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Surface chemical analysis — Data transfer format

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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.

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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.

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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-identifier*.

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 m², 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.

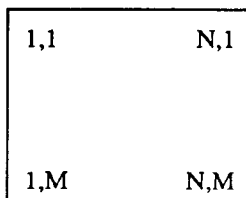
The above two entries are inserted if and only if the value of *experiment mode* is 'MAP', 'MAPDP', 'MAPSV', 'MAPSVDP' or 'SEM'. *),

- (*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 lifetime-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;

analyser work function or acceptance energy of atom or ion = real number;
 analysis source azimuth = real number;
 analysis source beam width x = real number;
 analysis source beam width y = real number;
 analysis source characteristic energy = real number;
 analysis source label = text line;
 analysis source polar angle of incidence = real number;
 analysis source strength = real number;
 analysis width x = real number;
 analysis width y = real number;
 block identifier = text line;
 carriage return = ? 7-bit ASCII character CARRIAGE RETURN followed by 7-bit ASCII character LINE FEED?;
 character =

' '	'!'	'"'	'#'	'\$'	'%'	'&'	'"'	'('	)'	'*'	'+'	'.'	'/'	'0'	'1'	'2'	'3'	'4'	'5'	'6'	'7'	'8'	'9'	':'	','	'<'	'='	'>'	'?'
'@'	'A'	'B'	'C'	'D'	'E'	'F'	'G'	'H'	'I'	'J'	'K'	'L'	'M'	'N'	'O'														
'P'	'Q'	'R'	'S'	'T'	'U'	'V'	'W'	'X'	'Y'	'Z'	'['	'\'	']'	'^'	'_'														
'`'	'a'	'b'	'c'	'd'	'e'	'f'	'g'	'h'	'i'	'j'	'k'	'l'	'm'	'n'	'o'														
'p'	'q'	'r'	's'	't'	'u'	'v'	'w'	'x'	'y'	'z'	'{'	' '	'}'	'~'															

(* A character is the character SPACE or any of the 94 graphic characters specified in the American National Standard for Information Systems - Coded character sets - 7-bit American national standard code for information interchange (7-Bit ASCII), ANSI X3.4-1986. 7-bit ASCII is the American national version of the International Standard - Information processing - ISO 7-bit coded character set for information interchange, ISO 646-1983. Other versions of ISO 646 may substitute different characters for '#', '\$', '@', '[', '\', ']', '^', '_', '{', '|', '}' or '~'.*);

charge of detected particle = integer;

comment line = text line;

corresponding variable label = text line;

corresponding variable units = units;

day of month = integer;

decimal number = [sign], [{digit}, '.'], {digit} -

(* The minus-sign followed by the empty-sequence indicates that there must be at least one digit in *decimal number*.*);

differential width = real number;

digit = '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7' | '8' | '9';

experiment identifier = text line;

experiment mode = ('MAP' | 'MAPDP' | 'MAPSV' | 'MAPSVDP' | 'NORM' | 'SDP' | 'SDPSV' | 'SEM'),

carriage return

(* The contents of each block in the experiment are indicated by the values of *experiment mode* as follows:

'MAP' A spectrum which refers to a specified point in a regular two-dimensional spatial array.

'MAPDP' A spectrum which refers to a specified point in a regular two-dimensional spatial array and to a specified layer in a depth profile.

'MAPSV' A complete set of single values of a fixed number of variables for every point in a regular two-dimensional spatial array. Note that an x linescan consists of a map with the value of *number of analysis positions* equal to the value of *number of discrete x coordinates available in full map*, that is, the number of discrete y coordinates is unity; in a y linescan the rôles of x and y are reversed.

'MAPSVDP' A complete set of single values of a fixed number of variables for every point in a regular two-dimensional array for one layer in a depth profile. Successive blocks refer to successive layers in the depth profile.

'NORM' Either independent data or data which refers to a specified set of single values of one or more experimental variables; the data may be spectral or non-spectral.

'SDP' A spectrum which refers to a specified layer in a depth profile.

'SDPSV' A complete set of single values of a fixed number of variables for every layer in a depth profile.

'SEM' An electron emission intensity for every point in a regular two-dimensional spatial array.

*);

experiment terminator = 'end of experiment', carriage return;

experimental variable label = text line;
 experimental variable units = units;
 field of view x = real number;
 field of view y = real number;
 first linescan finish x coordinate = integer;
 first linescan finish y coordinate = integer;
 first linescan start x coordinate = integer;
 first linescan start y coordinate = integer;
 format identifier = 'VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4', carriage return;
 future upgrade block entry = text line;
 future upgrade experiment entry = text line;
 hours = integer;
 institution identifier = text line;
 instrument model identifier = text line;
 integer = [sign], {digit} - , carriage return

(* The value of *integer* must be in the range -1E37 to 1E37.

The minus-sign followed by the empty-sequence indicates that there must be at least one digit in *integer*. *);

last linescan finish x coordinate = integer;
 last linescan finish y coordinate = integer;
 magnification of analyser transfer lens = real number;
 maximum ordinate value = real number;
 minimum ordinate value = real number;
 minutes = integer;
 month = integer;
 number of additional numerical parameters = zero or more;
 number of analysis positions = one or more;
 number of atoms in sputtering ion or atom particle = one or more;
 number of blocks = one or more;
 number of corresponding variables = one or more;
 number of discrete x coordinates available in full map = one or more;
 number of discrete y coordinates available in full map = one or more;
 number of experimental variables = zero or more;
 number of future upgrade block entries = zero or more;
 number of future upgrade experiment entries = zero or more;
 number of hours in advance of Greenwich Mean Time = real number;
 number of lines in block comment = zero or more;
 number of lines in comment = zero or more;
 number of manually entered items in block = zero or more;
 number of ordinate values = one or more;
 number of scans to compile this block = one or more;
 number of spectral regions = one or more;
 one or more = integer

(* The value of *one or more* must be greater than zero. *);

operator identifier = text line;
 ordinate value = real number;
 prefix number of manually entered item = one or more;
 real number = decimal number, ['E', [sign], {digit} -], carriage return

(* The value of *real number* must be in the range -1E37 to -1E-37, or zero, or in the range 1E-37 to 1E37.

The minus-sign followed by the empty-sequence indicates that the exponent part, if present, must contain at least one digit. *);

sample identifier = text line;
 sample normal polar angle of tilt = real number;
 sample normal tilt azimuth = real number;
 sample rotation angle = real number;
 scan mode = ('REGULAR' | 'IRREGULAR' | 'MAPPING'), carriage return

(* If the value of *experiment mode* is 'MAPSV', 'MAPSVDP' or 'SEM' then the value of *scan mode* must be

'MAPPING', otherwise if the data is in the form of an abscissa start, an abscissa increment and a number of complete sets of values of one or more experimental variables then the value of *scan mode* is 'REGULAR', otherwise the value of *scan mode* is 'IRREGULAR'. *);

seconds = integer;

sign = '+' | '-';

signal collection time = real number;

signal mode = ('analogue' / 'pulse counting'), carriage return
 (* Analogue signals, while recorded digitally, may be of either sign and have a gain which may be noted in the block comment. Pulse counting signals are integers with values equal to or greater than zero. *);

signal time correction = real number;

species label = text line;

sputtering ion or atom atomic number = one or more;

sputtering ion or atom charge sign and number = integer;

sputtering mode = ('continuous' | 'cyclic'), carriage return;

sputtering source azimuth = real number;

sputtering source beam current = real number;

sputtering source energy = real number;

sputtering source polar angle of incidence = real number;

sputtering source width x = real number;

sputtering source width y = real number;

target bias = real number;

technique = ('AES diff' | 'AES dir' | 'EDX' | 'ELS' | 'FABMS' | 'FABMS energy spec' | 'ISS' | 'SIMS' | 'SIMS energy spec' | 'SNMS' | 'SNMS energy spec' | 'UPS' | 'XPS' | 'XRF'), carriage return;
 (* these techniques are as follows

AES diff	differentiated Auger electron spectroscopy
AES dir	direct Auger electron spectroscopy
EDX	energy dispersive X-ray spectroscopy
ELS	electron energy loss spectroscopy
FABMS	fast atom bombardment mass spectroscopy
ISS	ion scattering spectroscopy
SIMS	secondary ion mass spectroscopy
SNMS	sputtered neutral mass spectroscopy
UPS	ultra-violet photoelectron spectroscopy
XPS	X-ray photoelectron spectroscopy
XRF	X-ray fluorescence spectroscopy

*)

text line = 80*[character], carriage return;

transition or charge state label = text line;

units = ('c/s' | 'd' | 'degree' | 'eV' | 'K' | 'micro C' | 'micro m' | 'm/s' | 'n' | 'nA' | 'ps' | 's' | 'u' | 'V'), carriage return
 (* These values are abbreviations for the units listed below:

'c/s'	counts per second
'd'	dimensionless - just a number, eg, counts per channel
'degree'	angle in degrees
'eV'	electron volts
'K'	Kelvin
'micro C'	microcoulombs
'micro m'	micrometres
'm/s'	metres per second
'n'	not defined here - may be given in a label
'nA'	nanoamps
'ps'	picoseconds
's'	seconds
'u'	unified atomic mass units
'V'	volts

*)

value of experimental variable = real number;

x coordinate = one or more;

y coordinate = one or more;

year in full = integer;

zero or more = integer

(* The value of *zero or more* must be equal to or greater than zero. *);

2.5 Specification of the spectrometer geometry

All angles of the analysis source, the analyser axis, the sputtering source and the sample are defined in figure 1, referred to the fixed orthogonal co-ordinate system of the sample stage x, y and z shift directions. If the sample has no x, y and z stage, the z direction is taken as the upward vertical, the x direction is the direction in the horizontal plane to the operator's right and the y direction is in the same horizontal plane but away from the operator when standing in front of the instrument. The choice of the front may be arbitrary but shall be clearly defined at the time the system geometry is evaluated.

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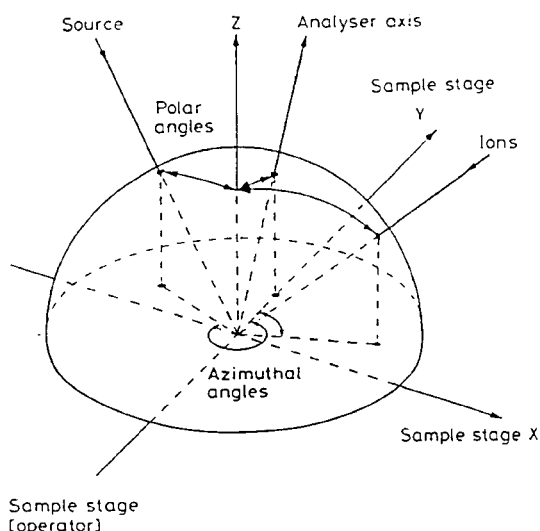


Figure 1 - The relationships of geometrical orientations for specifying angular values.

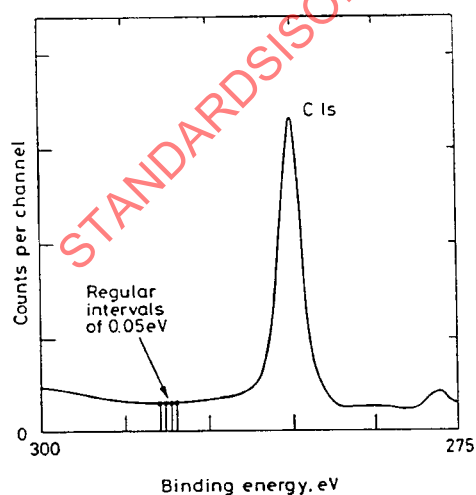


Figure A.1 - An XPS spectrum of one region over 25 eV around the C1s peak. This illustrates the example in B.2.1.

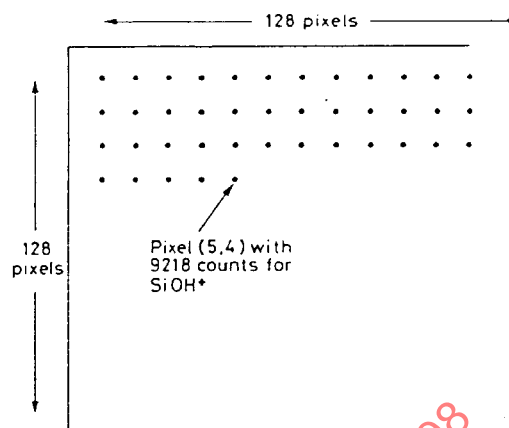


Figure A.2 - A SIMS map of one element setting the mass spectrometer to 45 amu. This illustrates the first block of the example in B.2.3.

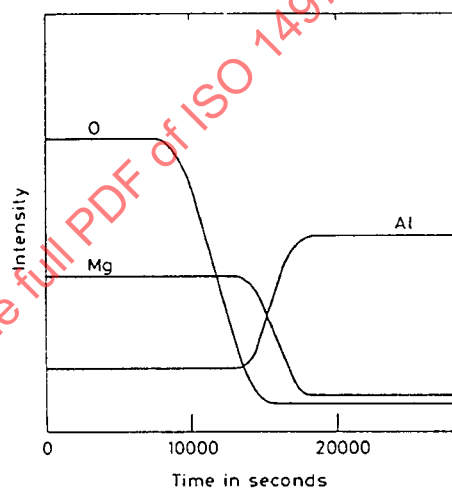


Figure A.3 - An AES cyclic sputter depth profile at one point with differential spectrum single values for each of three elements over 1000 depths lasting eight hours. This illustrates the example in B.2.6.

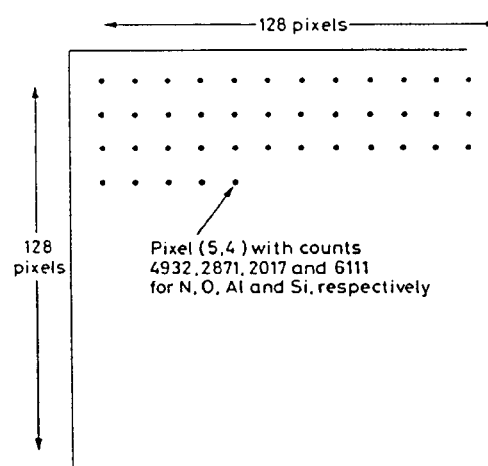


Figure A.4 - An AES map for four elements which may be transferred as one block. The data for the four elements may be transferred sequentially at each point, the counts for the elements being corresponding variables.

Annex A (informative)

Design of the format

Surface analysis provides the scientist with a wide range of techniques and many operating-parameters to vary. Usually the whole of the instrument, not just the spectrometer, is under computer control, allowing all the parameters to be automatically recorded. The complexity of the data-processing required for interpretation makes it essential to keep a complete record, and the transferred data should be equally complete. If all parameters are included in the format then each parameter can be identified by its position and the number of repetitions of a parameter can be indicated explicitly.

It is advantageous to use only those characters that appear on a normal display or printer since there is no difficulty in transferring these by communications protocols and manual checking of the data is possible. This is the principle upon which the design of the present Format is based⁽²⁾.

For data transfer it is envisaged that the procedure would be for the sending computer to write the formatted data to a text-file, for the text-file to be transferred to the receiving computer, and for the receiving computer to convert the data into its own data-structures, as three separate operations. The text-file could be transferred over a communications-link using a standard file-transfer protocol such as KERMIT, XMODEM or local area network protocol, or by writing it to a portable storage medium such as a floppy disk and exchanging the medium between compatible systems. The text-file could also be used as an intermediary between two incompatible programs running on the same computer. File-transfer details such as data-compression or error-checking are not specified in the format since these should be effected by the communications protocol. The present format simply defines the order in which the characters are to be assembled by the data-capture computer for transmission and in which they are expected to be received by the data-receiving computer.

The Format encompasses several kinds of experiment. The simplest experiment is a single spectrum of counts versus some regularly-scanned variable such as energy or mass, and the Format can encode this kind of data as an abscissa start, an abscissa increment and a list of ordinate values. The Format also covers a spectrum in which there is a complete set of single values of a fixed number of variables at each abscissa value. For rare cases in which there is no regularly-scanned variable the Format can encode data consisting of complete sets of corresponding values of two or more variables. These two *scan modes* are called REGULAR and IRREGULAR, respectively. A third scan mode, MAPPING, is used when the data are in the form of a map.

Any of the above types of spectrum can be encoded as a block of data, and provided that all have the same scan mode any number of such spectra can be assembled into a single overall experiment. Each spectrum may be obtained by any of the following *techniques*: AES diff (differentiated Auger electron spectroscopy), AES dir (direct Auger electron spectroscopy), EDX (energy dispersive X-ray spectroscopy), ELS (electron energy loss spectroscopy), FABMS (fast atom bombardment mass spectroscopy), ISS (ion scattering spectroscopy), SIMS (secondary ion mass spectroscopy), SNMS (sputtered neutral mass spectroscopy), UPS (ultra-violet photoelectron spectroscopy), XPS (X-ray photoelectron spectroscopy) and XRF (X-ray fluorescence spectroscopy). In the mass spectroscopies the spectrum is usually a function of mass but may instead be a function of the emitted particle energy at a given mass, and the corresponding techniques are distinguished as FABMS energy spec, SIMS energy spec and SNMS energy spec, respectively.

It is common in a surface analysis experiment for each spectrum to refer to a different point on the sample surface, as in a map, or to a different depth below the sample surface, as in sputter depth profiling. This kind of relationship between the spectra in an experiment is encoded by means of an *experiment mode*. Four of these experiment modes are MAP, SDP, MAPDP, and NORM. In MAP each spectrum refers to a specified point in a regular two-dimensional spatial array. In SDP each spectrum refers to a specified layer in a composition sputter depth profile. In MAPDP each spectrum refers to a specified point in a regular two-dimensional spatial array in a specified layer in a composition sputter depth profile. In NORM each spectrum may be independent of the others, or each spectrum may refer to a specified set of single values of one or more experimental variables such as temperature or time. NORM can also be used for data not in spectral form.

As a result of data-reduction in the data-capture computer, or because of the design of the experiment, instead of having spectra we may have a complete set of single values of a fixed number of variables for every point in a map or depth in a profile. In this case we can encode the map or profile as a single block instead of as a whole experiment. For this we include the four experiment modes MAPSV, SDPSV, SEM and MAPSVDP. In MAPSV each set of values refers to one point in a regular two-dimensional spatial array. In SDPSV each set of values refers to one layer in a composition depth profile. SEM is a map

of electron emission intensities. In MAPSVDP each set of values in a block refers to one point in a regular two-dimensional spatial array, and successive blocks refer to successive layers in a composition sputter depth profile. For a map, the block includes information on how the sets of values are to be arranged in rows and columns.

Very many kinds of experiment are covered by the above options. For instance, a linescan is a restricted case of MAPSV, and a multi-point depth profile with spectra may involve selecting only a few of the possible positions in MAPDP. The Format also covers non-standard applications such as spectrometer intensity/energy response functions and ratio scatter diagrams for AES and EDX.

In many experiments it is important to know the angles of incidence and emission of the various radiations. Here these angles are specified with respect to the fixed orthogonal coordinate system of the sample-stage x, y and z shift directions as shown in figure 1, rather than with respect to a coordinate system established with reference to the sample itself. Although angles referred to the sample itself would be more significant physically, only the fixed reference system is directly available to the data-capture computer. The angles of the sample may be deduced from settings of parameters of the instrument but the converse is not always true. The propagation of errors and the reduction of mistakes are both best effected by the recording of primary data rather than deduced data.

It may help to give the broad outline of the structure of the Format here. What is defined by the Format is an *experiment*. This consists of a set of parameters that apply to the experiment as a whole, followed by a number of *blocks*, followed by an experiment terminator. Each block consists of a set of parameters that apply only to that block, followed by a series of ordinate values representing a curve, spectrum or map. The parameters that apply to the experiment as a whole fall into the following groups in the order in which they appear:

- identity of the experiment in its research environment
- optional comments
- experiment mode
- number of blocks and how they are arranged
- pointers to manually-entered parameters
- future-upgrade parameters.

The parameters that apply to a block fall into the following groups in the order in which they appear:

- identity of the block in the experiment
- identity of the sample
- date and time
- optional comments
- technique
- analysis
- analyser
- spectral-recording
- sputtering
- sample orientation
- additional parameters and future-upgrade parameters

To illustrate the use of the Format a wide range of examples are given in Annex B. To aid the busy programmer who may be provided with no more than a very limited suite of options by his surface analysis instrument Annex C gives selected simple partially-encoded versions of the Format, derived from the Format of Clause 2, which may be used in certain traditional straightforward circumstances. This Format is based on the earlier VAMAS Standard Data Transfer Format⁽²⁾ but has three changes: (i) the spectrometer geometry description is based on a right handed rather than left handed co-ordinate system (ii) the number of entries in the parameter inclusion or exclusion list has been set to zero to simplify the format and (iii) the carriage return sequence has been changed from the single 7 bit ASCII character CARRIAGE RETURN to the two character sequence CARRIAGE RETURN followed by LINE FEED. The latter is the correct "end of line marker" in text files on a range of computer types. To assist programmers to decode this Format, skeleton programs are provided in reference (2). Note, however, that those programs can read and make use of a non-zero number of entries in the parameter inclusion or exclusion list, ie they can read both this and the original VAMAS Format. Additionally, those programs do not, of course, allow for item (iii) above.

Annex B (informative)

Examples of the format

B.1 General

Examples of the Format are given in B.2.1 to B.2.12. The items beginning an experiment, that is, from *format identifier* up to and including the comment lines, and the last item, that is, the experiment terminator, have been omitted in all cases. Similarly, the items beginning the blocks, namely *block identifier*, *number of lines in block comment* and the block comment lines have been omitted. The characters in the transferred text are shown indented, and to save space in printing here, *carriage return* is replaced by COMMA plus SPACE. Examples of items from *institution identifier* to *experiment identifier* could be NPL, VG ESCALAB 2, P J Cumpson, Mass Study; in the block the items *years to number of hours in advance of Greenwich Mean Time* would be 1986, 5, 1, 18, 45,21, 0. These are straightforward and so are not repeated.

B.2 Archetypal applications

Clause B.3 provides a detailed annotation of examples B.2.1 to B.2.4, respectively.

B.2.1 An XPS spectrum of one region over 25 eV around the C 1s peak.

The experiment parameters are as above plus

NORM, REGULAR, 1, 0, 0, 0, 0, 0, 1,

There is one block with parameters as above plus

XPS, Al, 1486.6, 300, 500, 500, 45, 90, FAT, 20, 3, 4.5, 0, 1000, 5000, 15, 0, C, 1s, -1, binding energy, eV, 275, 0.05, 1, counts per channel, d, pulse counting, 0.5, 1, 400E-9, 0, 0, 0, 0, 501, 3214, 33008,

followed by the 501 ordinate values.

B.2.2 An AES depth profile at one point with narrow-scan direct spectra of three elements, the first being oxygen.

The experiment parameters are

SDP, REGULAR, 3, 1, time in seconds, s, 0, 0, 0, 0, 300,

There are 300 blocks. The parameters of the first block are

AES dir, 0, electron gun, 18, 1, 1, 5000, 10, 3, 3, 45, 180, FRR, 4, 3, 4.5, 0, 2000, 5000, 15, 0, O, KLL, -1, kinetic energy, eV, 530, -0.5, 1, counts per channel, d, pulse counting, 0.5, 1, 400E-9, 2000, 120, 500, 500, 20, 270, continuous, 0, 0, 0, 0, 100, 20154, 31192,

followed by the 100 ordinate values.

B.2.3 Two SIMS maps of elements, setting the mass spectrometer to two discrete settings of mass, the first being 45 amu.

The experiment parameters are

MAPSV, MAPPING, 1, unified atomic mass units, u, 0, 0, 0, 0, 2,

There are two blocks. The parameters of the first block are

SIMS, 45, gallium gun, 31, 1, 1, 10000, 1.3, 0.1, 0.1, 12.8, 12.8, 1, 1, 128, 1, 128, 128, 20, 270, constant delta m, 0.9, 1, 4.3, 0, 12.8, 12.8, 0, 180, SiOH, 1, 1, 1, counts per pixel, d, pulse counting, 0.03, 1, 400E-9, 0, 0, 0, 0, 16384, 294, 681,

B.2.4 An AES depth profile of differential spectra of three elements, the first being oxygen, at four points on an integrated circuit.

This is an example where some positions in the map are left empty.

The experiment parameters are

MAPDP, REGULAR, 3, 4, 128, 128, 1, time in seconds, s, 0, 0, 0, 0, 1200,

There are 1200 blocks. The parameters of the first block are

AES diff, 15, 38, 0, electron gun, 18, 1, 1, 5000, 1020, 2, 2, 300, 300, 45, 180, FRR, 4, 5, 3, 4.5, 0, 2000, 5000,

15, 0, O, KLL, -1, kinetic energy, eV, 530, -0.5, 1, counts per channel, d, analogue, 0.5, 1, 400E-9, 2000, 120, 500, 500, 20, 270, cyclic, 0, 0, 0, 0, 100, 381, 4320, followed by the 100 ordinate values.

B.2.5 Five SNMS spectral regions of a stainless steel containing tin as a function of ten oxygen exposures.

The experiment parameters are

NORM, REGULAR, 5, 1, oxygen exposure in seconds, s, 0, 0, 0, 0, 50,

There are 50 blocks. The parameters of the first block are

SNMS, 0, argon, 18, 1, 1, 100, 10000, 3000, 3000, 0, 0, constant delta m, 0.9, 1, 5.1, 0, 1000, 1000, 30, 180, Sn, 0, 0, mass, u, 120.5, -0.1, 1, counts per channel, d, pulse counting, 0.03, 1, 400E-9, 0, 0, 0, 0, 31, 15, 38941,

followed by the 31 ordinate values.

B.2.6 An AES cyclic sputter depth profile at one point with differential spectrum single values for each of three elements over 1000 depths lasting eight hours.

The experiment parameters are

SDPSV, REGULAR, 0, 0, 0, 0, 0, 1,

There is one block with parameters

AES diff, electron gun, 18, 1, 1, 5000, 1020, 100, 100, 45, 180, FRR, 4, 5, 3, 4.5, 0, 1000, 5000, 15, 0, Al Mg O, KLL, -1, time in seconds, s, 0, 28.8, 3, Al intensity, d, Mg intensity, d, O intensity, d, analogue, 3, 1, 400E-9, 2000, 120, 3000, 3000, 20, 270, cyclic, 0, 0, 0, 0, 3000, 381, 4320, 23, 9793, 782, 5640,

followed by the 3000 ordinate values. Alternatively this could have been sent as three blocks corresponding to Al, Mg and O respectively. This would be equally valid.

B.2.7 SIMS Energy spectra 0 to 100 eV of three elements at five positions on an integrated circuit followed over 100 depths in a profile lasting one hour.

The spectral region, 0 to 100 eV, no longer defines the element uniquely so we use the experimental variables to do this.

The experiment parameters are

MAPDP, REGULAR, 1, 5, 128, 128, 2, unified atomic mass units, u, time in seconds, s, 0, 0, 0, 0, 1500,

There are 1500 blocks. The parameters of the first block are

SIMS energy spec, 37, 21, 28, 0, argon, 18, 1, 1, 1000, 100, 0.5, 0.5, 300, 300, 20, 270, constant delta m, 0.9, 1, 2.0, 0, 1E37, 1E37, 0, 0, Si, 1, 1, electron volts, eV, 0, 0.2, 1, counts per channel, d, pulse counting, 0.03, 1, 400E-9, 0, 0, 0, 0, 501, 0, 4927,

followed by the 501 ordinate values.

B.2.8 Combined AES spectra of three elements and one EDX spectrum for a full map as a function of sputtering depth at 100 depths.

The experiment parameters are

MAPDP, REGULAR, 4, 16384, 128, 128, 1, time in seconds, s, 0, 0, 0, 0, 6553600,

There are 6553600 blocks! The parameters of the first block are

AES dir, 1, 1, 0, electron gun, 18, 1, 1, 20000, 25, 0.2, 0.2, 300, 300, 45, 180, FRR, 2, 3, 4, 5, 2000, 5000, 15, 0, O, KLL, -1, electron volts, eV, 520, -1, 1, counts per channel, d, pulse counting, 0.03, 1, 400E-9, 2000, 1020, 3000, 3000, 20, 270, cyclic, 0, 0, 0, 0, 31, 831, 5420,

followed by the 31 ordinate values.

B.2.9 AES x linescan of four elements at peak and background in the direct spectrum mode across an integrated circuit about 2/3 of way down screen.

The experiment parameters are

MAPSV, MAPPING, 1, kinetic energy eV, eV, 0, 0, 0, 0, 8,

There are eight blocks. The parameters of the first block are

AES dir, 530, electron gun, 5000, 10, 0.1, 0.1, 12.8, 12.8, 1, 40, 128, 40, 128, 40, 45, 180, FRR, 2, 3, 4.5, 0, 2000,

5000, 15, 0, 0, KLL, -1, 1, counts per channel, d, pulse counting, 0.01, 1, 400E-9, 0, 0, 0, 0, 128, 3081, 34333, followed by the 128 ordinate values. Alternatively, we could use one block of eight corresponding variables followed by 1024 ordinate values. C.2.6 shows how the corresponding variable approach works.

B.2.10 A correction curve for scaling AES spectra.

The experiment parameters are

NORM, REGULAR, 1, 0, 0, 0, 0, 0, 1,

There is one block with parameters

AES dir, electron gun, 1E37, 1E37, 1E37, 1E37, 1E37, 1E37, FRR, 4, 3, 4.5, 0, 2000, 5000, 15, 0, all elements, any, -1, kinetic energy eV, eV, 0, 0.5, 1, normalising factor, d, pulse counting, 3, 1, 0, 0, 0, 0, 0, 4001, 0, 10000,

followed by the 4001 ordinate values.

B.2.11 A sputter-depth profile following two SIMS intensities, target bias and sputtering-time at irregular intervals.

The experiment parameters are

SDPSV, IRREGULAR, 1, unified atomic mass units, u, 0, 0, 0, 0, 2,

There are two blocks. The parameters of the first block are

SIMS, 11, oxygen, 8, 2, 1, 5000, 900, 500, 500, 20, 270, constant delta m, 0.9, 1, 3, 0, 1E37, 300, 300, 0, 0, boron, 1, 1, 3, counts per channel, d, target bias, V, sputtering time, s, pulse counting, 2, 1, 400E-9, 0, 0, 0, 0, 300, 2, 100517, -2.8, -1.7, 0, 3581,

followed by the 300 ordinate values.

B.2.12 A ratio scatter diagram in AES for 100 analyses of three elements

The experiment parameters are

NORM, IRREGULAR, 0, 0, 0, 0, 0, 0, 1,

There is one block with parameters

AES dir, electron gun, 20000, 10, 0.01, 0.01, 45, 180, FAT, 50, 1, 4.5, 0, 2000, 5000, 15, 0, Al Mg Si, KLL, -1, 3, Al intensity $(N1-N2)/(N1+N2)$, d, Mg intensity $(N1-N2)/(N1+N2)$, d, Si intensity $(N1-N2)/(N1+N2)$, d, pulse counting, 1, 1, 400E-9, 0, 0, 0, 0, 300, 0, 1, 0, 1, 0, 1,

followed by the 300 ordinate values.

B.3 Annotated examples

Dummy headings and some comments have been added, and the *format identifier* has been abbreviated to save space. Particular instrument and identifiers are given in the examples but these have no particular significance beyond illustrating the text of the entry.

B.3.1 Annotation of example in B.2.1

format identifier	VAMAS Surface Chemical <i>etc</i>
institution identifier	NPL
instrument model identifier	Kratos XSAM 800
operator identifier	WAD
experiment identifier	Gold medal contamination
number of lines in comment	1
comment line	example 1
experiment mode	NORM
scan mode	REGULAR
number of spectral regions	1
number of experimental variables	0
	0
number of manually entered items in block	0
number of future upgrade experiment entries	0
number of future upgrade block entries	0

number of blocks	1
block identifier	1st block id
sample identifier	1st sample id
year in full	1986
month	5
day of month	1
hours	18
minutes	45
seconds	21
number of hours in advance of Greenwich Mean Time	0
number of lines in block comment	0
technique	XPS
analysis source label	Al
analysis source characteristic energy	1486.6
analysis source strength	300
analysis source beam width x	500
analysis source beam width y	500
analysis source polar angle of incidence	45
analysis source azimuth	90
analyser mode	FAT
analyser pass energy or retard ratio or mass resolution	20
magnification of analyser transfer lens	3
analyser work function or acceptance energy of atom or ion	4.5
target bias	0
analysis width x	1000
analysis width y	5000
analyser axis take off polar angle	15
analyser axis take off azimuth	0
species label	C
transition or charge state label	1s
charge of detected particle	-1
abscissa label	binding energy
abscissa units	eV
abscissa start	275
abscissa increment	0.05
number of corresponding variables	1
corresponding variable label	counts per channel
corresponding variable units	d
signal mode	pulse counting
signal collection time	0.5
number of scans to compile this block	1
signal time correction	400E-9
sample normal polar angle of tilt	0
sample normal tilt azimuth	0
sample rotation angle	0
number of additional numerical parameters	0
number of ordinate values	501
minimum ordinate value	3214
maximum ordinate value	33008
<i>followed by 501 ordinate values and</i>	
experiment terminator	end of experiment

B.3.2 Annotation of example B.2.2

format identifier	VAMAS Surface Chemical <i>etc</i>
institution identifier	NPL

instrument model identifier	Riber MAC 2
operator identifier	WAD
experiment identifier	Tantalum pentoxide standard
number of lines in comment	1
comment line	example 2
experiment mode	SDP
scan mode	REGULAR
number of spectral regions	3
number of experimental variables	1
experimental variable label	time in seconds
experimental variable units	s
	0
number of manually entered items in block	0
number of future upgrade experiment entries	0
number of future upgrade block entries	0
number of blocks	300
block identifier	1st block id
sample identifier	1st sample id
year in full	1986
month	5
day of month	1
hours	18
minutes	45
seconds	21
number of hours in advance of Greenwich Mean Time	0
number of lines in block comment	0
technique	AES dir
value of experimental variable	0
analysis source label	electron gun
sputtering ion or atom atomic number	18
number of atoms in sputtering ion or atom particle	1
sputtering ion or atom charge sign and number	1
analysis source characteristic energy	5000
analysis source strength	10
analysis source beam width x	3
analysis source beam width y	3
analysis source polar angle of incidence	45
analysis source azimuth	180
analyser mode	FRR
analyser pass energy or retard ratio or mass resolution	4
magnification of analyser transfer lens	3
analyser work function or acceptance energy of atom or ion	4.5
target bias	0
analysis width x	2000
analysis width y	5000
analyser axis take off polar angle	15
analyser axis take off azimuth	0
species label	O
transition or charge state label	KLL
charge of detected particle	-1
abscissa label	kinetic energy
abscissa units	eV
abscissa start	530
abscissa increment	-0.5
number of corresponding variables	1
corresponding variable label	counts per channel

corresponding variable units	d
signal mode	pulse counting
signal collection time	0.5
number of scans to compile this block	1
signal time correction	400E-9
sputtering source energy	2000
sputtering source beam current	120
sputtering source width x	500
sputtering source width y	500
sputtering source polar angle of incidence	20
sputtering source azimuth	270
sputtering mode	continuous
sample normal polar angle of tilt	0
sample normal tilt azimuth	0
sample rotation angle	0
number of additional numerical parameters	0
number of ordinate values	100
minimum ordinate value	20154
maximum ordinate value	31192

*followed by 100 ordinate values, 299 more blocks and
experiment terminator*

end of experiment

B.3.3 Annotation of example B.2.3

format identifier	VAMAS Surface Chemical <i>etc</i>
institution identifier	NPL
instrument model identifier	VG SIMSLAB MIG 300
operator identifier	WAD
experiment identifier	IC 4261
number of lines in comment	1
comment line example	3
experiment mode	MAPSV
scan mode	MAPPING
number of experimental variables	1
experimental variable label	unified atomic mass units
experimental variable units	u
	0
number of manually entered items in block	0
number of future upgrade experiment entries	0
number of future upgrade block entries	0
number of blocks	2
block identifier	1st block id
sample identifier	1st sample id
year in full	1986
month	5
day of month	1
hours	18
minutes	45
seconds	21
number of hours in advance of Greenwich Mean Time	0
number of lines in block comment	0
technique	SIMS
value of experimental variable	45
analysis source label	gallium gun
sputtering ion or atom atomic number	31
number of atoms in sputtering ion or atom particle	1

sputtering ion or atom charge sign and number	1
analysis source characteristic energy	10000
analysis source strength	1.3
analysis source beam width x	0.1
analysis source beam width y	0.1
field of view x	12.8
field of view y	12.8
first linescan start x coordinate	1
first linescan start y coordinate	1
first linescan finish x coordinate	128
first linescan finish y coordinate	1
last linescan finish x coordinate	128
last linescan finish y coordinate	128
analysis source polar angle of incidence	20
analysis source azimuth	270
analyser mode	constant delta m
analyser pass energy or retard ratio or mass resolution	0.9
magnification of analyser transfer lens	1
analyser work function or acceptance energy of atom or ion	4.3
target bias	0
analysis width x	12.8
analysis width y	12.8
analyser axis take off polar angle	0
analyser axis take off azimuth	180
species label	SiOH
transition or charge state label	1
charge of detected particle	1
number of corresponding variables	1
corresponding variable label	counts per pixel
corresponding variable units	d
signal mode	pulse counting
signal collection time	0.03
number of scans to compile this block	1
signal time correction	400E-9
sample normal polar angle of tilt	0
sample normal tilt azimuth	0
sample rotation angle	0
number of additional numerical parameters	0
number of ordinate values	16384
minimum ordinate value	294
maximum ordinate value	681

*followed by 16384 ordinate values, the second block and
experiment terminator*

end of experiment

B.3.4 Annotation of example B.2.4

format identifier	VAMAS Surface Chemical <i>etc</i>
institution identifier	NPL
instrument model identifier	PHI Multiprobe 610
operator identifier	WAD
experiment identifier	IC failure diagnoses
number of lines in comment	1
comment line	example 4
experiment mode	MAPDP
scan mode	REGULAR
number of spectral regions	3

number of analysis positions	4
number of discrete x coordinates available in full map	128
number of discrete y coordinates available in full map	128
number of experimental variables	1
experimental variable label	time in seconds
experimental variable units	s
	0
number of manually entered items in block	0
number of future upgrade experiment entries	0
number of future upgrade block entries	0
number of blocks	1200
block identifier	1st block id
sample identifier	1st sample id
year in full	1986
month	5
day of month	1
hours	18
minutes	45
seconds	21
number of hours in advance of Greenwich Mean Time	0
number of lines in block comment	0
technique	AES diff
x coordinate	15
y coordinate	38
value of experimental variable	0
analysis source label	electron gun
sputtering ion or atom atomic number	18
number of atoms in sputtering ion or atom particle	1
sputtering ion or atom charge sign and number	1
analysis source characteristic energy	5000
analysis source strength	1020
analysis source beam width x	2
analysis source beam width y	2
field of view x	300
field of view y	300
analysis source polar angle of incidence	45
analysis source azimuth	180
analyser mode	FRR
analyser pass energy or retard ratio or mass resolution	4
differential width	5
magnification of analyser transfer lens	3
analyser work function or acceptance energy of atom or ion	4.5
target bias	0
analysis width x	2000
analysis width y	5000
analyser axis take off polar angle	15
analyser axis take off azimuth	0
species label	O
transition or charge state label	KLL
charge of detected particle	-1
abscissa label	kinetic energy
abscissa units	eV
abscissa start	530
abscissa increment	-0.5
number of corresponding variables	1
corresponding variable label	counts per channel

corresponding variable units	d
signal mode	analogue
signal collection time	0.5
number of scans to compile this block	1
signal time correction	400E-9
sputtering source energy	2000
sputtering source beam current	120
sputtering source width x	500
sputtering source width y	500
sputtering source polar angle of incidence	20
sputtering source azimuth	270
sputtering mode	cyclic
sample normal polar angle of tilt	0
sample normal tilt azimuth	0
sample rotation angle	0
number of additional numerical parameters	0
number of ordinate values	100
minimum ordinate value	381
maximum ordinate value	4320

*followed by 100 ordinate values, 1199 more blocks and
experiment terminator*

end of experiment

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Annex C (informative)

Partially encoded versions of the format

C.1 General

A partially-encoded version of the Format may be more appropriate for users whose instruments only provide a limited range of options. In these versions constants replace the variables defining the kind of experiment, and parameters that the Format would automatically omit because of these values are omitted. In C.2 to C.4 are partially-encoded versions for three frequently-used kinds of experiment. It should be stressed that these versions produce exactly the same output as that produced by the Format in Clause 2 for the same kind of experiment; the only difference is in their range of applicability. These versions do not cover manually entered items.

C.2 An experiment involving a number of regularly-scanned spectra or spectral regions for one technique as a function of one experimental variable, the analysis not being at a specifically-addressed point on the sample.

The example from B.2.5 illustrates this.

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. *),
'NORM', carriage return,
'REGULAR', carriage return,
number of spectral regions,
'1', carriage return,
experimental variable label,
experimental variable units,
'0', carriage return,
'0', carriage return,
'0', carriage return,
'0', carriage return,
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,
year in full
(* Gregorian calendar year, for example, '1987' *),
month,
day of month,
hours,
minutes,
seconds
(* If the value of any of the above six items is not known the value -1 should be entered as a dummy value.*),
number of hours in advance of Greenwich Mean Time,

number of lines in block comment,
{comment line}

(* The number of occurrences of *comment line* is specified by the value of *number of lines in block comment* above. *),

technique,

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 m², 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*. *),

analysis source label,

[sputtering ion or atom atomic number,

number of atoms in sputtering ion or atom particle,

sputtering ion or atom charge sign and number]

(* The above three entries are inserted if and only if the value of *technique* is 'FABMS', 'FABMS energy spec', 'SIMS', 'SIMS energy spec', 'SNMS', 'SNMS energy spec' or 'ISS'. *),

analysis source characteristic energy

(* energy in electron volts *),

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 *),

analysis source beam width x

(* width in micrometres at the sample in the plane perpendicular to the source beam *),

analysis source beam width y

(* width in micrometres at the sample in the plane perpendicular to the source beam *),

analysis source polar angle of incidence

(* degrees from upward z-direction, defined by the sample stage *),

analysis source azimuth

(* degrees clockwise from the y-direction, defined by the sample stage*),

analyser mode,

analyser pass energy or retard ratio or mass resolution

(* energy in electron volts, mass in amu *),

[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'. *),

magnification of analyser transfer lens,

analyser work function or acceptance energy of atom or ion

(* positive value for work function in electron volts for AES, XPS, UPS, ELS and ISS. The acceptance energy of an ion is the energy filter pass energy of the mass spectrometer for SIMS, SNMS and FABMS.*),

target bias

(* *target bias* is in volts, including the sign. *),

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. *),

analysis width y

(* As *analysis width x* but for y. *),

analyser axis take off polar angle

(* degrees from upward z-direction, defined by the sample stage *),

analyser axis take off azimuth

(* degrees clockwise from the y-direction, defined by the sample stage*),

species label

(* elemental symbol or molecular formula *),

transition or charge state label

(* for example, 'KLL' for AES, '1s' for XPS, '-1' for SIMS *),
charge of detected particle

(* for example, -1 for AES and XPS, +1 for positive SIMS *),

abscissa label,

abscissa units,

abscissa start,

abscissa increment,

'1', carriage return,

corresponding variable label

(* The corresponding variable will be intensity in this case *),

corresponding variable units,

signal mode,

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 *),

number of scans to compile this block,

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. *),

sample normal polar angle of tilt

(* degrees from upward z-direction, defined by the sample stage *),

sample normal tilt azimuth

(* degrees clockwise from the y-direction, defined by the sample stage*),

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 block comment line. *),

number of additional numerical parameters,

{additional numerical parameter label,

additional numerical parameter units,

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. *),

number of ordinate values,

minimum ordinate value,

maximum ordinate value,

{ordinate value} -

(* The number of occurrences of *ordinate value* is specified by the value of *number of ordinate values* above.*);

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* as a guide but is not mandatory.

technique	units
AES diff, AES dir, EDX, ELS, ISS, UPS, XPS, XRF	'eV'
FABMS, SIMS, SNMS	'u' or 's'
FABMS energy spec, SIMS energy spec, SNMS energy spec	'eV'

*);

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;
 analyser work function or acceptance energy of atom or ion = real number;
 analysis source azimuth = real number;
 analysis source beam width x = real number;
 analysis source beam width y = real number;
 analysis source characteristic energy = real number;
 analysis source label = text line;
 analysis source polar angle of incidence = real number;
 analysis source strength = real number;
 analysis width x = real number;
 analysis width y = real number;
 block identifier = text line;
 carriage return = ? 7-bit ASCII character CARRIAGE RETURN followed by 7-bit ASCII character LINE FEED?;
 character = ' ' | '!' | '"' | '#' | '\$' | '%' | '&' | "'" | '(' | ')' | '*' | '+' | ',' | '-' | '.' | '/'
 | '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7' | '8' | '9' | ':' | ';' | '<' | '=' | '>' | '?'
 | '@' | 'A' | 'B' | 'C' | 'D' | 'E' | 'F' | 'G' | 'H' | 'I' | 'J' | 'K' | 'L' | 'M' | 'N' | 'O'
 | 'P' | 'Q' | 'R' | 'S' | 'T' | 'U' | 'V' | 'W' | 'X' | 'Y' | 'Z' | '[' | ']' | '^' | '_' | '
 | '`' | 'a' | 'b' | 'c' | 'd' | 'e' | 'f' | 'g' | 'h' | 'i' | 'j' | 'k' | 'l' | 'm' | 'n' | 'o'
 | 'p' | 'q' | 'r' | 's' | 't' | 'u' | 'v' | 'w' | 'x' | 'y' | 'z' | '{' | '|' | '}' | '~'
 (* A character is the character SPACE or any of the 94 graphic characters specified in the American National
 Standard for Information Systems - Coded character sets - 7-bit American national standard code for information
 interchange (7-Bit ASCII), ANSI X3.4-1986. 7-bit ASCII is the American national version of the International
 Standard - Information processing - ISO 7-bit coded character set for information interchange, ISO 646-1983.
 Other versions of ISO 646 may substitute different characters for '#', '\$', '@', '[', '\', ']', '^', '~', '{', '|', '}'
 or '~'. *);
 charge of detected particle = integer;
 comment line = text line;
 corresponding variable label = text line;
 corresponding variable units = units;
 day of month = integer;
 decimal number = [sign], [{digit}, '.'], {digit} -
 (* The minus-sign followed by the empty-sequence indicates that there must be at least one digit in decimal
 number.*);
 differential width = real number;
 digit = '0' | '1' | '2' | '3' | '4' | '5' | '6' | '7' | '8' | '9';
 experiment identifier = text line;
 experiment terminator = 'end of experiment', carriage return;
 experimental variable label = text line;
 experimental variable units = units;
 format identifier = 'VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4', carriage return;
 hours = integer;
 institution identifier = text line;
 instrument model identifier = text line;
 integer = [sign], {digit} - , carriage return
 (* The value of integer must be in the range -1E37 to 1E37. *);
 magnification of analyser transfer lens = real number;
 maximum ordinate value = real number;
 minimum ordinate value = real number;
 minutes = integer;
 month = integer;

number of additional numerical parameters = zero or more;
 number of atoms in sputtering ion or atom particle = one or more;
 number of blocks = one or more;
 number of hours in advance of Greenwich Mean Time = real number;
 number of lines in block comment = zero or more;
 number of lines in comment = zero or more;
 number of ordinate values = one or more;
 number of scans to compile this block = one or more;
 number of spectral regions = one or more;
 one or more = integer
 (* The value of *one or more* must be greater than zero. *);
 operator identifier = text line;
 ordinate value = real number;
 real number = decimal number, ['E', [sign], {digit} -], carriage return
 (* The value of *real number* must be in the range -1E37 to -1E-37, or zero, or in the range 1E-37 to 1E37.
 The minus-sign followed by the empty-sequence indicates that the exponent part, if present, must contain at least one digit. *);
 sample identifier = text line;
 sample normal polar angle of tilt = real number;
 sample normal tilt azimuth = real number;
 sample rotation angle = real number;
 seconds = integer;
 sign = '+' | '-';
 signal collection time = real number;
 signal mode = ('analogue' | 'pulse counting'), carriage return
 (* Analogue signals, while recorded digitally, may be of either sign and have a gain which may be noted in the block comment. Pulse counting signals are integers with values equal to or greater than zero. *);
 signal time correction = real number;
 species label = text line;
 sputtering ion or atom atomic number = one or more;
 sputtering ion or atom charge sign and number = integer;
 target bias = real number;
 technique = ('AES diff' | 'AES dir' | 'EDX' | 'ELS' | 'FABMS' | 'FABMS energy spec' | 'ISS' | 'SIMS' | 'SIMS energy spec' | 'SNMS' | 'SNMS energy spec' | 'UPS' | 'XPS' | 'XRF'), carriage return;
 text line = 80*[character], carriage return;
 transition or charge state label = text line;
 units = ('c/s' | 'd' | 'degree' | 'eV' | 'K' | 'micro C' | 'micro m' | 'm/s' | 'n' | 'nA' | 'ps' | 's' | 'u' | 'V'), carriage return
 return
 (* These values are abbreviations for the units listed below:
 'c/s' counts per second
 'd' dimensionless - just a number, eg, counts per channel
 'degree' angle in degrees
 'eV' electron volts
 'K' Kelvin
 'micro C' microcoulombs
 'micro m' micrometres
 'm/s' metres per second
 'n' not defined here - may be given in a label
 'nA' nanoamps
 'ps' picoseconds
 's' seconds
 'u' unified atomic mass units
 'V' volts
 *);
 value of experimental variable = real number;
 year in full = integer;

zero or more = integer

(* The value of *zero or more* must be equal to or greater than zero. *);

C.3 An experiment involving a number of regularly-scanned spectral regions as a function of sputtering as in a sputter depth profile by one technique such as AES or SIMS, the analysis not being at a particularly addressed point on the sample.

The example from B.2.2 illustrates this.

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. *),
'SDP', carriage return,
'REGULAR', carriage return,
number of spectral regions,
'1', carriage return,
'time in seconds', carriage return,
's', carriage return,
'0', carriage return,
'0', carriage return,
'0', carriage return,
'0', carriage return,
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,
year in full
(* Gregorian calendar year, for example, '1987' *),
month,
day of month,
hours,
minutes,
seconds
(* If the value of any of the above six items is not known the value -1 should be entered as a dummy value. *),
number of hours in advance of Greenwich Mean Time,
number of lines in block comment,
{comment line}
(* The number of occurrences of *comment line* is specified by the value of *number of lines in block comment* above. *),
technique,
value of experimental variable
(* *value of experimental variable* may be, for example, total sputtering time in seconds at the start of recording each block *),
analysis source label,

sputtering ion or atom atomic number,
 number of atoms in sputtering ion or atom particle,
 sputtering ion or atom charge sign and number,
 analysis source characteristic energy
 (* energy in electron volts *),
 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 *),
 analysis source beam width x
 (* width in micrometres at the sample in the plane perpendicular to the source beam *),
 analysis source beam width y
 (* width in micrometres at the sample in the plane perpendicular to the source beam *),
 analysis source polar angle of incidence
 (* degrees from upward z-direction, defined by the sample stage *),
 analysis source azimuth
 (* degrees clockwise from the y-direction, defined by the sample stage *),
 analyser mode,
 analyser pass energy or retard ratio or mass resolution
 (* energy in electron volts, mass in amu *),
 [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'. *),
 magnification of analyser transfer lens,
 analyser work function or acceptance energy of atom or ion
 (* positive value for work function in electron volts for AES, XPS, UPS, ELS and ISS. The acceptance energy of an ion is the energy filter pass energy of the mass spectrometer for SIMS, SNMS and FABMS. *),
 target bias
 (* *target bias* is in volts, including the sign. *),
 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. *),
 analysis width y
 (* As *analysis width x* but for y. *),
 analyser axis take off polar angle
 (* degrees from upward z-direction, defined by the sample stage *),
 analyser axis take off azimuth
 (* degrees clockwise from the y-direction towards the operator, defined by the sample stage *),
 species label
 (* elemental symbol or molecular formula *),
 transition or charge state label
 (* for example, 'KLL' for AES, '1s' for XPS, '-1' for SIMS *),
 charge of detected particle
 (* for example, -1 for AES and XPS, +1 for positive SIMS *),
 abscissa label,
 abscissa units,
 abscissa start,
 abscissa increment,
 '1', carriage return,
 corresponding variable label
 (* The corresponding variable will be intensity in this case *),
 corresponding variable units,
 signal mode,
 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 *),
 number of scans to compile this block,
 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 $(1 - \text{measured rate} \times \text{dead time})$ whereas a negative value indicates a correction by multiplying by $\exp(\text{true count rate} \times \text{dead time})$). 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 elsewhere.
signal time correction is in seconds. *),
 [sputtering source energy
 (* energy in electron volts *),
 sputtering source beam current
 (* current in nanoamps or equivalent for neutrals *),
 sputtering source width x
 (* width in micrometres at the sample in the plane perpendicular to the sputtering source beam *),
 sputtering source width y
 (* width in micrometres at the sample in the plane perpendicular to the sputtering source beam *),
 sputtering source polar angle of incidence
 (* degrees from upward z-direction, defined by the sample stage *),
 sputtering source azimuth
 (* degrees clockwise from the y-direction, defined by the sample stage *),
 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 the value of *technique* is 'AES diff', 'AES dir', 'EDX', 'ELS', 'UPS', 'XPS' or 'XRF'. *),
 sample normal polar angle of tilt
 (* degrees from upward z-direction, defined by the sample stage *),
 sample normal tilt azimuth
 (* degrees clockwise from the y-direction towards the operator, defined by the sample stage *),
 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 block comment line. *),
 number of additional numerical parameters,
 {additional numerical parameter label,
 additional numerical parameter units,
 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. *),
 number of ordinate values,
 minimum ordinate value,
 maximum ordinate value,
 {ordinate value} -
 (* The number of occurrences of *ordinate value* is specified by the value of *number of ordinate values* above.*);
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* as a guide but is not mandatory.