cdot m^{-3}$
Wobbe index	to 0,01 $MJ \cdot m^{-3}$

For each property, it is the responsibility of the user to assess whether quoting this number of digits after the decimal point is justified and, if not, the number of digits reported shall be reduced accordingly. The number of digits reported shall not be increased.

11.6 Application of uncertainty

The earlier text of this clause provides the means by which to calculate a value for the expanded uncertainty to be associated with the corresponding calculated value of a physical property. Such a “stand-alone” analytical method result may satisfy fully a user’s requirement.

However, the usefulness and applicability of an uncertainty estimate may often depend upon the context in which the calculation is to be made. In this respect, it is possible to identify a number of distinct cases. These include, but are not limited to, the following:

a) Fitness-for-purpose: If the requirement is to demonstrate that a piece of analytical equipment performs within its specification of (property) uncertainty for a variety of test gases of known (property) uncertainty, then the relevant quantity to test this is the complete uncertainty as calculated in accordance with this clause, i.e. including both the compositional and non-compositional components of uncertainty.

b) Analytical compatibility: If the requirement is to demonstrate the concordance (within uncertainty) between the results from two (or more) sets of identical (or similar) analytical equipment on the same test gases, then it is necessary first to exclude those components of uncertainty that are common to each set of equipment, i.e. the non-compositional (component property) uncertainties. This may be achieved by setting each of the non-compositional uncertainties to zero in the relevant uncertainty formulae, so that the only difference between results arises from the compositional terms.

c) External compatibility: If the requirement is to test the concordance between results achieved by a set of analytical equipment and results achieved by direct measurement of a property on the same test gases, then the relevant measure of uncertainty for the analytical equipment is the complete uncertainty, i.e. again including both the compositional and non-compositional components of uncertainty.

d) Repeatability: If the requirement is to test the performance of a single piece of analytical equipment under repeatability conditions as defined in GUM,[5] then the repeatability of any (property) result may be evaluated directly from the set of calculated property values. Alternatively, it is also possible to determine the (property) uncertainty by determining the repeatability of each composition and then using these values as input to the relevant uncertainty formula. In this case, it is again necessary, since they are common throughout, to set the non-compositional uncertainty terms to zero.

12 Tables of data

Table 1 — Molar mass and atomic indices for components of natural gas

			Atomic index				
j	**Component**	**Molar mass**, M_j kg·kmol^{-1}	a_j	b_j	c_j	d_j	e_j
1	methane	16,042 46	1	4	0	0	0
2	ethane	30,069 04	2	6	0	0	0
3	propane	44,095 62	3	8	0	0	0
4	n-butane	58,122 20	4	10	0	0	0
5	2-methylpropane	58,122 20	4	10	0	0	0
6	n-pentane	72,148 78	5	12	0	0	0
7	2-methylbutane	72,148 78	5	12	0	0	0
8	2,2-dimethylpropane	72,148 78	5	12	0	0	0
9	n-hexane	86,175 36	6	14	0	0	0
10	2-methylpentane	86,175 36	6	14	0	0	0
11	3-methylpentane	86,175 36	6	14	0	0	0
12	2,2-dimethylbutane	86,175 36	6	14	0	0	0
13	2,3-dimethylbutane	86,175 36	6	14	0	0	0
14	n-heptane	100,201 94	7	16	0	0	0
15	n-octane	114,228 52	8	18	0	0	0
16	n-nonane	128,255 10	9	20	0	0	0
17	n-decane	142,281 68	10	22	0	0	0
56	n-undecane	156,308 26	11	24	0	0	0
57	n-dodecane	170,334 84	12	26	0	0	0
58	n-tridecane	184,361 42	13	28	0	0	0
59	n-tetradecane	198,388 00	14	30	0	0	0
60	n-pentadecane	212,414 58	15	32	0	0	0
18	ethene	28,053 16	2	4	0	0	0
19	propene	42,079 74	3	6	0	0	0
20	1-butene	56,106 32	4	8	0	0	0
21	cis-2-butene	56,106 32	4	8	0	0	0
22	trans-2-butene	56,106 32	4	8	0	0	0
23	2-methylpropene	56,106 32	4	8	0	0	0
24	1-pentene	70,132 90	5	10	0	0	0
25	propadiene	40,063 86	3	4	0	0	0
26	1,2-butadiene	54,090 44	4	6	0	0	0
27	1,3-butadiene	54,090 44	4	6	0	0	0
28	ethyne	26,037 28	2	2	0	0	0
29	cyclopentane	70,132 90	5	10	0	0	0
30	methylcyclopentane	84,159 48	6	12	0	0	0
31	ethylcyclopentane	98,186 06	7	14	0	0	0

NOTE The values of the molar mass given above have been obtained by weighted summation of the atomic masses (atomic weights) of the elements involved, as listed in Table A.1 and in ISO/TR 29922. All decimal digits have been retained in this table, i.e. no rounding to a fixed number of decimal places has been applied (except for air). Values of standard uncertainty for molar masses are not included in this table. Where required, they are calculated using Formula (25).

Table 1 *(continued)*

			Atomic index				
j	**Component**	**Molar mass**, M_j kg·kmol^{-1}	a_j	b_j	c_j	d_j	e_j
32	cyclohexane	84,159 48	6	12	0	0	0
33	methylcyclohexane	98,186 06	7	14	0	0	0
34	ethylcyclohexane	112,212 64	8	16	0	0	0
35	benzene	78,111 84	6	6	0	0	0
36	toluene	92,138 42	7	8	0	0	0
37	ethylbenzene	106,165 00	8	10	0	0	0
38	o-xylene	106,165 00	8	10	0	0	0
39	methanol	32,041 86	1	4	0	1	0
40	methanethiol	48,107 46	1	4	0	0	1
41	hydrogen	2,015 88	0	2	0	0	0
42	water	18,015 28	0	2	0	1	0
43	hydrogen sulfide	34,080 88	0	2	0	0	1
44	ammonia	17,030 52	0	3	1	0	0
45	hydrogen cyanide	27,025 34	1	1	1	0	0
46	carbon monoxide	28,010 1	1	0	0	1	0
47	carbonyl sulfide	60,075 1	1	0	0	1	1
48	carbon disulfide	76,140 7	1	0	0	0	2
49	helium	4,002 602	0	0	0	0	0
50	neon	20,179 7	0	0	0	0	0
51	argon	39,948	0	0	0	0	0
52	nitrogen	28,013 4	0	0	2	0	0
53	oxygen	31,998 8	0	0	0	2	0
54	carbon dioxide	44,009 5	1	0	0	2	0
55	sulfur dioxide	64,063 8	0	0	0	2	1
	air	28,965 46					

NOTE The values of the molar mass given above have been obtained by weighted summation of the atomic masses (atomic weights) of the elements involved, as listed in Table A.1 and in ISO/TR 29922. All decimal digits have been retained in this table, i.e. no rounding to a fixed number of decimal places has been applied (except for air). Values of standard uncertainty for molar masses are not included in this table. Where required, they are calculated using Formula (25).

Table 2 — Summation factors for components of natural gas at various metering reference temperatures

		Summation factor s_j at various metering reference temperatures				$u(s_j)$
j	**Component**	0 °C	15 °C	15,55 °C	20 °C	
1	methane	0,048 86	0,044 52	0,044 37	0,043 17	0,000 5
2	ethane	0,099 7	0,091 9	0,091 6	0,089 5	0,001 1
3	propane	0,146 5	0,134 4	0,134 0	0,130 8	0,001 6
4	n-butane	0,202 2	0,184 0	0,183 4	0,178 5	0,003 9
5	2-methylpropane	0,188 5	0,172 2	0,171 7	0,167 3	0,003 1
6	n-pentane	0,258 6	0,236 1	0,235 4	0,229 5	0,010 7
7	2-methylbutane	0,245 8	0,225 1	0,224 4	0,218 9	0,008 8
8	2,2-dimethylpropane	0,224 5	0,204 0	0,203 3	0,197 9	0,006 0
9	n-hexane	0,331 9	0,300 1	0,299 0	0,290 7	0,027 1
10	2-methylpentane	0,311 4	0,282 6	0,281 6	0,274 0	0,022 1
11	3-methylpentane	0,299 7	0,276 2	0,275 4	0,269 0	0,023 4
12	2,2-dimethylbutane	0,253 0	0,235 0	0,234 4	0,229 5	0,017 3
13	2,3-dimethylbutane	0,283 6	0,263 2	0,262 5	0,256 9	0,020 7
14	n-heptane	0,407 6	0,366 8	0,365 4	0,354 7	0,100 1
15	n-octane	0,484 5	0,434 6	0,432 9	0,419 8	0,100 2
16	n-nonane	0,561 7	0,503 0	0,501 0	0,485 6	0,100 6
17	n-decane	0,671 3	0,599 1	0,596 7	0,577 8	0,100 6
56	n-undecane	0,722 8	0,640 2	0,637 4	0,615 9	0,100 6
57	n-dodecane	0,856 7	0,761 5	0,758 3	0,733 5	0,100 6
58	n-tridecane	0,912 9	0,806 1	0,802 6	0,774 8	0,100 6
59	n-tetradecane	1,013 5	0,894 0	0,890 0	0,858 9	0,100 6
60	n-pentadecane	1,117 6	0,984 9	0,980 4	0,945 9	0,100 6
18	ethene	0,086 8	0,079 9	0,079 7	0,077 8	0,001 0
19	propene	0,138 1	0,126 7	0,126 3	0,123 2	0,001 6
20	1-butene	0,196 4	0,177 6	0,177 0	0,172 1	0,004 1
21	cis-2-butene	0,207 5	0,187 0	0,186 3	0,181 0	0,004 5
22	trans-2-butene	0,207 2	0,186 8	0,186 2	0,180 9	0,004 3
23	2-methylpropene	0,196 6	0,177 7	0,177 0	0,172 1	0,003 7
24	1-pentene	0,262 2	0,229 7	0,228 7	0,220 8	0,010 2
25	propadiene	0,141 7	0,131 3	0,131 0	0,128 2	0,002 5
26	1,2-butadiene	0,206 3	0,186 2	0,185 5	0,180 3	0,011 0
27	1,3-butadiene	0,199 3	0,173 9	0,173 1	0,167 3	0,003 8
28	ethyne	0,093 6	0,083 6	0,083 3	0,080 8	0,002 4
29	cyclopentane	0,240 9	0,222 1	0,221 5	0,216 4	0,013 7
30	methylcyclopentane	0,281 7	0,261 2	0,260 5	0,254 8	0,026 2
31	ethylcyclopentane	0,422 7	0,368 4	0,366 6	0,353 1	0,100 6
32	cyclohexane	0,293 9	0,268 6	0,267 7	0,261 0	0,032 5
33	methylcyclohexane	0,366 7	0,331 7	0,330 5	0,321 3	0,066 8
34	ethylcyclohexane	0,527 5	0,454 7	0,452 4	0,434 5	0,100 6
35	benzene	0,275 2	0,252 7	0,252 0	0,246 0	0,027 4

NOTE The values of s_j and $u(s_j)$ given above have all been derived by the methods described in ISO/TR 29922. All values refer to a pressure p_0 of 101,325 kPa (14,696 psi).

Table 2 *(continued)*

		Summation factor s_j at various metering reference temperatures				$u(s_j)$
j	**Component**	0 °C	15 °C	15,55 °C	20 °C	
36	toluene	0,372 6	0,335 9	0,334 7	0,325 1	0,100 2
37	ethylbenzene	0,412 9	0,379 7	0,378 5	0,369 4	0,100 2
38	o-xylene	0,485 2	0,441 1	0,439 6	0,427 7	0,100 4
39	methanol	0,580 6	0,446 4	0,442 3	0,411 7	0,023 3
40	methanethiol	0,190 9	0,170 0	0,169 3	0,164 0	0,011 7
41	hydrogen	−0,01	−0,01	−0,01	−0,01	0,025 0
42	water	0,309 3	0,256 2	0,254 6	0,241 9	0,015 0
43	hydrogen sulfide	0,100 6	0,092 3	0,092 0	0,089 8	0,002 3
44	ammonia	0,123 0	0,110 0	0,109 6	0,106 2	0,002 1
45	hydrogen cyanide	0,317 5	0,276 5	0,275 1	0,264 4	0,007 6
46	carbon monoxide	0,025 8	0,021 7	0,021 5	0,020 3	0,001 0
47	carbonyl sulfide	0,121 1	0,111 4	0,111 0	0,108 4	0,005 4
48	carbon disulfide	0,218 2	0,195 8	0,195 1	0,189 4	0,009 8
49	helium	−0,01	−0,01	−0,01	−0,01	0,025 0
50	neon	−0,01	−0,01	−0,01	−0,01	0,025 0
51	argon	0,030 7	0,027 3	0,027 2	0,026 2	0,001 0
52	nitrogen	0,021 4	0,017 0	0,016 9	0,015 6	0,001 0
53	oxygen	0,031 1	0,027 6	0,027 5	0,026 5	0,001 0
54	carbon dioxide	0,082 1	0,075 2	0,074 9	0,073 0	0,002 0
55	sulfur dioxide	0,157 9	0,140 6	0,140 0	0,135 6	0,003 5

NOTE The values of s_j and $u(s_j)$ given above have all been derived by the methods described in ISO/TR 29922. All values refer to a pressure p_0 of 101,325 kPa (14,696 psi).

Table 3 — Gross calorific values on a molar basis for components of natural gas in the ideal gas state at various combustion reference temperatures

		Gross calorific value $\left[\left(Hc\right)_{G}^{o}\right]_{j}\left(t_{1}\right)$ **kJ·mol^{-1} of the ideal gas at various reference temperatures**					$u(Hc)$
j	**Component**	0 °C	15 °C	15,55 °C	20 °C	25 °C	
1	methane	892,92	891,51	891,46	891,05	890,58	0,19
2	ethane	1 564,35	1 562,14	1 562,06	1 561,42	1 560,69	0,51
3	propane	2 224,03	2 221,10	2 220,99	2 220,13	2 219,17	0,51
4	n-butane	2 883,35	2 879,76	2 879,63	2 878,58	2 877,40	0,72
5	2-methylpropane	2 874,21	2 870,58	2 870,45	2 869,39	2 868,20	0,72
6	n-pentane	3 542,91	3 538,60	3 538,45	3 537,19	3 535,77	0,23
7	2-methylbutane	3 536,01	3 531,68	3 531,52	3 530,25	3 528,83	0,23
8	2,2-dimethylpropane	3 521,75	3 517,44	3 517,28	3 516,02	3 514,61	0,25
9	n-hexane	4 203,24	4 198,24	4 198,06	4 196,60	4 194,95	0,32
10	2-methylpentane	4 195,64	4 190,62	4 190,44	4 188,97	4 187,32	0,53
11	3-methylpentane	4 198,27	4 193,22	4 193,04	4 191,56	4 189,90	0,53
12	2,2-dimethylbutane	4 185,86	4 180,83	4 180,65	4 179,17	4 177,52	0,48
13	2,3-dimethylbutane	4 193,68	4 188,61	4 188,43	4 186,94	4 185,28	0,46
14	n-heptane	4 862,88	4 857,18	4 856,98	4 855,31	4 853,43	0,67
15	n-octane	5 522,41	5 516,01	5 515,78	5 513,90	5 511,80	0,76
16	n-nonane	6 182,92	6 175,82	6 175,56	6 173,48	6 171,15	0,81
17	n-decane	6 842,69	6 834,90	6 834,62	6 832,33	6 829,77	0,87
56	n-undecane	7 502,22	7 493,73	7 493,42	7 490,93	7 488,14	1,54
57	n-dodecane	8 162,43	8 153,24	8 152,91	8 150,21	8 147,19	1,13
58	n-tridecane	8 821,88	8 811,99	8 811,63	8 808,73	8 805,48	1,21
59	n-tetradecane	9 481,71	9 471,12	9 470,73	9 467,63	9 464,15	1,32
60	n-pentadecane	10 141,65	10 130,23	10 129,82	10 126,52	10 122,82	1,44
18	ethene	1 413,55	1 412,12	1 412,07	1 411,65	1 411,18	0,21
19	propene	2 061,57	2 059,43	2 059,35	2 058,73	2 058,02	0,34
20	1-butene	2 721,57	2 718,71	2 718,60	2 717,76	2 716,82	0,39
21	cis-2-butene	2 714,88	2 711,94	2 711,83	2 710,97	2 710,00	0,50
22	trans-2-butene	2 711,09	2 708,26	2 708,16	2 707,33	2 706,40	0,47
23	2-methylpropene	2 704,88	2 702,06	2 701,96	2 701,13	2 700,20	0,42

NOTE 1 All values of $\left[\left(Hc\right)_{G}^{o}\right]_{j}\left(t_{1}\right)$ for t_1 = 25 °C are taken from Reference [6] except for methane (j = 1), which is discussed in detail as a special case in ISO/TR 29922, water (see Note 3) and the C11 to C15 n-alkanes (see ISO/TR 29922). Values of $\left[\left(Hc\right)_{G}^{o}\right]_{j}\left(t_{1}\right)$ for t_1 = 20 °C, 15,55 °C, 15 °C and 0 °C have been obtained from the corresponding values at 25 °C by means of prescribed calculations of the type described in ISO/TR 29922.

NOTE 2 The value of $u(Hc)$ for methane is taken from ISO/TR 29922:—, 8.1.5. For every other component, the value of $u(Hc)$ has been estimated according to the methods described elsewhere in ISO/TR 29922.

NOTE 3 The non-zero calorific value of water vapour (j = 42) derives formally from the definition of gross calorific value, which requires condensation to the liquid state of all water vapour in the products of combustion. Thus, any water vapour present in a gas contributes its latent heat of vaporization to the gross calorific value of the mixture. The values given are taken from A.4. See ISO/TR 29922 for a fuller explanation.

Table 3 *(continued)*

j	Component	Gross calorific value $\left[\left(Hc\right)_G^o\right]_j\left(t_1\right)$ kJ·mol^{-1} of the ideal gas at various reference temperatures					$u(Hc)$
		0 °C	15 °C	15,55 °C	20 °C	25 °C	
24	1-pentene	3 381,32	3 377,76	3 377,63	3 376,59	3 375,42	0,73
25	propadiene	1 945,26	1 943,97	1 943,92	1 943,54	1 943,11	0,60
26	1,2-butadiene	2 597,15	2 595,12	2 595,05	2 594,46	2 593,79	0,40
27	1,3-butadiene	2 544,14	2 542,11	2 542,03	2 541,44	2 540,77	0,41
28	ethyne	1 301,86	1 301,37	1 301,35	1 301,21	1 301,05	0,32
29	cyclopentane	3 326,14	3 322,19	3 322,05	3 320,89	3 319,59	0,36
30	methylcyclopentane	3 977,05	3 972,46	3 972,29	3 970,95	3 969,44	0,56
31	ethylcyclopentane	4 637,20	4 631,93	4 631,74	4 630,20	4 628,47	0,71
32	cyclohexane	3 960,68	3 956,02	3 955,85	3 954,49	3 952,96	0,32
33	methylcyclohexane	4 609,33	4 604,08	4 603,89	4 602,36	4 600,64	0,71
34	ethylcyclohexane	5 272,76	5 266,90	5 266,69	5 264,97	5 263,05	0,95
35	benzene	3 305,12	3 302,90	3 302,81	3 302,16	3 301,43	0,27
36	toluene	3 952,77	3 949,83	3 949,72	3 948,86	3 947,89	0,51
37	ethylbenzene	4 613,16	4 609,54	4 609,40	4 608,34	4 607,15	0,66
38	o-xylene	4 602,18	4 598,64	4 598,52	4 597,48	4 596,31	0,76
39	methanol	766,60	765,09	765,03	764,59	764,09	0,13
40	methanethiol	1 241,64	1 240,28	1 240,23	1 239,84	1 239,39	0,32
41	hydrogen	286,64	286,15	286,13	285,99	285,83	0,02
42	water (see note 3)	45,064	44,431	44,408	44,222	44,013	0,004
43	hydrogen sulfide	562,93	562,38	562,36	562,19	562,01	0,23
44	ammonia	384,57	383,51	383,47	383,16	382,81	0,18
45	hydrogen cyanide	671,92	671,67	671,66	671,58	671,50	1,26
46	carbon monoxide	282,80	282,91	282,91	282,95	282,98	0,06
47	carbonyl sulfide	548,01	548,14	548,15	548,19	548,23	0,24
48	carbon disulfide	1 104,05	1 104,32	1 104,33	1 104,40	1 104,49	0,43

NOTE 1 All values of $\left[\left(Hc\right)_G^o\right]_j\left(t_1\right)$ for $t_1 = 25$ °C are taken from Reference [6] except for methane ($j = 1$), which is discussed in detail as a special case in ISO/TR 29922, water (see Note 3) and the C11 to C15 n-alkanes (see ISO/TR 29922). Values of $\left[\left(Hc\right)_G^o\right]_j\left(t_1\right)$ for $t_1 = 20$ °C, 15,55 °C, 15 °C and 0 °C have been obtained from the corresponding values at 25 °C by means of prescribed calculations of the type described in ISO/TR 29922.

NOTE 2 The value of $u(Hc)$ for methane is taken from ISO/TR 29922:—, 8.1.5. For every other component, the value of $u(Hc)$ has been estimated according to the methods described elsewhere in ISO/TR 29922.

NOTE 3 The non-zero calorific value of water vapour ($j = 42$) derives formally from the definition of gross calorific value, which requires condensation to the liquid state of all water vapour in the products of combustion. Thus, any water vapour present in a gas contributes its latent heat of vaporization to the gross calorific value of the mixture. The values given are taken from A.4. See ISO/TR 29922 for a fuller explanation.

Annex A

(normative)

Values of auxiliary constants

A.1 Gas constant

The value of the molar gas constant R (including the standard uncertainty) shall be taken from the current CODATA recommendation[7] as given in Table A.1.

Table A.1 — Molar gas constant

Molar gas constant $R/\text{J·mol}^{-1}\text{·K}^{-1}$	**Standard uncertainty** $u(R)/\text{J·mol}^{-1}\text{·K}^{-1}$
8,314 462 1	0,000 007 5

A.2 Atomic weights of the elements

The atomic mass in kg·kmol^{-1} of each of the elements, carbon, hydrogen, nitrogen, oxygen and sulfur, is required for the evaluation of Formula (25). The values shall be taken from the 2007 IUPAC recommendations[8] as given in Table A.2. A more detailed discussion of atomic masses is given in ISO/TR 29922.

Table A.2 — Atomic weights of the elements

Element		**Atomic weight** $A/\text{kg·kmol}^{-1}$	**Standard uncertainty** $u(A)/\text{kg·kmol}^{-1}$
carbon	C	12,010 7	0,000 4
hydrogen	H	1,007 94	0,000 035
nitrogen	N	14,006 7	0,000 1
oxygen	O	15,999 4	0,000 15
sulfur	S	32,065	0,002 5
helium	He	4,002 602	0,000 001
neon	Ne	20,179 7	0,000 3
argon	Ar	39,948	0,000 5

A.3 Properties of dry air

The value for the molar mass of dry air of fixed reference composition rounded to the fifth decimal place shall be taken as given in Table A.3[3][9].

Table A.3 — Molar mass of dry air

Molar mass $M_{\text{air}}/\text{kg·kmol}^{-1}$	**Standard uncertainty** $u(M_{\text{air}})/\text{kg·kmol}^{-1}$
28,965 46	0,000 17

The standard uncertainty quoted is that which derives solely from the known uncertainties in the molar masses of the constituents. No allowance has been made for uncertainties of composition, i.e. the composition of air is taken, for present purposes, as exact.

The value of the compression factor of dry air of reference composition at each of the four commonly used metering reference conditions shall be taken as given in Table A.4.

Table A.4 — Compression factor of dry air at various reference conditions

Reference condition	Compression factor Z_{air}	Standard uncertainty $u(Z_{\mathrm{air}})$
0 °C, 101,325 kPa	0,999 419	0,000 015
15 °C, 101,325 kPa	0,999 595	0,000 015
15,55 °C, 101,325 kPa	0,999 601	0,000 015
20 °C, 101,325 kPa	0,999 645	0,000 015

Each of these values has been calculated in accordance with the GERG-2004 formula as presented in References [1] and [10]. For the three highest temperatures, the values agree with those given by the more recent CIPM-2007 formulation[9] to within 2 to 3 parts per million, but that formulation is not valid at 0 °C. The values of standard uncertainty are taken directly from Reference [9].

A.4 Standard enthalpy of vaporization of water

The standard molar enthalpy of vaporization of water is required at each of the five commonly used combustion reference conditions in order to facilitate calculations of the difference between the ideal-gas gross calorific value and the ideal-gas net calorific value (molar basis) for each component. The values given in Table A.5, which have been calculated from the IAPWS-1995 formulation given in References [11] and [12] shall be used.

Table A.5 — Standard enthalpy of vaporization of water

Temperature/ °C	Enthalpy of vaporization $L^{\mathrm{o}}/\mathrm{kJ{\cdot}mol^{-1}}$	Standard uncertainty $u(L^{\mathrm{o}})/\mathrm{kJ{\cdot}mol^{-1}}$
0	45,064	0,004
15	44,431	0,004
15,55 (60 °F)	44,408	0,004
20	44,222	0,004
25	44,013	0,004

Annex B
(normative)

Formulae for uncertainty calculations

B.1 General

The formulae given in this annex shall be used in calculations of uncertainty for those properties that may be calculated by use of this document. Because the properties of the ideal gas are unlikely to be required as a final result, with an associated uncertainty, the formulae given apply specifically to the real gas.

In the event that the uncertainty associated with a property of the ideal gas is required, this may be obtained by setting $s = 0$ and $u(s) = 0$ in the appropriate formula.

B.2 Molar mass

$$u^2\left(M\right) = \left(\sum_{i=1}^{N}\sum_{j=1}^{N} M_i \cdot M_j \cdot u\left(x_i\right) \cdot u\left(x_j\right) \cdot r\left(x_i, x_j\right)\right) + \left(\sum_{i=1}^{N}\sum_{j=1}^{N} x_i \cdot x_j \cdot u\left(M_i\right) \cdot u\left(M_j\right) \cdot r\left(M_i, M_j\right)\right) \tag{B.1}$$

B.3 Summation factor

$$u^2\left(s\right) = \left(\sum_{i=1}^{N}\sum_{j=1}^{N} s_i \cdot u\left(x_i\right) \cdot r\left(x_i, x_j\right) \cdot s_j \cdot u\left(x_j\right)\right) + \sum_{i=1}^{N} x_i^2 \cdot u^2\left(s_i\right) \tag{B.2}$$

B.4 Compression factor

$$u^2\left(Z\right) = 4 \cdot s^2 \times \left(\left(\sum_{i=1}^{N}\sum_{j=1}^{N} s_i \cdot u\left(x_i\right) \cdot r\left(x_i, x_j\right) \cdot s_j \cdot u\left(x_j\right)\right) + \sum_{i=1}^{N} x_i^2 \cdot u^2\left(s_i\right)\right) \tag{B.3}$$

B.5 Molar-basis gross calorific value

$$u^2\left(\left(Hc\right)_G\right) = \sum_{i=1}^{N}\sum_{j=1}^{N} \left[\left(Hc\right)_G^o\right]_i \cdot u\left(x_i\right) \cdot r\left(x_i, x_j\right) \cdot \left[\left(Hc\right)_G^o\right]_j \cdot u\left(x_j\right) + \sum_{i=1}^{N} x_i^2 \cdot u^2\left(\left[\left(Hc\right)_G^o\right]_i\right) \tag{B.4}$$

B.6 Mass-basis gross calorific value

$$\left(\frac{u\left(\left(Hm\right)_G\right)}{\left(Hm\right)_G}\right)^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{\left[\left(Hc\right)_G^o\right]_i}{\left(Hc\right)_G} - \frac{M_i}{M}\right)\cdot u\left(x_i\right)\cdot r\left(x_i, x_j\right)\cdot\left(\frac{\left[\left(Hc\right)_G^o\right]_j}{\left(Hc\right)_G} - \frac{M_j}{M}\right)\cdot u\left(x_j\right) + \frac{\sum_{i=1}^{N} x_i^2 \cdot u^2\left(\left[\left(Hc\right)_G^o\right]_i\right)}{\left(Hc\right)_G^2} + \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} x_i \cdot u\left(M_i\right)\cdot r\left(M_i, M_j\right)\cdot x_j \cdot u\left(M_j\right)}{M^2} \tag{B.5}$$

B.7 Volume-basis gross calorific value

$$\left(\frac{u\left(\left(Hv\right)_G\right)}{\left(Hv\right)_G}\right)^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{\left[\left(Hc\right)_G^o\right]_i}{\left(Hc\right)_G} + \frac{2\cdot s_i \cdot s}{Z}\right)\cdot u\left(x_i\right)\cdot r\left(x_i, x_j\right)\cdot \left(\frac{\left[\left(Hc\right)_G^o\right]_j}{\left(Hc\right)_G} + \frac{2\cdot s_j \cdot s}{Z}\right)\cdot u\left(x_j\right) + \frac{\sum_{i=1}^{N} x_i^2 \cdot u^2\left(\left[\left(Hc\right)_G^o\right]_i\right)}{\left(Hc\right)_G^2} + \frac{4\cdot s^2 \cdot \sum_{i=1}^{N} x_i^2 \cdot u^2\left(s_i\right)}{Z^2} + \left(\frac{u\left(R\right)}{R}\right)^2 \tag{B.6}$$

where

$$s = \left(\left(1 - Z\right)\times\frac{p_2}{p_0}\right)^{1/2} \tag{B.7}$$

B.8 Molar-basis net calorific value

$$u^2\left(\left(Hc\right)_N\right) = \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\left[\left(Hc\right)_G^o\right]_i - \frac{L^o}{2}\cdot b_i\right)\cdot u\left(x_i\right)\cdot r\left(x_i, x_j\right)\cdot\left(\left[\left(Hc\right)_G^o\right]_j - \frac{L^o}{2}\cdot b_j\right)\cdot u\left(x_j\right) + \sum_{i=1}^{N} x_i^2 \cdot u^2\left(\left[\left(Hc\right)_G^o\right]_i\right) + \left(\frac{\sum_{i=1}^{N} x_i \cdot b_i}{2}\right)^2 \cdot u^2\left(L^o\right) \tag{B.8}$$

B.9 Mass-basis net calorific value

$$\left(\frac{u\left(\left(Hm\right)_N\right)}{\left(Hm\right)_N}\right)^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{\left(\left[\left(Hc\right)_G^o\right]_i - \frac{L^o}{2}\cdot b_i\right)}{\left(Hc\right)_N} - \frac{M_i}{M}\right)\cdot u\left(x_i\right)\cdot r\left(x_i, x_j\right)\cdot \left(\frac{\left(\left[\left(Hc\right)_G^o\right]_j - \frac{L^o}{2}\cdot b_j\right)}{\left(Hc\right)_N} - \frac{M_j}{M}\right)\cdot u\left(x_j\right) + \frac{\sum_{i=1}^{N} x_i^2\cdot u^2\left(\left[\left(Hc\right)_G^o\right]_i\right)}{\left(Hc\right)_N^2} + \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} x_i\cdot u\left(M_i\right)\cdot r\left(M_i, M_j\right)\cdot x_j\cdot u\left(M_j\right)}{M^2} + \left(\frac{\sum_{i=1}^{N} x_i\cdot b_i}{2\cdot\left(Hc\right)_N}\right)^2\cdot u^2\left(L^o\right) \tag{B.9}$$

B.10 Volume-basis net calorific value

$$\left(\frac{u\left(\left(Hv\right)_N\right)}{\left(Hv\right)_N}\right)^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{\left(\left[\left(Hc\right)_G^o\right]_i - \frac{L^o}{2} b_i\right)}{\left(Hc\right)_N} + \frac{2\cdot s_i\cdot s}{Z}\right)\cdot u\left(x_i\right)\cdot r\left(x_i, x_j\right)\cdot \left(\frac{\left(\left[\left(Hc\right)_G^o\right]_j - \frac{L^o}{2}\cdot b_j\right)}{\left(Hc\right)_N} + \frac{2\cdot s_i\cdot s}{Z}\right)\cdot u\left(x_j\right) + \frac{\sum_{i=1}^{N} x_i^2\cdot u^2\left(\left[\left(Hc\right)_G^o\right]_i\right)}{\left(Hc\right)_N^2} + \frac{4\cdot s^2\cdot\sum_{i=1}^{N} x_i^2\cdot u^2\left(s_i\right)}{Z^2} + \left(\frac{u\left(R\right)}{R}\right)^2 + \left(\frac{\sum_{i=1}^{N} x_i\cdot b_i}{2\cdot\left(Hc\right)_N}\right)^2\cdot u^2\left(L^o\right) \tag{B.10}$$

B.11 Density

$$\left(\frac{u(D)}{D}\right)^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{M_i}{M}+\frac{2\cdot s_i\cdot s}{Z}\right)\cdot u(x_i)\cdot r(x_i,x_j)\cdot u(x_j)\cdot\left(\frac{M_j}{M}+\frac{2\cdot s_j\cdot s}{Z}\right)+$$
$$\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{x_i\cdot u(M_i)\cdot r(M_i,M_j)\cdot u(M_j)\cdot x_j}{M^2}+ \tag{B.11}$$
$$\frac{4\cdot s^2\cdot\sum_{i=1}^{N}x_i^2\cdot u^2(s_i)}{Z^2}+\left(\frac{u(R)}{R}\right)^2$$

B.12 Relative density

$$\left(\frac{u(G)}{G}\right)^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{M_i}{M}+\frac{2\cdot s_i\cdot s}{Z}\right)\cdot u(x_i)\cdot r(x_i,x_j)\cdot\left(\frac{M_j}{M}+\frac{2\cdot s_j\cdot s}{Z}\right)\cdot u(x_j)+$$
$$\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{x_i\cdot u(M_i)\cdot r(M_i,M_j)\cdot u(M_j)\cdot x_j}{M^2}+$$
$$\frac{4\cdot s^2\cdot\sum_{i=1}^{N}x_i^2\cdot u^2(s_i)}{Z^2}+ \tag{B.12}$$
$$\left(\frac{u(M_{\mathrm{air}})}{M_{\mathrm{air}}}\right)^2+\left(\frac{u(Z_{\mathrm{air}})}{Z_{\mathrm{air}}}\right)^2$$

B.13 Gross Wobbe index

$$\begin{aligned}\left(\frac{u\left(W_G\right)}{W_G}\right)^2 = {} & \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{\left[\left(Hc\right)_G^o\right]_i}{\left(Hc\right)_G}+\frac{s_i\cdot s}{Z}-\frac{M_i}{2\cdot M}\right)\cdot u\left(x_i\right)\cdot \\ & r\left(x_i,x_j\right)\cdot u\left(x_j\right)\cdot\left(\frac{\left[\left(Hc\right)_G^o\right]_j}{\left(Hc\right)_G}+\frac{s_j\cdot s}{Z}-\frac{M_j}{2\cdot M}\right)+ \\ & \frac{\sum_{i=1}^{N}x_i^2\cdot u^2\left[\left(Hc\right)_G^o\right]_i}{\left(Hc\right)_G^2}+\frac{s^2\cdot\sum_{i=1}^{N}x_i^2\cdot u^2\left(s_i\right)}{Z^2}+ \\ & \frac{\sum_{i=1}^{N}\sum_{j=1}^{N}x_i\cdot u\left(M_i\right)\cdot r\left(M_i,M_j\right)\cdot u\left(M_j\right)\cdot x_j}{4\cdot M^2}+ \\ & \left(\frac{u\left(R\right)}{R}\right)^2+\left(\frac{u\left(M_{\text{air}}\right)}{2\cdot M_{\text{air}}}\right)^2+\left(\frac{u\left(Z_{\text{air}}\right)}{2\cdot Z_{\text{air}}}\right)^2\end{aligned} \tag{B.13}$$

B.14 Net Wobbe index

$$\begin{aligned}\left(\frac{u\left(W_N\right)}{W_N}\right)^2 = {} & \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{\left(\left[\left(Hc\right)_G^o\right]_i-\frac{L^o}{2}\cdot b_i\right)}{\left(Hc\right)_N}+\frac{s_i\cdot s}{Z}-\frac{M_i}{2\cdot M}\right)\cdot u\left(x_i\right)\cdot r\left(x_i,x_j\right)\cdot u\left(x_j\right)\cdot \\ & \left(\frac{\left(\left[\left(Hc\right)_G^o\right]_j-\frac{L^o}{2}\cdot b_j\right)}{\left(Hc\right)_N}+\frac{s_j\cdot s}{Z}-\frac{M_j}{2\cdot M}\right)+\frac{\sum_{i=1}^{N}x_i^2\cdot u^2\left[\left(Hc\right)_G^o\right]_i}{\left(Hc\right)_N^2}+ \\ & \frac{s^2\cdot\sum_{i=1}^{N}x_i^2\cdot u^2\left(s_i\right)}{Z^2}+\frac{\sum_{i=1}^{N}\sum_{j=1}^{N}x_i\cdot u\left(M_i\right)\cdot r\left(M_i,M_j\right)\cdot u\left(M_j\right)\cdot x_j}{4\cdot M^2}+ \\ & \left(\frac{u\left(R\right)}{R}\right)^2+\left(\frac{u\left(M_{\text{air}}\right)}{2\cdot M_{\text{air}}}\right)^2+\left(\frac{u\left(Z_{\text{air}}\right)}{2\cdot Z_{\text{air}}}\right)^2+\left(\frac{\sum_{i=1}^{N}x_i\cdot b_i}{2\cdot\left(Hc\right)_N}\right)^2\cdot u^2\left(L^o\right)\end{aligned} \tag{B.14}$$

Annex C
(informative)

Conversion factors

C.1 General

In several known applications, the value of quantities covered by this document are required in units other than the SI units used in the main body. In such cases, the following numerical factors shall be used to convert quantities from the SI units given in the main body to the same quantities in the required non-SI units.

In the following tables, to obtain the value of a quantity in the non-SI unit from the value of the quantity in the SI unit, divide by the conversion factor given and, using the normal rules of rounding, express the result to the rounding precision indicated.

Conversion factors given in normal typeface are approximate but of sufficient accuracy for the purposes of this document when values in SI units, obtained by use of the contingency method (11.5.4), are to be converted to non-SI units and quoted to the rounding precision indicated. Conversion factors given in italic are exact.

Conversion factors for volume-basis properties apply only when the property expressed in SI units and non-SI units refers to the same pressure and temperature.

C.2 Molar-basis calorific values

Table C.1

SI unit	Non-SI unit	Conversion factor	Rounding precision
kJ·mol^{-1}	Btu$_{IT}$·lb-mol^{-1}	*0,002 326*	1

C.3 Mass-basis calorific values

Table C.2

SI unit	Non-SI unit	Conversion factor	Rounding precision
MJ·kg^{-1}	Btu$_{IT}$·lb^{-1}	*0,002 326*	1

C.4 Volume-basis calorific values and Wobbe indices

Table C.3

SI unit	Non-SI unit	Conversion factor	Rounding precision
MJ·m^{-3}	kWh·m^{-3}	*3,6*	0,001
	Btu$_{IT}$·ft^{-3}	0,037 258 9	0,1

C.5 Density

Table C.4

SI unit	Non-SI unit	Conversion factor	Rounding precision
kg·m^{-3}	lb·ft^{-3}	16,018 46	0,000 01

Annex D
(informative)

Example calculations

D.1 General

This annex gives example calculations for the properties included in this document. These examples provide validated results that may be used to verify implementations of the methods. In order to assist in the verification of any implementation and to ensure that no rounding errors compromise the final results, more decimal places have been retained at each intermediate step than may strictly be necessary.

Further to this, an Excel® spreadsheet *ISO6976examples.xlsx*, with which the examples may be examined in greater numerical detail, is available for download at http://standards.iso.org/iso/ as an optional adjunct to this document.

D.2 Example 1: A simple mixture of five components

D.2.1 General

In this example calculation, results of the intermediate steps in the calculation of a limited selection of properties are provided for a simple five-component mixture. The mixture is necessarily simplified so as to restrict the size of the matrices containing the values of $r(x_i,x_j)$ and $r(M_i,M_j)$. Properties are calculated for combustion reference conditions of 15 °C and 101,325 kPa, and metering reference conditions of 15 °C and 101,325 kPa (ISO Standard Reference Conditions).

D.2.2 Compositional analysis

The mole-fraction analysis report of a natural gas sample provided the following information for the normalized composition (rounded to six decimal places) and associated uncertainties:

Component	x_i	$u(x_i)$
methane	0,933 212	0,000 346
ethane	0,025 656	0,000 243
propane	0,015 368	0,000 148
nitrogen	0,010 350	0,000 195
carbon dioxide	0,015 414	0,000 111
sum	1,000 000	

D.2.3 Calculation of molar mass

Component	x_i	M_i	$x_i \cdot M_i$
methane	0,933 212	16,042 46	14,971 016 2
ethane	0,025 656	30,069 04	0,771 451 3
propane	0,015 368	44,095 62	0,677 661 5
nitrogen	0,010 350	28,013 40	0,289 938 7
carbon dioxide	0,015 414	44,009 50	0,678 362 4
sum	1,000 000		17,388 430 1

from Formula (5) — molar mass M = 17,388 430 kg·kmol^{-1}

D.2.4 Calculation of real-gas molar volume

Component	x_i	s_i	$x_i \cdot s_i$
methane	0,933 212	0,044 52	0,041 546 6
ethane	0,025 656	0,091 90	0,002 357 8
propane	0,015 368	0,134 40	0,002 065 5
nitrogen	0,010 350	0,017 00	0,000 176 0
carbon dioxide	0,015 414	0,075 20	0,001 159 1
sum	1,000 000		0,047 305 0

p_2 = 101,325 kPa

p_0 = 101,325 kPa

from Formula (1) — compression factor Z = 0,997 762 24

from Formula (B.7) — summation factor s = 0,047 305

T_2 = 288,15 K

from A.1 — gas constant R = 8,314 462 1 J·mol^{-1}·K^{-1}

from Formula (11) — molar volume V = 0,023 591 917 m^3·mol^{-1}

D.2.5 Calculation of molar-basis gross calorific value

Component	x_i	$\left((Hc)_G^o\right)_i$	$x_i \cdot \left((Hc)_G^o\right)_i$
methane	0,933 212	891,51	831,967 830 1
ethane	0,025 656	1 562,14	40,078 263 8
propane	0,015 368	2 221,10	34,133 864 8
nitrogen	0,010 350	0,00	0,000
carbon dioxide	0,015 414	0,00	0,000
sum	1,000 000		906,179 958 8

from Formula (2) — molar-basis gross calorific value $(Hc)_G$ = 906,179 959 kJ·mol^{-1}

D.2.6 Calculation of uncertainty in molar-basis gross calorific value

Component	$\left((Hc)_G^o\right)_i$	$u(x_i)$	$\left((Hc)_G^o\right)_i \cdot u\left(x_i\right)$	$\left[\left((Hc)_G^o\right)_i \cdot u\left(x_i\right)\right]^2$
methane	891,51	0,000 346	0,308 462 46	0,095 149 089
ethane	1 562,14	0,000 243	0,379 600 02	0,144 096 175
propane	2 221,10	0,000 148	0,328 722 80	0,108 058 679
nitrogen	0,00	0,000 195	0,000 000 00	0,000 000 000
carbon dioxide	0,00	0,000 111	0,000 000 00	0,000 000 000
sum				0,347 303 943

	$r(x_i,x_j)$				
	CH_4	C_2H_6	C_3H_8	N_2	CO_2
CH_4	1	0	0	0	0
C_2H_6	0	1	0	0	0
C_3H_8	0	0	1	0	0
N_2	0	0	0	1	0
CO_2	0	0	0	0	1

Component	x_i	x_i^2	$u\left(\left(Hc\right)_G^o\right)_I$	$u^2\left(\left(Hc\right)_G^o\right)_I$	$x_i^2 \cdot u^2\left(\left(Hc\right)_G^o\right)_i$
methane	0,933 212	0,870 884 637	0,19	0,036 1	0,031 438 935
ethane	0,025 656	0,000 658 230	0,51	0,260 1	0,000 171 206
propane	0,015 368	0,000 236 175	0,51	0,260 1	0,000 061 429
nitrogen	0,010 350	0,000 107 123	0,00	0,000 0	0,000 000 000
carbon dioxide	0,015 414	0,000 237 591	0,00	0,000 0	0,000 000 000
sum	1,000 000				0,031 671 570

from Formula (B.4) — $u^2((Hc)_G)$ = 0,347 303 943 + 0,031 671 570

= 0,378 975 513

$u((Hc)_G)$ = 0,615 609 872 kJ·mol^{-1}

$U((Hc)_G)$ = 1,2 kJ·mol^{-1} (using a coverage factor of k = 2 and expressing the result to two significant figures)

D.2.7 Calculation of mass-basis gross calorific value

from D.2.5 — $(Hc)_G$ = 906,179 959 kJ·mol^{-1}

from D.2.3 — M = 17,388 430 kg·kmol^{-1}

from Formula (4) — mass-basis gross calorific value $(Hm)_G$ = 52,113 961 MJ·kg^{-1}

D.2.8 Calculation of uncertainty in mass-basis gross calorific value

Component	$\left(\left(Hc\right)_G^o\right)_I / \left(Hc\right)_G$	M_i/M	$\left[\left(\left(Hc\right)_G^o\right)_I / \left(Hc\right)_G\right] - \left[M_1 / M\right]$	$u(x_i)$	{column 4 value} · $u(x_i)$	{column 6 value}$^2 \times 10^8$
methane	0,983 811 2	0,922 593 9	0,061 217 3	0,000 346	0,000 021 2	0,044 864
ethane	1,723 873 9	1,729 255 6	−0,005 381 7	0,000 243	−0,000 001 3	0,000 171
propane	2,451 058 4	2,535 917 3	−0,084 858 9	0,000 148	−0,000 012 6	0,015 773
nitrogen	0,000 000 0	1,611 036 8	−1,611 036 8	0,000 195	−0,000 314 2	9,869 159
carbon dioxide	0,000 000 0	2,530 964 6	−2,530 964 6	0,000 111	−0,000 280 9	7,892 564
sum						17,822 531

NOTE Assuming correlation matrix $r(x_i,x_j)$ is the same as in D.2.6.

Component	x_i	x_i^2	$u\left(\left(Hc\right)_G^o\right)_I$	$u^2\left(\left(Hc\right)_G^o\right)_I$	$x_i^2 \cdot u^2\left(\left(Hc\right)_G^o\right)_I$	$x_i^2 \cdot u^2\left(\left(Hc\right)_G^o\right)_I / \left(\left(Hc\right)_G\right)^2 \times 10^8$
methane	0,933 212	0,870 884 637	0,19	0,036 1	0,031 438 935	3,828 591
ethane	0,025 656	0,000 658 230	0,51	0,260 1	0,000 171 206	0,020 849
propane	0,015 368	0,000 236 175	0,51	0,260 1	0,000 061 429	0,007 481
nitrogen	0,010 350	0,000 107 123	0,00	0,000 0	0,000 000 000	0,000 000
carbon dioxide	0,015 414	0,000 237 591	0,00	0,000 0	0,000 000 000	0,000 000
sum	1,000 000				0,031 671 570	3,856 921

	$r(M_i,M_j)$				
	methane	ethane	propane	nitrogen	carbon dioxide
methane	1,000 000 000 000 0	0,996 804 383 768 0	0,994 233 563 614 8	0,000 000 000 000 0	0,755 086 685 092 8
ethane	0,996 804 383 768 0	1,000 000 000 000 0	0,999 622 547 547 1	0,000 000 000 000 0	0,773 784 772 303 5
propane	0,994 233 563 614 8	0,999 622 547 547 1	1,000 000 000 000 0	0,000 000 000 000 0	0,779 072 967 793 4
nitrogen	0,000 000 000 000 0	0,000 000 000 000 0	0,000 000 000 000 0	1,000 000 000 000 0	0,000 000 000 000 0
carbon dioxide	0,755 086 685 092 8	0,773 784 772 303 5	0,779 072 967 793 4	0,000 000 000 000 0	1,000 000 000 000 0

Component	x_i	$u(M_i)$	$x_i \cdot u(M_i)$	$[x_i \cdot u(M_i) \cdot r(M_i,M_j) \cdot\ x_j \cdot u(M_j)] \ / \ M^2$
methane	0,933 212	0,000 423 79	0,000 395 5	
ethane	0,025 656	0,000 827 10	0,000 021 2	
propane	0,015 368	0,001 232 23	0,000 018 9	
nitrogen	0,010 350	0,000 200 00	0,000 002 1	
carbon dioxide	0,015 414	0,000 500 00	0,000 007 7	
sum	1,000 000			$0{,}064\ 425 \times 10^{-8}$

$$\begin{aligned}
\text{from Formula (B.5) — } u((Hm)_G) \ / \ (Hm)_G]^2 &= [17{,}822\ 531 + 3{,}856\ 921 + 0{,}064\ 425] \times 10^{-8} \\
&= 21{,}743\ 877 \times 10^{-8} \\
u((Hm)_G) &= [21{,}743\ 877 \times 10^{-8} \times (52{,}113\ 961)^2]^{1/2} \\
&= 0{,}024\ 301\ \text{MJ}\cdot\text{kg}^{-1} \\
U((Hm)_G) &= 0{,}049\ \text{MJ}\cdot\text{kg}^{-1}\ \text{(using a coverage factor of } k = 2 \text{ and expressing the result to two significant figures)}
\end{aligned}$$

D.2.9 Calculation of real-gas volume-basis gross calorific value

from D.2.5 — $(Hc)_G$ = 906,179 959 kJ·mol^{-1}

from D.2.4 — V = 0,023 591 917 m^3·mol^{-1}

from Formula (10) — $(Hv)_G$ = 38,410 611 MJ·m^{-3}

D.2.10 Calculation of uncertainty in volume-basis gross calorific value

Component	$\left(\left(Hc\right)_G^o\right)_i / \left(Hc\right)_G$	$2 \cdot s_i \cdot s / Z$	$\left[\left(\left(Hc\right)_G^o\right)_i / \left(Hc\right)_G\right] + \left[2 \cdot s_i \cdot s / Z\right]$	$u(x_i)$	$\left\{\left[\left(\left(Hc\right)_G^o\right)_I / \left(Hc\right)_G\right] + \left[2 \cdot s_i \cdot s / Z\right]\right\} \cdot u\left(x_i\right)$	{column 6 value}$^2 \times 10^8$
methane	0,983 811 2	0,004 221 5	0,988 032 7	0,000 346	0,000 341 859	11,686 779
ethane	1,723 873 9	0,008 714 2	1,732 588 1	0,000 243	0,000 421 019	17,725 692
propane	2,451 058 4	0,012 744 1	2,463 802 5	0,000 148	0,000 364 643	13,296 435
nitrogen	0,000 000 0	0,001 612 0	0,001 612 0	0,000 195	0,000 000 314	0,000 010
carbon dioxide	0,000 000 0	0,007 130 6	0,007 130 6	0,000 111	0,000 000 791	0,000 063
sum	NOTE Assuming correlation matrix $r(x_i,x_j)$ is the same as in D.2.6.					42,708 979

Component	x_i	x_i^2	$u\left(\left(Hc\right)_G^o\right)_I$	$u^2\left(\left(Hc\right)_G^o\right)_i$	$x_i^2 \cdot u^2\left(\left(Hc\right)_G^o\right)_I$	$x_i^2 \cdot u^2\left(\left(Hc\right)_G^o\right)_I / \left(Hc\right)_G^2 \times 10^8$
methane	0,933 212	0,870 884 637	0,19	0,036 1	0,031 438 935	3,828 591
ethane	0,025 656	0,000 658 230	0,51	0,260 1	0,000 171 206	0,020 849
propane	0,015 368	0,000 236 175	0,51	0,260 1	0,000 061 429	0,007 481
nitrogen	0,010 350	0,000 107 123	0,00	0,000 0	0,000 000 000	0,000 000
carbon dioxide	0,015 414	0,000 237 591	0,00	0,000 0	0,000 000 000	0,000 000
sum	1,000 000				0,031 671 570	3,856 921

Component	x_i	$u(s_i)$	$x_i^2 \cdot u^2\left(s_i\right) \times 10^8$	$4 \cdot s^2 \cdot x_i^2 \cdot u^2\left(s_i\right) / Z^2 \times 10^8$
methane	0,933 212	0,000 5	21,772 212	0,195 758
ethane	0,025 656	0,001 1	0,079 646	0,000 716
propane	0,015 368	0,001 6	0,060 461	0,000 544
nitrogen	0,010 350	0,001 0	0,010 712	0,000 096
carbon dioxide	0,015 414	0,002 0	0,095 037	0,000 854
sum	1,000 000			0,197 968

from A.1 — $[u(R) / R]^2$ $= 0{,}000\ 081\ 4 \times 10^{-8}$

from Formula (B.6) — $[u(Hv)_G / (Hv)_G]^2$ $= [42{,}708\ 979 + 3{,}856\ 921 + 0{,}197\ 968 + 0{,}000\ 081] \times 10^{-8}$

$= 46{,}763\ 949 \times 10^{-8}$

$u(Hv)_G = [46{,}763\ 949 \times 10^{-8} \times (38{,}410\ 611)^2]^{1/2}$

$= 0{,}026\ 267$ MJ·m^{-3}

$U(Hv)_G = 0{,}053$ MJ·m^{-3} (using a coverage factor of $k = 2$ and expressing the result to two significant figures)

D.3 Example 2: A simple mixture containing water vapour

D.3.1 General

This example follows the same procedures and is in the same presentational style as for example 1, but differs in that the simple five-component mixture now excludes propane and, in its place, contains water vapour at a known mole fraction. In addition, the combustion reference conditions and metering reference conditions are both changed to 15,55 °C (60 °F) and 101,325 kPa (14,696 psi).

D.3.2 Compositional analysis

The mole-fraction analysis report of a natural gas sample provided the following information for the normalized composition (rounded to six decimal places) and associated uncertainties:

Component	x_i	$u(x_i)$
methane	0,931 819	0,000 350
ethane	0,025 618	0,000 243
nitrogen	0,010 335	0,000 195
carbon dioxide	0,015 391	0,000 111
water	0,016 837	0,000 162
sum	1,000 000	

D.3.3 Calculation of molar mass

Component	x_i	M_i	$x_i \cdot M_i$
methane	0,931 819	16,042 46	14,948 669 0
ethane	0,025 618	30,069 04	0,770 308 7
nitrogen	0,010 335	28,013 40	0,289 518 5
carbon dioxide	0,015 391	44,009 50	0,677 350 2
water	0,016 837	18,015 28	0,303 323 3
sum	1,000 000		16,989 169 7

from Formula (7) — molar mass $M = 16{,}989\ 170\ \mathrm{kg \cdot kmol^{-1}}$

D.3.4 Calculation of real-gas molar volume

Component	x_i	s_i	$x_i \cdot s_i$
methane	0,931 819	0,044 37	0,041 344 8
ethane	0,025 618	0,091 60	0,002 346 6
nitrogen	0,010 335	0,016 90	0,000 174 7
carbon dioxide	0,015 391	0,074 90	0,001 152 8
water	0,016 837	0,254 60	0,004 286 7
sum	1,000 000		0,049 305 6

$p_2 = 101{,}325$ kPa

$p_0 = 101{,}325$ kPa

from Formula (1) — compression factor $Z = 0{,}997\ 569\ 0$

from Formula (B.7) — summation factor $s = 0{,}049\ 306$

T_2 = 288,706 K

from A.1 — gas constant R = 8,314 462 1 J·mol^{-1}·K^{-1}

from Formula (11) — molar volume V = 0,023 632 824 m^3·mol^{-1}

D.3.5 Calculation of molar-basis gross calorific value

Component	x_i	$\left(\left(Hc\right)_G^o\right)_i$	$x_i \cdot \left(\left(Hc\right)_G^o\right)_i$
methane	0,931 819	891,460	830,679 365 7
ethane	0,025 618	1562,060	40,016 853 1
nitrogen	0,010 335	0,000	0,000
carbon dioxide	0,015 391	0,000	0,000
water	0,016 837	44,408	0,747 697 5
sum	1,000 000		871,443 916 3

from Formula (2) — molar-basis gross calorific value $\left(Hc\right)_G^o$ = 871,443 916 kJ·mol^{-1}

D.3.6 Calculation of uncertainty in molar-basis gross calorific value

Component	$\left(\left(Hc\right)_G^o\right)_i$	$u\left(x_i\right)$	$\left(\left(Hc\right)_G^o\right)_i \cdot u\left(x_i\right)$	$\left[\left(\left(Hc\right)_G^o\right)_i \cdot u\left(x_i\right)\right]^2$
methane	891,460	0,000 350	0,312 011 00	0,097 350 864
ethane	1 562,060	0,000 243	0,379 580 58	0,144 081 417
nitrogen	0,000	0,000 195	0,000 000 00	0,000 000 000
carbon dioxide	0,000	0,000 111	0,000 000 00	0,000 000 000
water	44,408	0,000 162	0,007 194 10	0,000 051 755
sum				0,241 484 036

	$r(x_i,x_j)$				
	CH_4	C_2H_6	N_2	CO_2	H_2O
CH_4	1	0	0	0	0
C_2H_6	0	1	0	0	0
N_2	0	0	1	0	0
CO_2	0	0	0	1	0
H_2O	0	0	0	0	1

Component	x_i	x_i^2	$u\left(\left(Hc\right)_G^o\right)_I$	$u\left(\left(Hc\right)_G^o\right)_I$	$x_i^2 \cdot u^2\left(\left(Hc\right)_G^o\right)_i$
methane	0,931 819	0,868 286 649	0,190	0,036 10	0,031 345 148
ethane	0,025 618	0,000 656 282	0,510	0,260 10	0,000 170 699
nitrogen	0,010 335	0,000 106 812	0,000	0,000 00	0,000 000 000
carbon dioxide	0,015 391	0,000 236 883	0,000	0,000 00	0,000 000 000
water	0,016 837	0,000 283 485	0,004	0,000 02	0,000 000 005
sum	1,000 000				0,031 515 852

from Formula (B.4) —

$u^2((Hc)_G)$ = 0,241 484 036 + 0,031 515 852

= 0,272 999 888

$u((Hc)_G)$ = 0,522 493 911 kJ·mol^{-1}

$U((Hc)_G)$ = 1,0 kJ·mol^{-1} (using a coverage factor of $k = 2$ and expressing the result to two significant figures)

D.3.7 Calculation of mass-basis gross calorific value

from D.3.5 — $(Hc)_G$ = 871,443 916 kJ·mol^{-1}

from D.3.3 — M = 16,989 170 kg·kmol^{-1}

from Formula (4) — mass-basis gross calorific value $(Hm)_G$ = 51,294 085 MJ·kg^{-1}

D.3.8 Calculation of uncertainty in mass-basis gross calorific value

Component	$\left(\left(Hc\right)_G^o\right)_I / \left(Hc\right)_G$	M_i / M	$\left[\left(\left(Hc\right)_G^o\right)_I / \left(Hc\right)_G\right] - \left[M_i / M\right]$	$u\left(x_i\right)$	{column 4 value} · $u(x_i)$	{column 6 value}^{2} × 10^8
methane	1,022 968 9	0,944 275 7	0,078 693 2	0,000 350	0,000 027 5	0,075 860
ethane	1,792 496 3	1,769 894 6	0,022 601 7	0,000 243	0,000 005 5	0,003 016
nitrogen	0,000 000 0	1,648 897 5	−1,648 897 5	0,000 195	−0,000 321 5	10,338 476
carbon dioxide	0,000 000 0	2,590 444 4	−2,590 444 4	0,000 111	−0,000 287 5	8,267 887
water	0,050 959 1	1,060 397 9	−1,009 438 8	0,000 162	−0,000 163 5	2,674 176
sum						21,359 415

NOTE Assuming correlation matrix $r(x_i,x_j)$ is the same as in D.3.6.

Component	x_i	x_i^2	$u\left(\left(Hc\right)_G^o\right)_I$	$u^2\left(\left(Hc\right)_G^o\right)_I$	$x_i^2 \cdot u^2\left(\left(Hc\right)_G^o\right)_I$	$x_i^2 \cdot u^2\left(\left(Hc\right)_G^o\right)_I / \left(\left(Hc\right)_G\right)^2 \times 10^8$
methane	0,931 819	0,868 286 649	0,190	0,036 10	0,031 345 148	4,127 541
ethane	0,025 618	0,000 656 282	0,510	0,260 10	0,000 170 699	0,022 478
nitrogen	0,010 335	0,000 106 812	0,000	0,000 00	0,000 000 000	0,000 000
carbon dioxide	0,015 391	0,000 236 883	0,000	0,000 00	0,000 000 000	0,000 000
water	0,016 837	0,000 283 485	0,004	0,000 02	0,000 000 005	0,000 001
sum	1,000 000				0,031 515 852	4,150 020

	$r(M_i,M_j)$				
	methane	ethane	nitrogen	carbon dioxide	water
methane	1,000 000 000 000 0	0,996 804 383 768 0	0,000 000 000 000 0	0,755 086 685 092 8	0,139 700 393 083 5
ethane	0,996 804 383 768 0	1,000 000 000 000 0	0,000 000 000 000 0	0,773 784 772 303 5	0,107 369 828 180 3
nitrogen	0,000 000 000 000 0	0,000 000 000 000 0	1,000 000 000 000 0	0,000 000 000 000 0	0,000 000 000 000 0
carbon dioxide	0,755 086 685 092 8	0,773 784 772 303 5	0,000 000 000 000 0	1,000 000 000 000 0	0,543 709 883 997 2
water	0,139 700 393 083 5	0,107 369 828 180 3	0,000 000 000 000 0	0,543 709 883 997 2	1,000 000 000 000 0

Component	x_i	$u(M_i)$	$x_i \cdot u(M_i)$	$[x_i \cdot u(M_i) \cdot r(M_i,M_j) \cdot x_j \cdot u(M_j)] / M^2$
methane	0,931 819	0,000 423 79	0,000 394 9	
ethane	0,025 618	0,000 827 10	0,000 021 2	
nitrogen	0,010 335	0,000 200 00	0,000 002 1	
carbon dioxide	0,015 391	0,000 500 00	0,000 007 7	
water	0,016 837	0,000 166 00	0,000 002 8	
sum	1,000 000			$0{,}061\ 785 \times 10^{-8}$

from Formula (B.5) — $u((Hm)_G) / (Hm)_G]^2$ $= [21{,}359\ 415 + 4{,}150\ 020 + 0{,}061\ 785] \times 10^{-8}$

$= 25{,}571\ 220 \times 10^{-8}$

$u((Hm)_G)$ $= [25{,}571\ 220 \times 10^{-8} \times (51{,}294\ 085)^2]^{1/2}$

$= 0{,}025\ 938$ MJ·kg^{-1}

$U((Hm)_G)$ $= 0{,}052$ MJ·kg^{-1} (using a coverage factor of $k = 2$ and expressing the result to two significant figures)

D.3.9 Calculation of real-gas volume-basis gross calorific value

from D.3.5 — $(Hc)_G$ = 871,443 916 kJ·mol^{-1}

from D.3.4 — V = 0,023 632 824 m^3·mol^{-1}

from Formula (10) — $(Hv)_G$ = 36,874 304 MJ·m^{-3}

D.3.10 Calculation of uncertainty in volume-basis gross calorific value

Component	$\left((Hc)_G^o\right)_I / (Hc)_G$	$2 \cdot s_i \cdot s / Z$	$\left[\left((Hc)_G^o\right)_I / (Hc)_G\right] + \left[2 \cdot s_i \cdot s / Z\right]$	$u(x_i)$	$\left\{\left[\left((Hc)_G^o\right)_I / (Hc)_G\right] + \left[2 \cdot s_i \cdot s / Z\right]\right\} \cdot u(x_i)$	{column 6 value}^{2} × 10^8
methane	1,022 968 9	0,004 386 0	1,027 354 9	0,000 350	0,000 359 574	12,929 362
ethane	1,792 496 3	0,009 054 8	1,801 551 1	0,000 243	0,000 437 777	19,164 863
nitrogen	0,000 000 0	0,001 670 6	0,001 670 6	0,000 195	0,000 000 326	0,000 011
carbon dioxide	0,000 000 0	0,007 404 0	0,007 404 0	0,000 111	0,000 000 822	0,000 068
water	0,050 959 1	0,025 167 6	0,076 126 7	0,000 162	0,000 012 333	0,015 209
sum						32,109 513

NOTE Assuming correlation matrix $r(x_i,x_j)$ is the same as in D.3.6.

Component	x_i	x_i^2	$u\left(\left((Hc)_G^o\right)_I\right)$	$u^2\left(\left((Hc)_G^o\right)_i\right)$	$x_i^2 \cdot u^2\left(\left((Hc)_G^o\right)_I\right)$	$x_i^2 \cdot u^2\left(\left((Hc)_G^o\right)_I\right) / (Hc)_G^2 \times 10^8$
methane	0,931 819	0,868 286 649	0,190	0,036 10	0,031 345 148	4,127 541
ethane	0,025 618	0,000 656 282	0,510	0,260 10	0,000 170 699	0,022 478
nitrogen	0,010 335	0,000 106 812	0,000	0,000 00	0,000 000 000	0,000 000
carbon dioxide	0,015 391	0,000 236 883	0,000	0,000 00	0,000 000 000	0,000 000
water	0,016 837	0,000 283 485	0,004	0,000 02	0,000 000 005	0,000 001
sum	1,000 000				0,031 515 852	4,150 020

Component	x_i	$u\left(s_i\right)$	$x_i^2 \cdot u^2\left(s_i\right) \times 10^8$	$4 \cdot s^2 \cdot x_i^2 \cdot u^2\left(s_i\right) / Z^2 \times 10^8$
methane	0,931 819	0,000 5	21,707 166	0,212 114
ethane	0,025 618	0,001 1	0,079 410	0,000 776
nitrogen	0,010 335	0,001 0	0,010 681	0,000 104
carbon dioxide	0,015 391	0,002 0	0,094 753	0,000 926
water	0,016 837	0,015 0	6,378 403	0,062 327
sum	1,000 000			0,276 247

from A.1 — $[u(R) / R]^2 = 0{,}000\ 081\ 4 \times 10^{-8}$

from Formula (B.6) — $[u(Hv)_G / (Hv)_G)]^2 = [32{,}109\ 513 + 4{,}150\ 020 + 0{,}276\ 247 + 0{,}000\ 081] \times 10^{-8}$

$= 36{,}535\ 861 \times 10^{-8}$

$u(Hv)_G = [36{,}535\ 861 \times 10^{-8} \times (36{,}874\ 304)^2]^{1/2}$

$= 0{,}022\ 289\ \mathrm{MJ \cdot m^{-3}}$

$U(Hv)_G = 0{,}045\ \mathrm{MJ \cdot m^{-3}}$ (using a coverage factor of $k = 2$ and expressing the result to two significant figures)

D.3.11 Conversion to non-SI units

The results obtained in D.3.5 to D.3.10 for the molar-basis, mass-basis and volume-basis gross calorific values $(Hc)_G$, $(Hm)_G$ and $(Hv)_G$, respectively, may be summarized and properly reported as

$$(Hc)_G = (871{,}4 \pm 1{,}0)\ \text{kJ}\cdot\text{mol}^{-1}$$

$$(Hm)_G = (51{,}294 \pm 0{,}052)\ \text{MJ}\cdot\text{kg}^{-1}$$

$$(Hv)_G = (36{,}874 \pm 0{,}045)\ \text{MJ}\cdot\text{m}^{-3}$$

Conversion of these values to non-SI units is achieved by use of Annex C as follows:

— using Table C.1:

$(Hc)_G = (871{,}4 \pm 1{,}0)\ \text{kJ}\cdot\text{mol}^{-1}$ $= [(871{,}4 \pm 1{,}0)\ /\ 0{,}002\ 326]\ \text{Btu}_{\text{IT}}\cdot\text{lb-mol}^{-1}$

$= (374\ 635 \pm 430)\ \text{Btu}_{\text{IT}}\cdot\text{lb-mol}^{-1}$

— using Table C.2:

$(Hm)_G = (51{,}294 \pm 0{,}052)\ \text{MJ}\cdot\text{kg}^{-1}$ $= [(51{,}294 \pm 0{,}052)\ /\ 0{,}002\ 326]\ \text{Btu}_{\text{IT}}\cdot\text{lb}^{-1}$

$= (22\ 052 \pm 22)\ \text{Btu}_{\text{IT}}\cdot\text{lb}^{-1}$

— using Table C.3:

$(Hv)_G = (36{,}874 \pm 0{,}045)\ \text{MJ}\cdot\text{m}^{-3}$ $= [(36{,}874 \pm 0{,}045)\ /\ 0{,}037\ 258\ 9]\ \text{Btu}_{\text{IT}}\cdot\text{ft}^{-3}$

$= (989{,}7 \pm 1{,}2)\ \text{Btu}_{\text{IT}}\cdot\text{ft}^{-3}$

D.4 Example 3: A more complex mixture of 11 components

D.4.1 General

In this example, calculation results of intermediate steps are not reported, but instead the final results of calculation of a wider range of properties are provided for a more complete 11-component mixture. The properties are calculated in D.4.3, for combustion reference conditions of 15 °C and 101,325 kPa, and metering reference conditions of 15 °C and 101,325 kPa (ISO Standard Reference Conditions), and in D.4.4, for combustion reference conditions of 25 °C and 101,325 kPa, and metering reference conditions of 0 °C and 101,325 kPa. For both sets of reference conditions, the calculations are made first by using the assumption of an identity matrix for mole fraction correlations, and then by using the more rigorous normalization matrix.

D.4.2 Compositional analysis

The mole-fraction analysis report of a natural gas sample provided the following information for the normalized composition (rounded to six decimal places) and associated uncertainties:

Component	x_i	$u(x_i)$
methane	0,922 393	0,000 348
ethane	0,025 358	0,000 247
propane	0,015 190	0,000 149
n-butane	0,000 523	0,000 018
2-methylpropane	0,001 512	0,000 027
n-pentane	0,002 846	0,000 007
2-methylbutane	0,002 832	0,000 009
2,2-dimethylpropane	0,001 015	0,000 004
n-hexane	0,002 865	0,000 008
nitrogen	0,010 230	0,000 195
carbon dioxide	0,015 236	0,000 112
sum	1,000 000	

D.4.3 Properties and uncertainties for ISO standard reference conditions

D.4.3.1 Results from use of an identity matrix for mole fraction correlations

Property	Units	Y	$u(Y)$	$U(Y)$
gross calorific value - volume basis	$\mathrm{MJ{\cdot}m^{-3}}$	39,733 51	0,026 917	0,053 833
(after rounding according to 11.5.2)		39,734		0,054
net calorific value - volume basis	$\mathrm{MJ{\cdot}m^{-3}}$	35,868 11	0,024 757	0,049 515
(after rounding according to 11.5.2)		35,868		0,050
density	$\mathrm{kg{\cdot}m^{-3}}$	0,764 62	0,000 586	0,001 172
(after rounding according to 11.5.2)		0,764 6		0,001 2
relative density		0,623 91	0,000 478	0,000 956
(after rounding according to 11.5.2)		0,623 91		0,000 96
gross Wobbe index	$\mathrm{MJ{\cdot}m^{-3}}$	50,303 18	0,021 588	0,043 177
(after rounding according to 11.5.2)		50,303		0,043
net Wobbe index	$\mathrm{MJ{\cdot}m^{-3}}$	45,409 54	0,020 151	0,040 302
(after rounding according to 11.5.2)		45,410		0,040

D.4.3.2 Results from use of the normalization matrix for mole fraction correlations

Values for the elements $r(x_i,x_j)$ of the mole fraction correlation coefficient (normalization) matrix, calculated according to ISO 14912:2003, 8.5.2.3, Formula (69) and rounded to six decimal places, are given in the following tabulation. Revised estimates for the various property value uncertainties obtained by use of this complete correlation coefficient matrix in place of an identity matrix are shown in the subsequent tabulation. It is clear that, for this typical example, these are, in general, substantially smaller than those given in D.4.3.1.

$r(x_i,x_j)$	CH_4	C_2H_6	C_3H_8	nC_4	iC_4	nC_5	iC_5	$neoC_5$	nC_6	N_2	CO_2
CH_4	1,000 000	−0,657 246	−0,377 458	−0,041 205	−0,056 924	0,099 228	0,061 961	0,064 295	0,080 202	−0,512 347	−0,265 664
C_2H_6	−0,657 246	1,000 000	−0,035 617	−0,007 450	−0,013 720	−0,085 690	−0,063 295	−0,054 908	−0,074 061	−0,030 668	−0,038 371
C_3H_8	−0,377 458	−0,035 617	1,000 000	−0,004 442	−0,007 810	−0,039 877	−0,029 677	−0,025 538	−0,034 574	−0,024 994	−0,023 925
nC_4	−0,041 205	−0,007 450	−0,004 442	1,000 000	−0,000 824	−0,000 592	−0,000 551	−0,000 372	−0,000 567	−0,005 703	−0,003 373
iC_4	−0,056 924	−0,013 720	−0,007 810	−0,000 824	1,000 000	0,002 803	0,001 827	0,001 811	0,002 303	−0,010 740	−0,005 392
nC_5	0,099 228	−0,085 690	−0,039 877	−0,000 592	0,002 803	1,000 000	0,079 557	0,071 180	0,094 670	−0,072 794	−0,014 019
iC_5	0,061 961	−0,063 295	−0,029 677	−0,000 551	0,001 827	0,079 557	1,000 000	0,051 085	0,067 927	−0,053 627	−0,010 845
$neoC_5$	0,064 295	−0,054 908	−0,025 538	−0,000 372	0,001 811	0,071 180	0,051 085	1,000 000	0,060 788	−0,046 653	−0,008 952
nC_6	0,080 202	−0,074 061	−0,034 574	−0,000 567	0,002 303	0,094 670	0,067 927	0,060 788	1,000 000	−0,062 845	−0,012 357
N_2	−0,512 347	−0,030 668	−0,024 994	−0,005 703	−0,010 740	−0,072 794	−0,053 627	−0,046 653	−0,062 845	1,000 000	−0,028 699
CO_2	−0,265 664	−0,038 371	−0,023 925	−0,003 373	−0,005 392	−0,014 019	−0,010 845	−0,008 952	−0,012 357	−0,028 699	1,000 000

Property	Units	Y	$u(Y)$	$U(Y)$
gross calorific value - volume basis	MJ·m^{-3}	39,733 51	0,016 316	0,032 631
(after rounding according to 11.5.2)		39,734		0,033
net calorific value – volume basis	MJ·m^{-3}	35,868 11	0,015 305	0,030 609
(after rounding according to 11.5.2)		35,868		0,031
density	kg·m^{-3}	0,764 62	0,000 277	0,000 554
(after rounding according to 11.5.2)		0,764 62		0,000 55
relative density		0,623 91	0,000 226	0,000 453
(after rounding according to 11.5.2)		0,623 91		0,000 45
gross Wobbe index	MJ·m^{-3}	50,303 18	0,019 823	0,039 646
(after rounding according to 11.5.2)		50,303		0,040
net Wobbe index	MJ·m^{-3}	45,409 54	0,018 498	0,036 996
(after rounding according to 11.5.2)		45,410		0,037

D.4.4 Properties and uncertainties for 25 °C/0 °C reference conditions

D.4.4.1 Results from use of an identity matrix for mole fraction correlations

Property	Units	Y	$u(Y)$	$U(Y)$
gross calorific value - volume basis	MJ·m^{-3}	41,893 60	0,028 425	0,056 850
(after rounding according to 11.5.2)		41,894		0,057
net calorific value - volume basis	MJ·m^{-3}	37,852 28	0,026 164	0,052 327
(after rounding according to 11.5.2)		37,852		0,052
density	kg·m^{-3}	0,807 01	0,000 619	0,001 238
(after rounding according to 11.5.2)		0,807 0		0,001 2
relative density		0,624 11	0,000 479	0,000 958
(after rounding according to 11.5.2)		0,624 11		0,000 96
gross Wobbe index	MJ·m^{-3}	53,029 30	0,022 783	0,045 566
(after rounding according to 11.5.2)		53,029		0,046
net Wobbe index	MJ·m^{-3}	47,913 76	0,021 278	0,042 557
(after rounding according to 11.5.2)		47,914		0,043

D.4.4.2 Results from use of the normalization matrix for mole fraction correlations

Of course, the change in reference conditions does not affect the mole fraction correlation coefficient (normalization) matrix, which remains unchanged from that presented in D.4.3.2. So too, as the results show, does the conclusion that use of an identity matrix in place of the normalization matrix results in a "safe" (over)estimate of the uncertainty for all properties.

Property	**Units**	Y	$u(Y)$	$U(Y)$
gross calorific value - volume basis	$MJ\cdot m^{-3}$	41,893 60	0,017 241	0,034 483
(after rounding according to 11.5.2)		41,894		0,034
net calorific value – volume basis	$MJ\cdot m^{-3}$	37,852 28	0,016 181	0,032 361
(after rounding according to 11.5.2)		37,852		0,032
density	$kg\cdot m^{-3}$	0,807 01	0,000 293	0,000 586
(after rounding according to 11.5.2)		0,807 01		0,000 59
relative density		0,624 11	0,000 227	0,000 454
(after rounding according to 11.5.2)		0,624 11		0,000 45
gross Wobbe index	$MJ\cdot m^{-3}$	53,029 30	0,020 914	0,041 828
(after rounding according to 11.5.2)		53,029		0,042
net Wobbe index	$MJ\cdot m^{-3}$	47,913 76	0,019 528	0,039 057
(after rounding according to 11.5.2)		47,914		0,039

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