



BSI Standards Publication

Gas analysis — Conversion of gas mixture composition data

National foreword

This British Standard is the UK implementation of EN ISO 14912:2025. It is identical to ISO 14912:2025. It supersedes BS EN ISO 14912:2006, which is withdrawn.

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

A list of organizations represented on this committee can be obtained on request to its committee manager.

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© The British Standards Institution 2025
Published by BSI Standards Limited 2025

ISBN 978 0 539 24465 6

ICS 71.040.40

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This British Standard was published under the authority of the Standards Policy and Strategy Committee on 31 May 2025.

Amendments/corrigenda issued since publication

Date	Text affected
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English Version

Gas analysis - Conversion of gas mixture composition data (ISO 14912:2025)

Analyse des gaz - Conversion des données de
composition de mélanges gazeux (ISO 14912:2025)

Gasanalyse - Umrechnung von
Zusammensetzungsangaben für Gasgemische (ISO
14912:2025)

This European Standard was approved by CEN on 8 May 2025.

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European foreword

This document (EN ISO 14912:2025) has been prepared by Technical Committee ISO/TC 158 "Analysis of gases" in collaboration with Technical Committee CEN/TC 238 "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of an identical text or by endorsement, at the latest by November 2025, and conflicting national standards shall be withdrawn at the latest by November 2025.

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The text of ISO 14912:2025 has been approved by CEN as EN ISO 14912:2025 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 document 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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This document was prepared by Technical Committee ISO/TC 158, *Analysis of gases*, in collaboration with the European Committee for Standardization (CEN) Technical Committee CEN/TC 238, *Test gases, test pressures, appliance categories and gas appliance types*, in accordance with the Agreement on technical cooperation between ISO and CEN (Vienna Agreement).

This second edition cancels and replaces the first edition (ISO 14912:2003 and ISO 14912:2003/Cor.1:2006), which has been technically revised.

The main changes are as follows:

- update of the molar mass data for mixture components in [Annex C](#) according to the 2019 to 2021 IUPAC/CIAAW atomic mass data;
- update of the value of the gas constant according to the 2018 revision of the International System of Units (SI);
- update of the bibliography and the corresponding references in the text;
- update of the information in [Annex E](#) on the computer programme CONVERT;
- correction of [Formulae \(37\)](#) and [\(39\)](#);
- recalculation of the examples in [Annex D](#);
- addition of a table of molar mass data for the relevant elements from which the molar mass data for mixture components were calculated;
- addition of information concerning data for synthetic air;
- editorial corrections.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

The composition of a gas mixture is given by the identity of the mixture components and their content in the mixture. For the purpose of expressing component contents, different quantities are in use, the most common ones being mass concentration, amount fraction and volume fraction. This diversity is due to the fact that in different applications, different quantities have decisive advantages. Therefore, procedures for conversion between different quantities are needed.

As far as these quantities involve volumes, their value depends on the state conditions, i.e., pressure and temperature, of the gas mixture. For these quantities, therefore, procedures for conversion between different state conditions are needed.

As a crude approximation, all of the conversions referred to above can be performed on the basis of the ideal gas law. In most cases, however, an accurate conversion shall take into account the real gas behaviour of the components and of the entire gas mixture. These calculations use values of the compression factor (or the density) of the components concerned and the entire gas mixture.

This document provides conversion procedures which fully account for real gas behaviour of pure gases and gas mixtures. In addition to these, approximate procedures for practical applications are described, designed for different levels of accuracy and available data. These procedures are based on approximate calculations of a) pure gas compression factors using virial coefficients and b) mixture compression factors using component data. Uncertainty estimates are given which account for the uncertainty due to approximations in the conversion procedures and the uncertainty of the input data.

Recently, advanced compression factor calculations for pure gases and gas mixtures, based on multi-parameter equations of state became publicly available (see e.g. NIST Reference Fluid and Transport Properties Database (REFPROP))^[17] and were even standardized (see e.g. ISO 20765-2). Concerning accuracy and uncertainty, these tools clearly outperform the simple approach used in ISO 14912 (truncated virial expansion, linear interpolation of virial coefficient data). However, for the intended use of ISO 14912, the performance is sufficient and the simplicity is beneficial for many users.

Gas analysis — Conversion of gas mixture composition data

1 Scope

This document defines the following quantities commonly used to express the composition of gas mixtures:

- amount fraction and concentration;
- mass fraction and concentration;
- volume fraction and concentration.

For these quantities of composition, this document specifies methods for:

- conversion between different quantities;
- conversion between different state conditions.

Conversion between different quantities means calculating the value of the content of a specified component in terms of one of the quantities listed above from the value of the same content, at the same pressure and temperature of the gas mixture, given in terms of another of these quantities. Conversion between different state conditions means calculating the value of the content of a specified component, in terms of one of the quantities listed above, under one set of state conditions from the value of the same quantity under another set of state conditions, i.e., pressure and temperature, of the gas mixture. Gas mixture composition can be converted simultaneously between different quantities of composition and different state conditions by combination of the two types of conversion.

This document is applicable only to homogeneous and stable gas mixtures. Therefore, any state conditions (pressure and temperature) considered need to be well outside the condensation region of the gas mixture. In addition, volume concentrations can only be used if the component under consideration is completely gaseous, and for the use of volume fractions, all components need to be completely gaseous. Further restrictions of state conditions apply for approximations of compression factors using virial coefficients (see [Annex A](#)).

2 Normative references

There are no normative references in this document.

3 Terms and definitions

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

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

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

NOTE Further information concerning the terms defined in [3.1](#) is given in [5.1](#).

3.1 Quantities for the expression of gas mixture composition

3.1.1

amount fraction

amount-of-substance fraction

x

quotient of the amount of substance of a specified component and the sum of the amounts of substance of all components of a gas mixture

Note 1 to entry: The amount fraction is independent of the pressure and the temperature of the gas mixture.

Note 2 to entry: In [5.1](#), this term is addressed mathematically and further discussed in context.

3.1.2

mass fraction

w

quotient of the mass of a specified component and the sum of the masses of all components of a gas mixture

Note 1 to entry: The mass fraction is independent of the pressure and the temperature of the gas mixture.

Note 2 to entry: In [5.1](#), this term is addressed mathematically and further discussed in context.

3.1.3

volume fraction

φ

quotient of the volume of a specified component and the sum of the volumes of all components of a gas mixture before mixing, all volumes referring to the pressure and the temperature of the gas mixture

Note 1 to entry: The volume fraction is a function of the pressure and the temperature of the gas mixture. Therefore, the pressure and the temperature have to be specified.

Note 2 to entry: The volume fraction can only be used for state conditions where all mixture components are completely gaseous.

Note 3 to entry: The (equivalent) definition in ISO 80000-9 is obtained by expressing the volume of the components as the product of the amount of substance and the molar volume of the components and then dividing the numerator and denominator of the defining quotient by the amount of substance of the gas mixture.

Note 4 to entry: In [5.1](#), this term is addressed mathematically and further discussed in context.

3.1.4

amount concentration

amount-of-substance concentration

c

quotient of the amount of substance of a specified component and the volume of a gas mixture

Note 1 to entry: The amount concentration is a function of the pressure and the temperature of the gas mixture. Therefore, the pressure and the temperature have to be specified.

Note 2 to entry: In [5.1](#), this term is addressed mathematically and further discussed in context.

3.1.5

mass concentration

γ

quotient of the mass of a specified component and the volume of a gas mixture

Note 1 to entry: The mass concentration is a function of the pressure and the temperature of the gas mixture. Therefore, the pressure and the temperature have to be specified.

Note 2 to entry: In [5.1](#), this term is addressed mathematically and further discussed in context.

3.1.6

volume concentration

σ

quotient of the volume of a specified component before mixing and the volume of a gas mixture, both volumes referring to the same pressure and the same temperature

Note 1 to entry: The volume concentration is a function of the pressure and the temperature of the gas mixture. Therefore, the pressure and the temperature have to be specified.

Note 2 to entry: The volume concentration can only be used at state conditions where the specified component is completely gaseous.

Note 3 to entry: The *volume fraction* (3.1.3) and *volume concentration* (3.1.6) take the same value if, at the same state conditions, the sum of the component volumes before mixing and the volume of the mixture are equal. However, because the mixing of two or more gases at the same state conditions is usually accompanied by a slight contraction or, less frequently, a slight expansion, this is not generally the case.

Note 4 to entry: In 5.1, this term is addressed mathematically and further discussed in context.

3.2 Additional quantities involved in conversions of gas mixture composition

3.2.1

compression factor

compressibility factor

Z

quotient of the volume of an arbitrary amount of gas at specified pressure and temperature and the volume of the same amount of an ideal gas at the same state conditions

Note 1 to entry: This definition is applicable to pure gases and to gas mixtures, therefore the term “gas” is used as a general term to be understood to cover pure gases as well as gas mixtures.

Note 2 to entry: By definition, the compression factor of an ideal gas is 1. At room temperature and atmospheric pressure, for many gases the compression factor differs only moderately from 1.

Note 3 to entry: The compression factor is a function of pressure, temperature and the amount fractions of the components.

3.2.2

mixing factor

f

quotient of the volume of an arbitrary amount of a gas mixture at specified pressure and temperature and the sum of the volumes of all mixture components, before mixing, at the same state conditions

Note 1 to entry: If the component volumes are strictly additive, i.e., if the sum of the component volumes before mixing is the same as the volume after mixing, the mixing factor is 1. At room temperature and atmospheric pressure, for many gas mixtures the mixing factor differs only slightly from 1.

3.2.3

density

ρ

quotient of the mass of an arbitrary amount of gas and its volume at specified pressure and temperature

Note 1 to entry: This definition is applicable to pure gases and to gas mixtures, therefore the term “gas” is used as a general term to be understood to cover pure gases and gas mixtures.

3.2.4

molar volume

V_{mol}

quotient of the volume of an arbitrary amount of gas at specified pressure and temperature and its amount of substance

Note 1 to entry: This definition is applicable to pure gases and to gas mixtures, therefore the term “gas” is used as a general term to be understood to cover pure gases and gas mixtures.

Note 2 to entry: The amount of substance of a mixture is given by the sum of the amounts of substance of the components.

Note 3 to entry: In ISO 80000-9 the symbol V_m is used for the molar volume.

Note 4 to entry: In ISO 80000-9 molar volume is restricted to pure substances.

3.2.5

virial coefficients

coefficients in the expansion of the compression factor in terms of powers of a quantity of state

Note 1 to entry: In practice, only two virial expansions are used, where the quantity of state is either the pressure, p , or the inverse molar volume, $1/V_{\text{mol}}$, as given in Formulae (1) and (2).

$$Z(V_{\text{mol}}, T) = 1 + \frac{B(T)}{V_{\text{mol}}} + \frac{C(T)}{V_{\text{mol}}^2} + \dots \quad (1)$$

$$Z(p, T) = 1 + B'(T)p + C'(T)p^2 + \dots \quad (2)$$

3.2.5.1

second molar-volume virial coefficient

B

coefficient of $1/V_{\text{mol}}$ in the expression of the compression factor as a series of inverse powers of the molar volume, V_{mol}

3.2.5.2

third molar-volume virial coefficient

C

coefficient of $1/V_{\text{mol}}^2$ in the expression of the compression factor as a series of inverse powers of the molar volume, V_{mol}

3.2.5.3

second pressure virial coefficient

B'

coefficient of p in the expression of the compression factor as a series of powers of the pressure p

3.2.5.4

third pressure virial coefficient

C'

coefficient of p^2 in the expression of the compression factor as a series of powers of the pressure p

4 Symbols and units

Symbol	Quantity	SI unit
α	$= p/(RT)$	mol/m ³
B	second molar-volume virial coefficient	m ³ /mol
B'	second pressure virial coefficient	1/Pa
γ	mass concentration	kg/m ³
c	amount concentration	mol/m ³
C	third molar-volume virial coefficient	m ⁶ /mol ²
C'	third pressure virial coefficient	1/Pa ²
D	dilution factor	1
f	mixing factor	1
φ	volume fraction	m ³ /m ³
m	mass	kg

Symbol	Quantity	SI unit
M	molar mass	kg/mol
n	amount of substance	mol
N	number of gas mixture components	1
p	pressure	Pa
p_{vap}	saturation vapour pressure	Pa
p_{dew}	dew pressure	Pa
R	gas constant (numerical value 8,314 462 618 153 24)	J/(mol·K)
ρ	density	kg/m ³
σ	volume concentration	m ³ /m ³
t	Celsius temperature	°C
T	thermodynamic temperature	K
V	volume	m ³
V_{mol}	molar volume	m ³ /mol
w	mass fraction	kg/kg
W	mass of a gas cylinder	kg
x	amount fraction	mol/mol
X_{ref}	reference value of state conditions ($X = p, T$)	same as for X
X_{crit}	critical property of a pure gas ($X = p, T, V, Z$)	same as for X
X_{pscrit}	pseudo-critical property of a gas mixture ($X = p, T$)	same as for X
Z	compression factor	1

Symbol	Index
i, j, k	for gas mixture components ($i, j, k = 1, \dots, N$)
S	(sample of) gas mixture

In addition to the symbols specified above, the following symbols are used to denote objects of generic mathematical expressions.

Symbol	Quantity
F	mathematical function expressing a conversion
I	input quantity of composition
O	output quantity of composition
Ω	conversion factor
K, L, P, Q, Y	general variables or quantities
$\partial F / \partial P$	partial derivative (sensitivity coefficient)
$r(P, Q)$	correlation coefficient of quantities P, Q
$\mathbf{R}$	correlation matrix
$u(P)$	standard uncertainty of quantity P
$u^2(P)$	variance of quantity P
$u(P, Q)$	covariance of quantities P, Q
$\mathbf{U}$	variance-covariance matrix
$v(P)$	relative standard uncertainty of quantity P $v(P) = u(P)/ P $

5 Basic Principles

5.1 Expression of gas mixture composition

The generic term for the amount of a component in a mixture is “content”. This term is intended for use only in a purely descriptive or qualitative sense.

Quantitative statements require the expression of content as a value (the product of a number and a unit) of a “quantity of composition”.

For the purposes of this document, six quantities of composition, subdivided into two distinct conceptual families, called fractions and concentrations, are defined in 3.1. The terms “fraction” and “concentration” are themselves incomplete, and shall not be used in quantitative statements of content without further qualification by one of the modifiers “amount”, “mass” or “volume”.

In quantitative expressions of gas mixture composition, the applicable quantity, for example the amount fraction or the mass concentration, shall be used in conjunction with the name or the chemical formula of the component.

EXAMPLE 1 The hydrogen content in a hydrogen/nitrogen mixture, expressed as amount fraction, is $x(\text{H}_2) = 0,1$ mol/mol.

EXAMPLE 2 The sulfur dioxide content in air at 101,325 kPa and 25 °C, expressed as mass concentration, is $\gamma(\text{SO}_2) = 1$ mg/m³.

Gas mixture composition may either relate to the preparation of gas mixtures or to the analysis of gas mixtures. In the first case, the composition expresses the formulation of a prepared mixture. Here the components are the parent gases that were mixed. These can be technically pure gases or specified gas mixtures. In the second case, the composition expresses the results of analysis. Here, the components are the analytes (i.e., the distinct chemical substances typically determined quantitatively) and the matrix (i.e., the complementary gas).

Fractions are often used in the expression of results of gas mixture preparation. If a gas mixture consists of N components, 1, 2, ..., N , and if the amounts of these components in the mixture are quantified by amount of substance, $n_1, n_2, \dots, n_N$, the amount fraction x_i of any component i is given by [Formula \(3\)](#):

$$x_i = \frac{n_i}{\sum_k n_k} \quad (3)$$

If the amounts of the mixture components are quantified by mass, $m_1, m_2, \dots, m_N$, the mass fraction w_i of any component i is given by [Formula \(4\)](#):

$$w_i = \frac{m_i}{\sum_k m_k} \quad (4)$$

If the amounts of the mixture components are quantified by volume, $V_1, V_2, \dots, V_N$, the volume fraction φ_i of any component i is given by [Formula \(5\)](#):

$$\varphi_i = \frac{V_i}{\sum_k V_k} \quad (5)$$

Concentrations are often used to express the results of chemical analysis of a mixture. If the amount of a specified component, i , found in the analysed sample is quantified by amount of substance, n_i , and if V_S is

the sample volume at specified pressure and temperature, the amount concentration (amount-of-substance concentration) c_i is given by [Formula \(6\)](#):

$$c_i = \frac{n_i}{V_S} \quad (6)$$

If the amount of the component is quantified by mass, m_i , the mass concentration γ_i is given by [Formula \(7\)](#):

$$\gamma_i = \frac{m_i}{V_S} \quad (7)$$

If the amount of the component is quantified by volume, V_i , the volume concentration σ_i is given by [Formula \(8\)](#):

$$\sigma_i = \frac{V_i}{V_S} \quad (8)$$

In all the above expressions, it shall be noted that the sample volume depends on pressure and temperature. In the expression for the volume concentration, the volume of the component also depends on pressure and temperature. For both volumes, the state conditions shall be the same.

The quantities of composition exhibit different behaviour concerning the dependence on pressure and temperature, as follows:

- amount concentration and mass concentration depend strongly on state conditions,
- volume fraction and volume concentration depend weakly on state conditions,
- amount fraction and mass fraction are strictly independent of state conditions.

Given the application to homogeneous gas mixtures only (see Scope), the state conditions (pressure and temperature) shall be such that the mixture is completely gaseous. In addition,

- a) the volume concentration is only applicable if the state conditions are such that the individual component under consideration, at those state conditions, is completely gaseous;
- b) the volume fraction is only applicable if the state conditions are such that all components, at those state conditions, are completely gaseous.

The expression “completely gaseous” means one homogeneous gas phase, i.e., for an individual component, that the pressure is well below the saturation vapour pressure at the given temperature or that the temperature is well above the critical temperature. For a mixture, the equivalent condition is that the pressure is well below the dew pressure at the given temperature or that the temperature is well above the cricondentherm. Thus, the state conditions are to be well outside the relevant condensation regions. Methods for assessing whether, at specified state conditions, gas mixtures and their components are completely gaseous are described in [Annex A](#).

NOTE For gas mixtures the applicable term is “cricondentherm”: maximum temperature at which condensation can occur (see ISO 7504).

5.2 Conversion between different quantities

The conversion between different quantities of composition uses the basic relations between the following quantities, which apply both to pure gases and to gas mixtures:

- amount of substance, n ;
- mass, m ;
- volume, V .

The relation between amount of substance and mass is given by [Formula \(9\)](#):

$$n = \frac{m}{M} \quad (9)$$

where M is the molar mass of the gas or gas mixture.

The molar masses of pure gases are calculated from the molar masses of the elements (see [8.1.1](#)). The molar masses of gas mixtures are calculated from the composition and the molar masses of the components (see [8.2.1](#)).

The relation between amount of substance and volume is given by [Formula \(10\)](#), which is the general equation of state for real gases.

$$n = \frac{pV}{ZRT} \quad (10)$$

where

- p is the pressure of the gas or gas mixture;
- T is the temperature of the gas or gas mixture;
- Z is the compression factor of the gas or gas mixture;
- R is the gas constant.

The relation between mass and volume is given by [Formula \(11\)](#):

$$m = \rho V \quad (11)$$

where ρ is the density of the gas or gas mixture.

The three quantities M , Z and ρ can be related by combining [Formulae \(9\)](#), [\(10\)](#) and [\(11\)](#) to give [Formula \(12\)](#):

$$\rho Z = \frac{Mp}{RT} \quad (12)$$

Therefore, only two of these quantities are independent. In this document, the conversion between quantities of composition is based on known values of M and Z .

In addition to the formulas above, conversions between fractions and concentrations require relations between the amount of a gas mixture and the amounts of its components.

If a gas mixture sample S consists of N components, 1, 2, ..., N , the amount of substance n_S of the gas mixture sample is given by the sum of the amounts of substance of the components, as in [Formula \(13\)](#):

$$n_S = \sum_k n_k \quad (13)$$

Analogously, the mass m_S of the gas mixture sample is given by the sum of the component masses, as in [Formula \(14\)](#):

$$m_S = \sum_k m_k \quad (14)$$

While amounts of substance and masses of mixture components are strictly additive, for component volumes additivity is only an approximation (though usually very good). The relation between the volume V_S of the gas mixture sample and the component volumes at identical state conditions is as follows in [Formula \(15\)](#):

$$V_S = f_S \sum_k V_k \quad (15)$$

where f_S is the mixing factor of the gas mixture S .

In the majority of applications, the mixing factor is assumed to be unity (see [8.2.3](#)).

5.3 Conversion between different state conditions

If gas mixture composition is expressed in terms of quantities which depend on pressure and temperature, reference conditions are necessary for comparison purposes. Therefore, procedures for converting any such mixture composition from given state conditions to specified reference conditions are required. The basic relation involved in these conversions is the relation between the volume $V(p, T)$ of a sample of a gas or gas mixture at given state conditions (p, T) and the volume $V(p_{\text{ref}}, T_{\text{ref}})$ of the same sample at specified reference conditions $(p_{\text{ref}}, T_{\text{ref}})$, using [Formula \(16\)](#).

$$\frac{V(p, T)}{V(p_{\text{ref}}, T_{\text{ref}})} = \frac{p_{\text{ref}} T Z(p, T)}{p T_{\text{ref}} Z(p_{\text{ref}}, T_{\text{ref}})} \quad (16)$$

6 Main procedures

6.1 Conversion between different quantities of composition

6.1.1 Conversion of the content of single components

Conversion between different quantities of composition refers to specified state conditions (pressure p , temperature T) of the gas mixture under consideration. Conversion is performed by multiplication with a conversion factor which in most cases is a quotient, composed of one or several quantities of the component i under consideration and the gas mixture S . For example, amount concentrations c_i are converted into mass fractions w_i as follows in [Formula \(17\)](#):

$$w_i = \frac{RTZ_S}{pM_S} M_i c_i \quad (17)$$

where

M_i and M_S are the molar masses of component i and mixture S ;

Z_S is the compression factor of mixture S at the specified state conditions of p and T .

Depending on which two of the three dependent quantities molar mass, M , compression factor, Z , and density, ρ , are selected, the conversion factors can be expressed differently. In this document, conversion factors are

always expressed in terms of M and Z . To utilize density data of pure gases and gas mixtures, these would be converted into compression factor data according to [Formula \(12\)](#).

In [Clause 8](#), the determination of the input quantities required for conversions is addressed.

[Table 1](#) specifies a complete set of conversion factors, expressed in terms of molar masses and compression factors of the component and the mixture under consideration. To obtain a desired quantity, take a given quantity and multiply it by the corresponding factor in [Table 1](#).

Table 1 — Conversion factors between quantities of composition

Desired quantity	Given quantity x_i	Given quantity φ_i	Given quantity w_i	Given quantity c_i	Given quantity σ_i	Given quantity γ_i
x_i	1	$\frac{Z_S}{f_S Z_i}$	$\frac{M_S}{M_i}$	$\frac{Z_S}{\alpha}$	$\frac{Z_S}{Z_i}$	$\frac{Z_S}{\alpha M_i}$
φ_i	$\frac{f_S Z_i}{Z_S}$	1	$\frac{f_S M_S Z_i}{Z_S M_i}$	$\frac{f_S Z_i}{\alpha}$	f_S	$\frac{f_S Z_i}{\alpha M_i}$
w_i	$\frac{M_i}{M_S}$	$\frac{Z_S M_i}{f_S M_S Z_i}$	1	$\frac{Z_S M_i}{\alpha M_S}$	$\frac{Z_S M_i}{M_S Z_i}$	$\frac{Z_S}{\alpha M_S}$
c_i	$\frac{\alpha}{Z_S}$	$\frac{\alpha}{f_S Z_i}$	$\frac{\alpha M_S}{Z_S M_i}$	1	$\frac{\alpha}{Z_i}$	$\frac{1}{M_i}$
σ_i	$\frac{Z_i}{Z_S}$	$\frac{1}{f_S}$	$\frac{M_S Z_i}{Z_S M_i}$	$\frac{Z_i}{\alpha}$	1	$\frac{Z_i}{\alpha M_i}$
γ_i	$\frac{\alpha M_i}{Z_S}$	$\frac{\alpha M_i}{f_S Z_i}$	$\frac{\alpha M_S}{Z_S}$	M_i	$\frac{\alpha M_i}{Z_i}$	1
x_i is the amount fraction of component i φ_i is the volume fraction of component i w_i is the mass fraction of component i c_i is the amount concentration of component i σ_i is the volume concentration of component i γ_i is the mass concentration of component i M_i is the molar mass of component i Z_i is the compression factor of component i M_S is the molar mass of gas mixture S Z_S is the compression factor of gas mixture S f_S is the mixing factor of gas mixture S α is the abbreviation of the quotient $p/(RT)$						
NOTE All quantities refer to the specified state conditions (pressure p , temperature T) of the gas mixture under consideration.						

6.1.2 Conversion of complete compositions

If the composition for a gas mixture is completely known, that is, if the content of all components of the mixture (including the matrix gas) is available, then the conversion factors may be largely reduced to component quantities. This is done by means of summation relations, expressing single or compound mixture quantities as sums over component quantities, for example as follows:

$$\frac{Z_S}{f_S} = \sum_k x_k Z_k \quad (18)$$

and

$$M_S = \sum_k x_k M_k \quad (19)$$

If the task is to convert amount fractions into another quantity of composition, and if the complete molar composition of the gas mixture under consideration is available, then [Formulae \(18\)](#) and [\(19\)](#) may be utilized to express any required conversion factor in terms of component data, i.e., amount fractions x_k , molar masses M_k and compression factors Z_k . As an exception, the mixing factor f_S cannot be expressed in terms of component data alone and has to be estimated separately, for instance by using equations of state.

[Table 2](#) specifies conversion factors, designed for conversion of complete composition data, based on summation relations for mixture quantities. The relevant summation relations are given in [Annex B](#). The given composition shall be specified in terms of fractions, while the desired composition can be expressed in fractions or in concentrations. To obtain a desired quantity, take a given quantity and multiply by the corresponding factor in [Table 2](#).

In principle, this approach is also applicable to conversion of complete compositions expressed in concentrations. However, the application range of such conversions is in practice restricted to specialized cases, since concentrations are normally not used for expressing complete compositions. Therefore, conversions of this kind are not considered in this document. Tables for conversion of concentrations into fractions based on summation relations can be found in DIN 51896-1[21].

Table 2 — Conversion factors between quantities of composition, based on summation relations, using component compression factors

Desired quantity	Given quantity x_i	Given quantity φ_i	Given quantity w_i
x_i	1	$\frac{1 / Z_i}{\sum \varphi_k / Z_k}$	$\frac{1 / M_i}{\sum w_k / M_k}$
φ_i	$\frac{Z_i}{\sum x_k Z_k}$	1	$\frac{Z_i / M_i}{\sum w_k Z_k / M_k}$
w_i	$\frac{M_i}{\sum x_k M_k}$	$\frac{M_i / Z_i}{\sum \varphi_k M_k / Z_k}$	1
c_i	$\frac{\alpha}{f_S \sum x_k Z_k}$	$\frac{\alpha}{f_S Z_i}$	$\frac{\alpha / M_i}{f_S \sum w_k Z_k / M_k}$
σ_i	$\frac{Z_i}{f_S \sum x_k Z_k}$	$\frac{1}{f_S}$	$\frac{Z_i / M_i}{f_S \sum w_k Z_k / M_k}$
γ_i	$\frac{\alpha M_i}{f_S \sum x_k Z_k}$	$\frac{\alpha M_i}{f_S Z_i}$	$\frac{\alpha}{f_S \sum w_k Z_k / M_k}$
$x_i (x_k)$ is the amount fraction of component $i (k)$ $\varphi_i (\varphi_k)$ is the volume fraction of component $i (k)$ $w_i (w_k)$ is the mass fraction of component $i (k)$ c_i is the amount concentration of component i σ_i is the volume concentration of component i γ_i is the mass concentration of component i $M_i (M_k)$ is the molar mass of component $i (k)$ $Z_i (Z_k)$ is the compression factor of component $i (k)$ f_S is the mixing factor of gas mixture S α is the abbreviation of the quotient $p/(RT)$			
NOTE All quantities refer to the specified state conditions (pressure p , temperature T) of the gas mixture under consideration.			

6.2 Conversion to reference conditions

Conversion to reference conditions applies only to volume fractions and to concentrations, as the values of these quantities vary with changes of pressure and temperature (see [5.1](#)).

Conversion of these quantities from given state conditions (p, T) to specified reference conditions ($p_{\text{ref}}, T_{\text{ref}}$) is performed by multiplication with a conversion factor as follows:

$$c_i(p_{\text{ref}}, T_{\text{ref}}) = \frac{p_{\text{ref}} T Z_S(p, T)}{p T_{\text{ref}} Z_S(p_{\text{ref}}, T_{\text{ref}})} c_i(p, T) \quad (20)$$

$$\gamma_i(p_{\text{ref}}, T_{\text{ref}}) = \frac{p_{\text{ref}} T Z_S(p, T)}{p T_{\text{ref}} Z_S(p_{\text{ref}}, T_{\text{ref}})} \gamma_i(p, T) \quad (21)$$

$$\sigma_i(p_{\text{ref}}, T_{\text{ref}}) = \frac{Z_S(p, T) Z_i(p_{\text{ref}}, T_{\text{ref}})}{Z_S(p_{\text{ref}}, T_{\text{ref}}) Z_i(p, T)} \sigma_i(p, T) \quad (22)$$

$$\varphi_i(p_{\text{ref}}, T_{\text{ref}}) = \frac{f_S(p_{\text{ref}}, T_{\text{ref}}) Z_S(p, T) Z_i(p_{\text{ref}}, T_{\text{ref}})}{f_S(p, T) Z_S(p_{\text{ref}}, T_{\text{ref}}) Z_i(p, T)} \varphi_i(p, T) \quad (23)$$

Instead of using [Formulae \(20\) to \(23\)](#), conversion to other state conditions can be performed using amount fractions or mass fractions, taking advantage of their independence of state conditions. For example, amount concentrations at given state conditions can first be converted to amount fractions which then are converted to amount concentrations at different state conditions.

7 Practical implementation

7.1 Conversion between quantities of composition

The factors by which different quantities of composition are mutually interconverted can include data for the component i under consideration (the molar mass M_i , the compression factor Z_i) and data for the entire mixture S (the molar mass M_S , the compression factor Z_S , the mixing factor f_S).

If the component and mixture data are available as required, the application of the factors specified in [6.1.1](#), [Table 1](#) is straightforward. In practice component compression factors will often not be available at the state conditions (pressure p , temperature T) under consideration. In this case, these quantities shall be calculated from available data, using for example virial coefficients (see [8.1](#)).

The main problem, however, is the lack of gas mixture data. With the exception of air, which for practical purposes can be treated like a well-characterized pure gas, neither the molar mass nor the required volumetric properties (compression factor, mixing factor) of the gas mixture will usually be available, and measurement of these data will not be practical. To overcome these problems, this document considers the following two main alternatives.

- a) If the composition of the gas mixture is specified completely by amount fractions, mass fractions or volume fractions, the relevant combinations of mixture property data required for conversion into other quantities of composition can be expressed almost completely by weighted averages of component property data. Using these summation rules, conversion of fractions into other fractions or concentrations can be performed using the conversion factors specified in [Table 2](#). The input required for these conversions is:

- complete mixture composition data;
- relevant component property data;
- an estimate of the mixing factor (only for conversion into concentrations).

These procedures will normally be applied in the case of synthetic mixtures, where the complete composition is available from the mixture preparation formulation. Additional details for conversions of this type are specified in [7.3](#).

Mixture components can be pure gases and specified gas mixtures. For example, as dry air is a well characterized gas with known molar mass and compression factor, a calibration gas mixture of trace levels of SO₂ in dry air is conveniently treated as a 2-component mixture instead of a mixture of SO₂, N₂, O₂, Ar, CO₂ etc.

- b) If the composition of the gas mixture is not specified completely, the strategy for estimating conversion factors depends on the mixture property data involved, the target conversion uncertainty and the