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Surface chemical analysis — Data transfer format

Analyse chimique des surfaces — Protocole pour le transfert des données

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Contents

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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.

Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

International Standard ISO 14976 was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee 3, *Data management and treatment.*

Annexes A to D of this International Standard are for information only.

Introduction

In surface analysis many commercial instruments are operated through a computer. This computer is also used for processing the captured data, using routines from a built-in set of options for peak synthesis, peak deconvolution, background subtraction, peak area measurement, quantification in various levels of sophistication, mapping, depth profile presentation, smoothing, differentiation and a host of other functions. However, many analysts wish to process their data on another computer in their own particular way using programs written to their specification and under their full control. They need to encode the data in the data-capture computer into a form suitable for transmission then decode it into the form required in the receiving computer. Manufacturer's data formats all differ and differ again from instrument model to instrument model for any given manufacturer. These formats are not published. A standard format for the transferring of data is required to enhance communication, reduce the number of programs required to effect the encoding and decoding and to reduce the uncertainty of data analysis.

Surface chemical analysis — Data transfer format

1 Scope

This International Standard specifies a Format to transfer data from computer to computer via parallel interfaces or via serial interfaces over direct wire, telephone line, local area network or other communications link. The transferred data is encoded only in those characters that appear on a normal display or printer. The format is suitable for AES, EDX, FABMS, ISS, SIMS, SNMS, UPS, XPS, XRF and similar analytical methods. It covers spectra, elemental maps, depth profiles and sequences of data resulting from a variety of experiments.

2 Description of the format

2.1 General

The design of this Format is presented in Annex A. The Format is described using components of the metalanguage defined in the British Standard - Method of defining syntactic metalanguage, BS 6154:1981[1], the appropriate elements of which are given in 2.2 and 2.3.

In this Format some parameters are relevant only to particular cases of the three items; experiment mode, scan mode or technique, and provision is made for including these parameters only where they are relevant. This conditional inclusion could be expressed in the metalanguage, but only at the expense of a more complicated structure than a simple list. To keep the structure simple these parameters are expressed as optional-sequences, and have the conditions under which each of these optional-sequences is to be included specified in an accompanying bracketed-textual-comment.

2.2 The Components of the metalanguage

The metalanguage comprises a notation for specifying a set of rules for generating a linear sequence of characters. Only characters generated by the rules are to be inserted in the sequence. The sequence may be considered as being a sequence of sub-sequences. A sub-sequence may be represented in the notation by enclosing the given characters within either a pair of APOSTROPHE or a pair of QUOTATION MARK characters. The sub-sequence together with these enclosing characters is called a *terminal-string*.

A terminal-string is one example of a *syntactic-primary*.

A syntactic-primary may be preceded by an integer followed by an ASTERISK to represent a specific number of successive occurrences of the same syntactic-primary. A syntactic-primary, together with a preceding integer and ASTERISK, if present, is called a *syntactic-factor*.

A syntactic-factor may be followed by a MINUS SIGN followed by another syntactic-factor. This sub-sequence is called a *syntactic term*.

A number of syntactic-terms may be given in succession but separated by COMMA characters to represent a sub-sequence generated by applying each of the syntactic-terms in turn. A single syntactic-term or group of syntactic-terms separated by COMMA characters is called a *single-definition*.

A number of single-definitions may be given in succession but separated by VERTICAL LINE characters to represent the generation of a sub-sequence by one and only one of the single-definitions, that is, to represent a list of alternative single-definitions. A single-definition or group of single-definitions separated by VERTICAL LINE characters is called a *definitions-list*.

What is represented by the MINUS SIGN followed by a second syntactic-factor when present in a syntactic-term may now be explained. It is to except from generation by the syntactic-term any sub-sequence that could be generated by the second syntactic-factor. The second syntactic-factor is called a *syntactic-exception*.

A unique name may be assigned to a particular definitions-list. The name may consist of one or more characters. The first character must be a letter. Any subsequent character may be a letter or a digit. Spaces and new lines included in the name are not significant. The name is called a *meta-identifer*.

A meta-identifier is assigned to a definitions-list by giving the meta-identifier followed by an EQUALS SIGN followed by the definitions-list followed by a SEMICOLON. This is called a *syntax-rule*.

One or more syntax-rules together make up the set of rules for generating the linear sequence of characters. The set of rules is called a *syntax*.

A syntactic-primary, which has been introduced as having a terminal-string as an example, may now be defined as consisting of one of the following:

(a) No characters at all, representing no characters being added to the sequence. This is called an *empty-sequence*.

(b) A LEFT BRACKET followed by a definitions-list followed by a RIGHT BRACKET, representing the generation of either an empty-sequence or one sub-sequence represented by the definitions-list. This is called an *optional-sequence*.

(c) A LEFT BRACE followed by a definitions-list followed by a RIGHT BRACE, representing either an empty-sequence or a succession of any number of sub-sequences each of which is a sub-sequence that may be generated by the definitions-list. This is called a *repeated-sequence*.

(d) A LEFT PARENTHESIS followed by a definitions-list followed by a RIGHT PARENTHESIS, representing any sub-sequence generated by the enclosed definitions-list. This is called a *grouped-sequence*.

(e) A meta-identifier, already described, representing any sub-sequence generated by the definitions-list to which it has been assigned in a syntax-rule.

(f) A terminal-string, already described, representing the enclosed sub-sequence.

(g) A QUESTION MARK followed by some text followed by another QUESTION MARK, representing a sub-sequence that is described in the enclosed text in another language because it cannot be represented in the metalanguage itself. This is called a *special-sequence*.

The characters LEFT PARENTHESIS and ASTERISK followed by some text followed by the characters ASTERISK and RIGHT PARENTHESIS is called a *bracketed-textual-comment*. This allows a comment for the benefit of the human reader to be added to a syntax without affecting its meaning. It may be inserted anywhere in a syntax except in a meta-identifier, an integer, a special-sequence or a terminal-string.

With the exception of terminal-strings the layout on the page does not affect the meaning of the syntax.

NOTE 1 The following is a summary of the special symbols of the metalanguage. The first six are given in the order of precedence implied in the description of 2.2 with highest precedence at the top, this order being overridden by the bracket-pairs that follow them.

*			follows an integer specifying the number of occurrences of the following syntactic-primary in a syntactic-factor.
-			precedes a syntactic-exception in a syntactic-term.
,			separates successive syntactic-terms in a single-definition.
|			separates alternative single-definitions in a definitions-list.
=			separates the definitions-list from the meta-identifier being defined in a syntax-rule.
;			terminates a syntax-rule.
'	and	'	or
"	and	"	enclose characters to form a terminal-string, representing the characters as they are generated.
(*	and	*)	enclose a comment to form a bracketed-textual-comment, giving additional information for the human reader.
(	and	)	enclose a definitions-list to form a grouped-sequence, grouping items together in the usual algebraic sense.
{	and	}	enclose a definitions-list to form a repeated-sequence, a syntactic-primary which may occur zero or more times.
[	and	]	enclose a definitions-list to form an optional-sequence, a syntactic-primary which may be omitted or included once.
?	and	?	enclose text to form a special-sequence, a syntactic-primary described in a language other than the metalanguage.

2.3 Additional rules

Some parameters need to be repeated a number of times, the actual number of repeats depending on the value of a parameter that has occurred earlier in the format. There is no provision in the metalanguage for expressing this dependence. In these cases the parameters are expressed as repeated-sequences, and the name of the parameter whose value gives the actual number of repeats is given in an accompanying bracketed-textual-comment.

A real number equal to 1E37 is to be taken as a dummy value indicating that the true value is not known. The only integer values that may not be known are those specifying elements of date or time of day and in these cases the value -1 is used as a dummy value.

NOTE 2 Where meta-identifiers are used inside bracketed-textual-comments they are printed in italics.

NOTE 3 Each meta-identifier in the definitions-lists in the syntax-rules defining *experiment* and *block* corresponds to a simple-variable or array-variable stored in the data-capture computer. When output in the Format each variable or array-element is represented by a sub-sequence ending in a *carriage return* composed of the ASCII characters with denary values 13 and 10, the widely-used CARRIAGE RETURN LINE FEED combination. The sub-sequence forms a normal integer or real-number representation of a stored numerical value or expresses an equivalent stored text string. Each of the meta-identifiers consists of a word or phrase chosen to be unambiguous, and additional explanation of its

meaning is given in a bracketed-textual-comment where necessary. These two syntax-rules have been given first, followed by the remaining syntax-rules in alphabetical order.

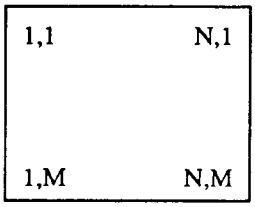
2.4 The format

experiment = format identifier,
institution identifier,
instrument model identifier,
operator identifier,
experiment identifier,
number of lines in comment,
{comment line}
(* The number of occurrences of *comment line* is specified by the value of *number of lines in comment* above.
The comment may include details of the last calibration of the instrument. *),
experiment mode,
scan mode,
[number of spectral regions]
(* Normally only one technique is used in an experiment but there may be more. The value of *number of spectral regions* is the sum for all techniques of the numbers of spectral regions in each technique.
number of spectral regions is inserted if and only if the value of *experiment mode* is 'MAP', 'MAPDP', 'NORM' or 'SDP'. *),
[number of analysis positions,
number of discrete x coordinates available in full map,
number of discrete y coordinates available in full map]
(* The above three entries are inserted if and only if the value of *experiment mode* is either 'MAP' or 'MAPDP'.
Note that if the product of the values of *number of discrete x coordinates available in full map* and *number of discrete y coordinates available in full map* is greater than the value of *number of analysis positions* then some positions in the map are left empty. *),
number of experimental variables
(* An experimental variable is a parameter which may be varied from block to block through the experiment but which remains constant within each block. *),
{experimental variable label,
experimental variable units}
(* The number of occurrences of the above pair of entries is specified by the value of *number of experimental variables* above. *),
'0', carriage return,
number of manually entered items in block,
{prefix number of manually entered item}
(* The number of occurrences of *prefix number of manually entered item* is specified by the value of *number of manually entered items in block* above. If this is greater than zero then the values of successive occurrences of *prefix number of manually entered item* should be in ascending order. Any of the items preceded by prefix numbers in comment brackets in the syntax-rule defining *block* which need to be evaluated by the operator and manually entered from the keyboard should be included in this list. If an item is to be expressed as a real number and the operator is unable to supply a value then the computer should enter the value 1E37. *),
number of future upgrade experiment entries,
number of future upgrade block entries
(* *number of future upgrade experiment entries* and *number of future upgrade block entries* are included in case the Format is upgraded in the future to include more non-optional, non-repeating parameters. The numbers of these new parameters will be entered here so that old programs can skip the new parameters in new data, and new programs will not try to read the new parameters in old data. For the present both of them would be set to zero. *),
{future upgrade experiment entry}
(* The number of occurrences of *future upgrade experiment entry* is given by the value of *number of*

future upgrade experiment entries above. It is defined as a *text line* so that any *integer*, *real number* or *text line* inserted here by a future upgrade of the Format can be read as a *text line* then discarded. *),
number of blocks,
{block} -
(* The minus-sign followed by the empty-sequence, that is, nothing but the separator, indicates that there must be at least one block.
The number of occurrences of *block* is specified by the value of *number of blocks* above. *),
experiment terminator;

block = block identifier,
sample identifier,
(* 1*) [year in full]
(* Gregorian calendar year, for example, '1987' *),
(* 2*) [month],
(* 3*) [day of month],
(* 4*) [hours]
(* 24-hour clock *),
(* 5*) [minutes],
(* 6*) [seconds]
(* If the value of any of the above six items is not known the value -1 should be entered as a dummy value. *),
(* 7*) [number of hours in advance of Greenwich Mean Time],
(* 8*) [number of lines in block comment,
(* 8*) {comment line}]
(* The number of occurrences of *comment line* is specified by the value of *number of lines in block comment* above. *),
(* 9*) [technique],
(*10*) [x coordinate
(* the ordinal number, starting with unity, of the point in the array along the analysis source deflection system x-axis *),
(*10*) y coordinate]
(* the ordinal number, starting with unity, of the point in the array along the analysis source deflection system y-axis.
The above two entries are inserted if and only if the value of *experiment mode* is either 'MAP' or 'MAPDP'.*),
(*11*) {value of experimental variable}
(* *value of experimental variable* may be, for example, total time in seconds, total sputtering time in seconds, total sputtering fluence in ions per m^2, temperature in Kelvin, energy in electron volts or mass in unified atomic mass units. Where this variable changes smoothly with time this value shall be the value at the start of recording the block data unless specified otherwise in the *experimental variable label*.
The number of occurrences of *value of experimental variable* is specified by the value of *number of experimental variables* above, and the order in which the values are given is the same as the order in which *experimental variable label* and *experimental variable units* are declared above. *),
(*12*) [analysis source label],
(*13*) [sputtering ion or atom atomic number,
(*13*) number of atoms in sputtering ion or atom particle,
(*13*) sputtering ion or atom charge sign and number]
(* The above three entries are inserted if and only if either (1) the value of *experiment mode* is 'MAPDP', 'MAPSVDP', 'SDP' or 'SDPSV', or (2) the value of *technique* is 'FABMS', 'FABMS energy spec', 'ISS', 'SIMS', 'SIMS energy spec', 'SNMS' or 'SNMS energy spec'.*),
(*14*) [analysis source characteristic energy]
(* energy in electron volts *),
(*15*) [analysis source strength]
(* power in watts for XPS and XRF; beam current in nanoamps for AES, EDX, ISS, SIMS and SNMS; beam equivalent for FABMS *),
(*16*) [analysis source beam width x
(* width in micrometres at the sample in the plane perpendicular to the source beam *),
(*16*) analysis source beam width y]
(* width in micrometres at the sample in the plane perpendicular to the source beam*),

(*17*) [field of view x
(* micrometres *),
(*17*) field of view y]
(* micrometres.
The above two entries are inserted if and only if the value of *experiment mode* is 'MAP', 'MAPDP', 'MAPSV', 'MAPSVDP' or 'SEM'. *),
(*18*) [first linescan start x coordinate,
(*18*) first linescan start y coordinate,
(*18*) first linescan finish x coordinate,
(*18*) first linescan finish y coordinate,
(*18*) last linescan finish x coordinate,
(*18*) last linescan finish y coordinate]
(* The above six entries are inserted if and only if the value of *experiment mode* is 'MAPSV', 'MAPSVDP' or 'SEM'.
They are required for specifying the size and shape of the map and for relating the order in the scan sequence to the position on the sample.
In the coordinate system to be used, x-values start at unity at the left-hand side of the frame and increase towards the right-hand side, and y-values start at unity at the top of the frame and increase towards the bottom of the frame, as shown below.



*),
(*19*) [analysis source polar angle of incidence]
(* degrees from upward z-direction, defined by the sample stage *),
(*20*) [analysis source azimuth]
(* degrees clockwise from the y-direction, defined by the sample stage*),
(*21*) [analyser mode],
(*22*) [analyser pass energy or retard ratio or mass resolution]
(* energy in electron volts, mass in amu *),
(*23*) [differential width]
(* electron volts peak-to-peak for sinusoidal modulation or computer differentiation.
differential width is inserted if and only if the value of *technique* is 'AES diff'. *),
(*24*) [magnification of analyser transfer lens],
(*25*) [analyser work function or acceptance energy of atom or ion]
(* positive value for work function in electron volts for AES, ELS, ISS, UPS and XPS. The acceptance energy of an ion is the energy filter pass energy of the mass spectrometer for FABMS, SIMS, and SNMS. *),
(*26*) [target bias]
(* *target bias* is in volts, including the sign. *),
(*27*) [analysis width x
(* The analysis width x is the gated signal width of the source in the x-direction in the plane perpendicular to the beam for FABMS, FABMS energy spec, ISS, SIMS, SIMS energy spec, SNMS and SNMS energy spec, the analyser slit length divided by the magnification of the analyser transfer lens to that slit for AES diff, AES dir, ELS, UPS and XPS, and is the source width in the x-direction for both EDX and XRF.
analysis width x is in micrometres. *),
(*27*) analysis width y]
(* As *analysis width x* but for y. *),
(*28*) [analyser axis take off polar angle
(* degrees from upward z-direction, defined by the sample stage *),

(*28*) analyser axis take off azimuth]
(* degrees clockwise from the y-direction, defined by the sample stage*),
(*29*) [species label]
(* elemental symbol or molecular formula *),
(*30*) [transition or charge state label
(* for example, 'KLL' for AES, '1s' for XPS, '-1' for SIMS *),
(*30*) charge of detected particle]
(* for example, -1 for AES and XPS, +1 for positive SIMS *),
(*31*) [abscissa label,
(*31*) abscissa units,
(*31*) abscissa start,
(*31*) abscissa increment]
(* The above four entries are inserted if and only if the value of *scan mode* is 'REGULAR'.*),
(*32*) [number of corresponding variables
(* If the data is in the form of sets of corresponding values of two or more variables then *number of corresponding variables* is equal to the number of variables, otherwise it is equal to unity. *),
(*32*) {corresponding variable label,
(*32*) corresponding variable units}]
(* The number of occurrences of the above pair of items is specified by the value of *number of corresponding variables* above. *),
(*33*) [signal mode],
(*34*) [signal collection time]
(* time in seconds per scan for each channel or array-point, except for both EDX and XRF where it is the total spectrum collection time *),
(*35*) [number of scans to compile this block],
(*36*) [signal time correction]
(* This is the system dead time, except for EDX and XRF where it is the livetime-corrected acquisition time. In the case of a dead time, a positive value indicates that the count rate should be corrected by dividing by (1 - measured rate x dead time) whereas a negative value indicates a correction by multiplying by (exp(true count rate x dead time)). If the spectra have already been corrected for dead time the value here will be zero and the value of the dead time used will be noted in a comment line or elsewhere.
signal time correction is in seconds. *),
(*37*) [sputtering source energy
(* energy in electron volts *),
(*37*) sputtering source beam current
(* current in nanoamps or equivalent for neutrals *),
(*37*) sputtering source width x
(* width in micrometres at the sample in the plane perpendicular to the sputtering source beam*),
(*37*) sputtering source width y
(* width in micrometres at the sample in the plane perpendicular to the sputtering source beam*),
(*37*) sputtering source polar angle of incidence
(* degrees from upward z-direction, defined by the sample stage *),
(*37*) sputtering source azimuth
(* degrees clockwise from the y-direction, defined by the sample stage*),
(*37*) sputtering mode]
(* The value of *sputtering mode* is either 'continuous', when sputtering continues while spectral data is being recorded, or 'cyclic', when sputtering is suspended while spectral data is being recorded.
The above seven entries are for a sputtering source used in addition to the analysis source, as in depth profiling, in AES diff, AES dir, EDX, ELS, UPS, XPS or XRF.
The above seven entries are inserted if and only if both (1) the value of *technique* is 'AES diff', 'AES dir', 'EDX', 'ELS', 'UPS', 'XPS' or 'XRF', and (2) the value of *experiment mode* is 'MAPDP', 'MAPSVDP', 'SDP' or 'SDPSV'. *),
(*38*) [sample normal polar angle of tilt
(* degrees from upward z-direction, defined by the sample stage *),
(*38*) sample normal tilt azimuth]
(* degrees clockwise from the y-direction, defined by the sample stage*),

(*39*) [sample rotation angle]
(* degrees clockwise rotation about the sample normal. If this is referenced to a particular direction on the sample this direction would be specified in a comment line at item number 8.*),
(*40*) [number of additional numerical parameters],
(*40*) {additional numerical parameter label,
(*40*) additional numerical parameter units,
(*40*) additional numerical parameter value}
(* The number of occurrences of the above group of three entries is specified by the value of *number of additional numerical parameters* above. *),
{future upgrade block entry}
(* The number of occurrences of *future upgrade block entry* is given by the value of *number of future upgrade block entries* above. It is defined as a *text line* so that any *integer*, *real number* or *text line* inserted at this point by a future upgrade of the Format can be read as a *text line* then discarded. *),
number of ordinate values
(* The value of *number of ordinate values* is equal to product of the value of *number of corresponding variables* and the number of sets of corresponding variables to be transferred.*),
{minimum ordinate value,
maximum ordinate value}
(* The number of occurrences of the above pair of entries is specified by the value of *number of corresponding variables* above. The order in which the pairs of entries appear is the same as the order in which the corresponding values of *corresponding variable label* are given above. *),
{ordinate value} -
(* The number of occurrences of *ordinate value* is specified by the value of *number of ordinate values* above. If the value of *number of corresponding variables* is greater than unity then the data is sent in the form of successive complete sets, each set consisting of an ordinate value for each of the corresponding variables arranged in the same order as that in which each value of *corresponding variable label* is given above.
The minus-sign followed by the empty-sequence indicates that there must be at least one ordinate value. *);
abscissa increment = real number
(* For units see the table under *abscissa start*. *);
abscissa label = text line;
abscissa start = real number;
abscissa units = units
(* The table below shows the usual values of *abscissa units* for values of *technique* and *experiment mode* as a guide but is not mandatory.

experiment mode	units corresponding to technique		
	AES diff, AES dir, EDX, ELS, ISS, UPS, XPS, XRF	FABMS, SIMS, SNMS	FABMS energy spec, SIMS energy spec, SNMS energy spec
MAP MAPDP NORM SDP	'eV'	'u' or 's'	'eV'
SDPSV	's'	's'	

*);
additional numerical parameter label = text line;
additional numerical parameter units = units;
additional numerical parameter value = real number;
analyser axis take off azimuth = real number;
analyser axis take off polar angle = real number;
analyser mode = ('FAT' | 'FRR' | 'constant delta m' | 'constant m/delta m'), carriage return;
analyser pass energy or retard ratio or mass resolution = real number;