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Coal and coke — Calculation of analyses to different bases

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National foreword

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**Coal and coke — Calculation of
analyses to different bases**

*Charbon et coke — Calculs pour les analyses par rapport à
différentes bases*



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Foreword

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The committee responsible for this document is ISO/TC 27, *Solid mineral fuels*, Subcommittee SC 5, *Methods of analysis*.

This third edition cancels and replaces the second edition (ISO 1170:2008), of which it constitutes a minor revision.

Coal and coke — Calculation of analyses to different bases

1 Scope

This International Standard gives equations that allow analytical data relating to coal and coke to be expressed on the various different bases in common use. Consideration is given to corrections that can be applied to certain determined values for coal prior to their calculation to other bases.

2 Normative references

The following documents, in whole or in part, are normatively referenced in this document and are indispensable for its application. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 602, *Coal — Determination of mineral matter*

ISO 17247, *Coal — Ultimate analysis*

3 Principle

In order to convert an analytical result expressed on one basis to another basis, it is multiplied by a factor calculated from the appropriate formulae (see [Table 1](#)) after insertion of the requisite numerical values.

4 Symbols

The symbols employed in the subsequent clauses are as follows, with suffixes (separated by a dot) “ad” (air-dried), “ar” (as-received), “d” (dry), “daf” (dry, ash-free) or “dmmf” (dry, mineral-matter-free) where appropriate.

w_A	ash, expressed as percent mass fraction
w_C	carbon content, expressed as percent mass fraction
w_{Cl}	chlorine content, expressed as percent mass fraction
$w_{Cl.inorg}$	inorganic chlorine content, expressed as percent mass fraction
w_{CO_2}	carbon dioxide content, expressed as percent mass fraction
w_H	hydrogen content, excluding hydrogen in the moisture, but including the hydrogen from water of hydration in minerals, expressed as percent mass fraction
w_{H_2O}	moisture content, expressed as percent mass fraction
w_h	water of hydration in the mineral matter, expressed as percent mass fraction
w_{MM}	mineral matter content, expressed as percent mass fraction (see Annex A)
w_N	nitrogen content, expressed as percent mass fraction
w_O	oxygen content, excluding oxygen in the moisture but including the oxygen from water of hydration in minerals, expressed as percent mass fraction
$w_{S,o}$	organic sulfur content, expressed as percent mass fraction

$w_{S,p}$	pyritic sulfur content, expressed as percent mass fraction
$w_{S,s}$	sulfate sulfur content, expressed as percent mass fraction
$w_{S,T}$	total sulfur content, expressed as percent mass fraction
w_V	volatile matter content, expressed as percent mass fraction
F_{Cl}	national correction factor for the estimation of the inorganic chlorine content
F_h	national correction factor for the estimation of water of hydration
F_{MM}	national correction factor for the estimation of the mineral matter (see Annex A)

5 Calculations for coal analyses

5.1 Introduction

In International Standards covering the analysis of coal, it is generally specified that the determination shall be carried out on an air-dried test sample. However, in making use of these analyses, it is sometimes necessary to express or report the results on some other basis. The bases in common use are “air-dried”, “as-received”, “dry”, “dry, ash-free”, and “dry, mineral-matter-free”.

5.2 Procedure

Any analytical value (except net calorific value) on a particular basis may be converted to any other basis by multiplying it by the appropriate factor calculated from the formulae given in Table 1, after insertion of the requisite numerical values for the symbols (for determination of moisture, see ISO 589 and ISO 11722; for ash, see ISO 1171). However, in some determinations, there is a direct involvement of the mineral matter and, in these cases, it is essential to apply a correction to the air-dried result prior to its calculation to the dry, mineral-matter-free basis. This correction is dependent on the nature, as well as the quantity, of the mineral matter present and, for any given sample, the formula recommended by the national standards organization of the country of origin of the sample should be used and should be quoted in full, together with the analysis. All the determinations that may be expressed on the dry, mineral-matter-free basis are considered individually below.

If it is necessary to calculate an analytical result expressed on the dry, mineral-matter-free basis back to any other basis, then it is essential that any correction deducted during the application of any Formulae (1) to (10) inclusive be added back to the dry, mineral-matter-free value before applying the appropriate formula from [Table 1](#).

5.3 Carbon

Total carbon, as determined in coal, comprises both organic carbon and carbonate carbon in the mineral matter. It is reported on the air-dried basis (see ISO 609, ISO 625, or ISO 29541). In order to convert the total carbon content as analysed to a dry, mineral-matter-free basis, subtract the carbonate carbon before the conversion as given in Formula (1):

$$w_{C,dmmf} = (w_{C,ad} - 0,273 w_{CO_2,ad}) \times \frac{100}{100 - (w_{H_2O,ad} + w_{MM,ad})} \quad (1)$$

5.4 Hydrogen

The hydrogen content reported on the air-dried basis includes the hydrogen of the coal substance and the hydrogen present (as water) in the mineral matter (see ISO 609, ISO 625 and ISO 29541). The hydrogen present as moisture in the air-dried sample shall be deducted before reporting $w_{H,ad}$. Before calculating

the hydrogen of the coal substance to a dry, mineral-matter-free basis, it is also necessary to deduct the hydrogen of the mineral matter as given in Formula (2):

$$w_{\text{H.dmmf}} = (w_{\text{H.ad}} - \frac{w_{\text{h.ad}}}{9}) \times \frac{100}{100 - (w_{\text{H}_2\text{O.ad}} + w_{\text{MM.ad}})} \quad (2)$$

Since the water of hydration in the mineral matter cannot readily be determined, it is generally estimated from a knowledge of the minerals likely to be present and the total mineral matter content as given in Formula (3):

$$w_{\text{h.ad}} = F_{\text{h}} \times w_{\text{A.ad}} \quad (3)$$

where F_{h} is a national factor, depending of the actual type of coal. If no national factor is available, a value of F_{h} equal to 0,1 may be used to achieve an approximate result.

5.5 Nitrogen

The nitrogen content is reported on the air-dried basis (see ISO 29541). There is no nitrogen in the mineral state normally associated with coal, and the calculation to a dry, mineral-matter-free-basis is as given in Formula (4):

$$w_{\text{N.dmmf}} = w_{\text{N.ad}} \times \frac{100}{100 - (w_{\text{H}_2\text{O.ad}} + w_{\text{MM.ad}})} \quad (4)$$

5.6 Sulfur

The total sulfur content, $w_{\text{S,T}}$, as reported on the air-dried basis (see ISO 334, ISO 351 or ISO 19579), includes organic sulfur, $w_{\text{S,o}}$, pyritic sulfur, $w_{\text{S,p}}$, and sulfate sulfur, $w_{\text{S,s}}$. The pyritic sulfur and the sulfate sulfur are determined and the organic sulfur is obtained by difference (see ISO 157). In order to convert the total sulfur content to a dry, mineral-matter-free basis, subtract the content of pyritic and sulfate sulfur as given in Formula (5):

$$w_{\text{S,o.dmmf}} = (w_{\text{S,T.ad}} - w_{\text{S,p.ad}} - w_{\text{S,s.ad}}) \times \frac{100}{100 - (w_{\text{H}_2\text{O.ad}} + w_{\text{MM.ad}})} \quad (5)$$

5.7 Oxygen

Although oxygen is a significant component of coal and coke, there has been insufficient demand for its direct determination to justify continuation of an ISO standard.

The oxygen content is calculated by difference on an air-dried basis as given in Formula (6), which is taken from ISO 17247:

$$w_{\text{O.ad}} = 100 - (w_{\text{C.ad}} + w_{\text{H.ad}} + w_{\text{N.ad}} + w_{\text{S,T.ad}} + w_{\text{A.ad}} + w_{\text{H}_2\text{O.ad}}) \quad (6)$$

The calculated "oxygen by difference" includes the oxygen in the coal substance, in the carbonate minerals (as carbon dioxide) and in the water of hydration of the mineral matter.

The oxygen content on a dry, mineral-matter-free basis can be calculated as given in Formula (7):

$$w_{\text{O.dmmf}} = 100 - (w_{\text{C.dmmf}} + w_{\text{H.dmmf}} + w_{\text{N.dmmf}} + w_{\text{S.T.dmmf}}) \quad (7)$$

It is necessary to exercise caution with the estimated result derived for "oxygen by difference" as it incorporates the summation of errors in the results of the other elements.

5.8 Chlorine

The chlorine content is reported on the air-dried basis (see ISO 587) and includes chlorine from the mineral matter and chlorine combined with the coal substance. It is, therefore, necessary to subtract the inorganic chlorine before calculating to the dry, mineral-matter-free basis as given in Formula (8):

$$w_{\text{Cl.dmmf}} = (w_{\text{Cl.ad}} - w_{\text{Cl.inorg.ad}}) \times \frac{100}{100 - (w_{\text{H}_2\text{O.ad}} + w_{\text{MM.ad}})} \quad (8)$$

The content of inorganic chlorine may be calculated using a national factor, F_{Cl} , as given in Formula (9):

$$w_{\text{Cl.inorg.ad}} = F_{\text{Cl}} \times w_{\text{Cl.ad}} \quad (9)$$

For higher rank coal, no chlorine combined with the coal matter has been found.^[1] Therefore, a value $F_{\text{Cl}} = 1$ may be used for these coals.

5.9 Volatile matter

The mineral matter associated with a sample also loses mass under the conditions of the volatile matter determination (see ISO 562), the magnitude of the loss being dependent on both the nature and the quantity of the minerals present.

Correction is, therefore, necessary prior to the calculation of the volatile matter to a dry, mineral-matter-free basis to take account of losses of sulfur, water of hydration, carbon dioxide and chlorine as given in Formula (10):

$$w_{\text{V.dmmf}} = (w_{\text{V.ad}} - w_{\text{CO}_2.\text{ad}} - 0.5 \times w_{\text{S,p.ad}} - w_{\text{h.ad}} - w_{\text{Cl.ad}}) \times \frac{100}{100 - (w_{\text{H}_2\text{O.ad}} + w_{\text{MM.ad}})} \quad (10)$$

The loss of mass from pyritic sulfur during devolatilization is approximately half of the sulfur bound in pyrite.

5.10 Net calorific value

The calculation of the net calorific value is dealt with in detail in ISO 1928, which, however, does not include calculation to a dry, mineral-matter-free basis as this basis is not of importance for net calorific values.

NOTE Net calorific values cannot be converted to any other basis by direct multiplying with the appropriate formulas in [Table 1](#) as net calorific values includes a correction for the heat of vaporization related to the actual moisture content.

6 Calculations for coke analyses

Coke analyses may be expressed on the “air-dried”, “as-received”, “dry” and “dry, ash-free” bases, and these values (except for net calorific value) are calculated by the use of the appropriate formulae given in [Table 1](#), after insertion of requisite numerical values for the symbols (for determination of moisture, see ISO 579 and ISO 687; for ash, see ISO 1171).

It is not proposed at present to recommend the calculation for the conversion of analytical results for coke to a dry, mineral-matter-free basis.

7 Table for calculation to different bases

Table 1 — Formulae for calculation of results to different bases

Basis of value given	Basis of value wanted				
	As analysed (air-dried) (ad)	As received ^a (ar)	Dry (d)	Dry, ash free (daf)	Dry, mineral matter free (dmmf)
As analysed (air-dried) (ad)	—	$\frac{100 - w_{H_2O,ar}}{100 - w_{H_2O,ad}}$	$\frac{100}{100 - w_{H_2O,ad}}$	$\frac{100}{100 - (w_{H_2O,ad} + w_{A,ad})}$	$\frac{100}{100 - (w_{H_2O,ad} + w_{MM,ad})}$
As received (ar)	$\frac{100 - w_{H_2O,ad}}{100 - w_{H_2O,ar}}$	—	$\frac{100}{100 - w_{H_2O,ar}}$	$\frac{100}{100 - (w_{H_2O,ar} + w_{A,ar})}$	$\frac{100}{100 - (w_{H_2O,ar} + w_{MM,ar})}$
Dry (d)	$\frac{100 - w_{H_2O,ad}}{100}$	$\frac{100 - w_{H_2O,ar}}{100}$	—	$\frac{100}{100 - w_{A,d}}$	$\frac{100}{100 - w_{MM,d}}$
Dry, ash-free (daf)	$\frac{100 - (w_{H_2O,ad} + w_{A,ad})}{100}$	$\frac{100 - (w_{H_2O,ar} + w_{A,ar})}{100}$	$\frac{100 - w_{A,d}}{100}$	—	$\frac{100 - w_{A,d}}{100 - w_{MM,d}}$
Dry, mineral-matter-free (dmmf)	$\frac{100 - (w_{H_2O,ad} + w_{MM,ad})}{100}$	$\frac{100 - (w_{H_2O,ar} + w_{MM,ar})}{100}$	$\frac{100 - w_{MM,d}}{100}$	$\frac{100 - w_{MM,d}}{100 - w_{A,d}}$	—

^a Note that the formulae given for calculating results for the “as received” basis may be used to calculate them for any other moisture basis, for example moisture-holding capacity or bed moisture.

Annex A (normative)

Mineral matter

In order to calculate analytical results for coal to a dry, mineral-matter-free basis, it is necessary to know the total amount of mineral matter present. This is normally determined on the air-dried test sample by the method specified in ISO 602. However, occasions can arise when it is expedient to estimate the amount of mineral matter from the ash by the application of equations that take account of the chemical changes occurring during the ashing process. The main changes are

- a) liberation of water of hydration from silicates,
- b) liberation of carbon dioxide from carbonates,
- c) liberation of chlorine from chlorides,
- d) oxidation of pyrites to iron(III) oxide with loss of sulfur,
- e) fixation of sulfur by basic oxides.

Correction values for the last four chemical changes can be calculated with reasonable accuracy from readily determined constituents. However, the correction for the water of hydration in the silicate minerals, which is frequently greater than the sum of the remainder, is normally not very precise nor accurate because the determination is complex and is seldom carried out. Concentrations of the water of hydration ranging from 5 % to 20 % have been reported in various parts of the world, and it is clear that no single equation can find universal approval. The equation can be simple, as given in Formula (A.1):

$$w_{\text{MM.ad}} = F_{\text{MM}} \times w_{\text{A.ad}} \quad (\text{A.1})$$

where F_{MM} is a national factor, depending on the actual type of coal. If no national factor is available, a value of F_{MM} equal to 1,1 may be used to calculate an estimated result.

The national equation may be more complex, i.e. including more variables than the ash, $w_{\text{A.ad}}$.

If it is necessary to use a calculated (instead of a determined) value for mineral matter, then the equation used should be that recommended by the national standards organization in the country of origin of the sample. The equation should be quoted whenever it is used.

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- [1] HUGGINS F.E., & HUFFMAN G.P. Chlorine in coal: an XAFS spectroscopic investigation. *Fuel*. 1995 April, **74** (Issue 4) pp. 556–569
- [2] ISO 157, *Coal — Determination of forms of sulfur*
- [3] ISO 334, *Solid mineral fuels — Determination of total sulfur — Eschka method*
- [4] ISO 351, *Solid mineral fuels — Determination of total sulfur — High temperature combustion method*
- [5] ISO 562, *Hard coal and coke — Determination of volatile matter*
- [6] ISO 579, *Coke — Determination of total moisture*
- [7] ISO 587, *Solid mineral fuels — Determination of chlorine using Eschka mixture*
- [8] ISO 589, *Hard coal — Determination of total moisture*
- [9] ISO 609, *Solid mineral fuels — Determination of carbon and hydrogen — High temperature combustion method*
- [10] ISO 625, *Solid mineral fuels — Determination of carbon and hydrogen — Liebig method*
- [11] ISO 687, *Solid mineral fuels — Coke — Determination of moisture in the general analysis test sample*
- [12] ISO 1171, *Solid mineral fuels — Determination of ash*
- [13] ISO 1928, *Solid mineral fuels — Determination of gross calorific value by the bomb calorimetric method and calculation of net calorific value*
- [14] ISO 11722, *Solid mineral fuels — Hard coal — Determination of moisture in the general analysis test sample by drying in nitrogen*
- [15] ISO 19579, *Solid mineral fuels — Determination of sulfur by IR spectrometry*
- [16] ISO 29541, *Solid mineral fuels — Determination of total carbon, hydrogen and nitrogen content — Instrumental method*

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