A Systematic Representation of Analytical Chemical Actions

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Received July 26, 1992

A representation formalism for analytical method descriptions is presented. Using this formalism, the semantic information of all the participants of a sentence in relation to the main verb is maintained. The logical basis of the representation is given as well as a routine for the graphical presentation.

During the past 20 years various publications appeared on the representation of (analytical) chemical actions. Malissa et al.[1,2] worked out a method using icons (the SSSAC). This method should facilitate a faster access to the fast growing stream of information. The method was not adopted by the analytical chemical community. The representation was criticized by Kateman.[3] His main criticism was that the representation was not complete enough to capture all information of an analytical method description.

In the publications on the development of the TOSAR system (which is part of a system for storage and retrieval of literature information), Fugmann et al.[4] presented a treelike graph. In this representation concepts are nodes which are connected by edges representing the relations between the concepts. The concepts are predominantly constituted by the chemical substances used in, and produced by, certain processes. The relations can be logical relations, such as 'and' and 'or'. The starting materials of a process are written above their products and linked to them by the edges (arcs). They can be labeled with a limited set of reaction-specific functions (participant, nonparticipant, accelerator, and inhibitor). The process itself and the process conditions are written between as nodes linked to the product or as nodes which connect the products. This way, a sequentially ordered representation of the process flow in a document is produced.

Fugmann et al. also stressed the use of graphs for the representation of documents as being "more lucid than natural language text".

A drawback of this representation is that most of the functional information of the chemicals and other circumstances playing a role within the actions is lost. Also, no explicit interpretation of quantifiers and sets of objects and actions is given. A pleasant feature of the representation is that every action leads to some product, a feature which is lost in later representations.

Zamora and Blower[5,6] represented synthesis information in a strict form which, in fact, could contain only one product and one synthesis/reaction step. The participants in the reaction were labeled with 'product', 'reactant', 'medium', 'temperature', 'yield', etc. Other information (on for instance the purification and identification procedures) were omitted.

Ai, Blower, and Ledwith[7] extended the notation to multistep reactions and identified the individual actions that had to be performed in order to obtain the described reaction but still omitted the workup procedures. However, some information will still be lost because all participants in the actions are classified as 'reactant', 'reagent', 'product', 'catalyst', or 'solvent', and the actions are mainly represented as one of five primitive actions (react, combine, prepare, workup, result).

Nishida et al.[8] use case structures to represent actions. The representation sticks closely to the original texts (although certain normalizations are executed). The order of the actions is the order of the presentation/storage of the actions.

As a consequence of current research on the automatic extraction of information from method descriptions[9] and because of current research on the development of a quality and database system for graphite furnace atomic absorption spectrometry, a well-defined format and representation of analytical method information is required which can represent information existing within the written method descriptions and can facilitate reasoning on mass flow during the analysis process. This last requirement will then facilitate the determination of the possible content of the sample solution after the sample preparation, which will enable automatic evaluation of sample preparation methods. A further requirement is that analytical chemists have no trouble understanding it.

REPRESENTATION: THEORY

The information describing an analytical method can be divided into factual and procedural information. Factual information is, for instance, information on the performance characteristics of the method, as well as information on brand, type, and settings of the instruments. Procedural information entails information on all the actions that have to be performed in order to obtain quantitative information on the analyte(s) using the described type of sample. Within the procedural information factual information exists as well. This information concerns the attributes of the objects that play a role in the actions, such as information on the content of solutions, instrumental parameters, etc. Factual information can be stored efficiently in databases in the following format: object–descriptive parameter–value, e.g., spectrometer–type–"single beam", spectrometer–background correction–"deuterium lamp". Within such a representation the type of the link/relation between object and descriptive parameter is (and can be) implicit. The relation can be attributive, has-part, or of a more complex structure. The choice of the descriptive parameter is completely free.

A representative of the procedural information on the other hand should contain clear information about the type of relation between the actions, its participants, and other concepts mentioned in relation to the action, in order to be a good representation of the semantic content of the original text. These relations are called cases or roles, and they are limited in number. We have chosen to represent the preparation procedures of chemicals and the sample preparation procedure,

0095-2338/93/1633-0350$04.00/0

Table I. Specification of the Cases and Their Definitions: (i) = Classified as Input; (o) = Classified as Output

actor	who or what carries out the action (hardly mentioned in analytical method descriptions)
object (i)	that which undergoes the action
applied (i)	the material (chemicals, powder, soil, etc.) that is used in the action; frequently marked with "with"
recipient (i)	the solid or liquid material which is the goal of the material having the object case (e.g., "add ... to a solution", "immerse in a solution")
location goal (i)	the container which is the goal of the material having the object case (e.g. "rinse ... in a flask")
source (i)	the starting material; frequently marked with "from" or with "in" (e.g. "... is prepared from ...", "... is determined in butter")
goal	the goal of the action not covered by the to- or result-case (e.g. "adapt to matrix")
from	describes the initial state of the object concept (as in "a gradient from 100% ..." and "heat from 40 °C to ...")
to	describes the end state of a concept because of the action (e.g. "heat from ... to 85 °C", "dilute to volume", "bleach to a faint ... color")
result (o)	the material being the result of the action; frequently marked with "to" (as in "complex to ...", "convert to ...", "decompose to ...")
instrument	the apparatus, glassware, etc., that is used in the action; frequently marked with "with"
location	the location of the action
means	a description of action by which the main action is performed, frequently marked with "by" (as in "determine by reducing ...")
method	the technique that is used within the action represented by the main verb and mentioned as adverb (e.g. "is titrated potentiometrically")
manner	the way in which the action is performed; frequently given as adverb or marked with "at" or "with" (e.g. "is titrated slowly", "... at a rate of", "add ... with care")
circumstance	the circumstances under which the action is performed; frequently marked with "in the presence of" or "at" plus temperature indication
time	when the action has to be executed
duration	how long the action has to be executed
interval	after which point in time the action has to be repeated continuously (e.g. "daily")
termination	until which time point the action has to be executed
condition	conditional statements frequently marked with "for" (e.g. "the method is sufficiently precise for routine analysis")
purpose	the purpose of undertaking the action; frequently marked with "to" or "for" followed by some verb (e.g. "add ... to stop the etching")
number	how many times the action has to be executed
logic	to indicate negations

Table II. Specification of the Implicit Cases and Their Definitions

input	the input of some (frequently physical) action which cannot be labeled with the as input classified cases of Table I
output	the output of some (frequently physical) action (more than one output is possible)
leaving output	the output that is taken out of (one of) the input stream(s) (useful for the graphical representation)
scheme	a list of action identifiers that comprise the current action
type	to indicate a type relation between some action or process and some previously mentioned and specified action or process (is also used between objects; in that case it frequently directs to a stock solution (description) implying that some portion has to be taken)

by the procedural representation format that is the topic of this paper. The preparation procedures of chemicals include descriptive information about chemicals and solutions. The other information like the performance characteristics of the method and the description of the instrumentation and its settings can be represented as factual information, and they are outside the scope of this article. A large part of this information can also be represented within the procedural format, as will be shown later.

Actions can efficiently be represented by using case structures.[8,9] These structures maintain the functional information between the verbs of a sentence and the other constituents. Actions (analytical) can also be regarded as processes with a certain input and a certain output, similar to chemical reactions.[4] This is evident for actions such as "filtrate", in which the object of the action is the input and in which the output is specified by words like "filtrate" and "residue". But, as this output is frequently not mentioned in direct relation to the verb which represents the action, the output relation is not represented by caselike relations. For other actions like "add" and "heat", the input is marked by cases, but the output is left implicit (and not referred to by linguistic reference resolution). A resulting state of the input is sometimes mentioned, e.g., in "heat the solution to 60 °C".

A specification of case information together with input and output will enable the correct representation of the analytical process for computer-based purposes: how the actions are performed, how they follow each other, and how they are linked to each other. This will facilitate the graphical representation and reasoning about the mass flow of chemicals along the action sequence. The latter will enable evaluation of existing sample preparations for other analytes and techniques, by checking on the existence of possible interferents introduced during the sample preparation. Another application is the development of analytical procedures as recently shown by Zhou et al.[10] This reasoning, however, can only be accurate when background information is used of the verbs which operate on the input. For physical action verbs such as "filtrate", the composition of the output streams can be determined exactly from the composition of the input stream(s); for "add" and "heat", however, this will be more complicated because of possible reactions. This means that for most of the actions chemical knowledge and/or physical–chemical knowledge of possible reactions and other processes are needed in order to determine the composition of the output stream(s). For addition-like actions, Zhou et al. implemented a chemical reaction generator within their analytical director robotic expert system for development and application of robotic analytical procedures. The use of partition coefficients could also be employed on extractions. For the most part, however, analytical method descriptions lack information on the content of, for example, solutions that intermediate two consecutive analytical actions.

The cases that are specified for the analytical chemistry domain are listed in Table I together with their definitions. We have tried to choose names for these cases that represent their meaning as much as possible. The subdivision of the cases is determined by the function of the sentence components

Table III. Specification of the Relations between Nonaction Concepts

attribute	for the representation of attributive relations between object and properties like concentration, valence, weight, etc.
attrib of	the reverse of the attribute relation
obj reverse	the reverse of the 'object' case
number	indicates that some concept is a set of objects and gives its number of elements, each of which conforms to the given description
num value	the numeric value of some attribute
min number	the lower limit of some numeric attribute value
max number	the upper limit of some numeric attribute value
unit	the unit of some attribute having a numeric value (e.g. concentration)
contains	a containment relation describing chemical composition
containment	the reverse 'contains' relation
of	representing a concept that belongs to or is strictly related to another concept as in "the resonance line of Sb"
location	the location of an object
locates	the reverse 'location' relation
link	for the representation of the internal relation between the input and the output streams
type	to indicate a type relation between some object and some previously mentioned and specified object (e.g. to indicate a unique portion of some solution that is used within various actions; the object inherits all attributes of its type)
role	the description of the role or function the object has in the current action; frequently marked with "as" (e.g. "... is added as oxidant")
and	indicates specified members of distributive or collective sets (conjunctions)
or	indicates specified members of disjunctions
element of	indicates that the object is an element of the specified set
element	the reverse 'element of' relation
class	the class of the concept
interpretation	the logical interpretation of some set or concept (e.g. collective, independent)

in relation to the central verb, the meaning of the verb, and the class or type of the sentence component. Influence of the meaning of the verb can be recognized in "...is added to a solution", which is represented by a 'recipient' case, and "...reacts to Fe^{2+}", which is represented by a 'result' case. Subdivision by the class of the sentence component can be recognized in the subdivision between 'source/result' and 'from/to'. This type of subdivision will help in reasoning on the mass flow. The difference between 'means' and 'manner' is motivated by the fact that the former will lead to a clear description of the steps by which a certain process is performed (they are listed under 'scheme', see Table II), whereas the latter will only yield a crude indication (a part of) the instrumental technique that is to be used. The location case can be subdivided, based on the information contained within the prepositions "on", "in", "under", "between", etc. Up to now the type of the location yielded sufficient information (e.g., "waterbath" indicates that it should be "on"; "oven" indicates that it should be "in"). The difference between 'location_goal' and 'recipient' should enable reasoning on the material flow along the actions.

Nominalized verbs (e.g., titration, addition) are represented as verbs. The tense of the verbs is implicitly the imperative mood of method descriptions.

A number of cases in Table I can be classified as input or output of the action. This classification holds for most verbs used in method descriptions. Some verbs like "take" have the value of the object case as output. In order to prevent contradictions in these cases the object-case values are represented by the output case. The other relations mainly give access to information on the conditions within which the action has to be executed.

In Table II, the implicit case like output relations are given, together with some other relations. The identification of the relation 'leaving_output' depends on the verb. It is used for verbs in which (one of) the output(s) is taken out of (one of) the input stream(s), e.g. for "take" ("take the vessel out of the container"). If facilitates a discrimination between various output streams.

Except for these relations, other relations exist between the nonaction concepts present within the sentence. These relations are listed in Table III. The class information is optional; it can be useful for reasoning on the flow of chemicals,

```
Sample preparation:
Milk (0.2 ml) was mixed with aq. 6.25 % La(NO3) (2 ml), and H2O was added to 25
ml.

['sample preparation',
        [id,    [$SAMPLE_PREP1]],
        [object, [$MILK1]],
        [means, [$MIX1]],
        [scheme, [$MIX1,$ADD1]],
        [output, [$SAMPLE_2]]].



[mix,   [id,    [$MIX1]],
        [object, [milk,  [id,    [$MILK1]],
                         [class,  [solution]],
                         [attrib, [volume, [num_value, [0.2]],
                                           [unit,   [ml]]]]]],
        [object, [H2O,   [id,    [$SOL1]],
                         [class,  [solution]],
                         [contains, [LaNO3, [class, [chemical]],
                                            [attrib, [concentration,
                                                      [num_value, [6.25]],
                                                      [unit,   [%]]]]]],
                         [attrib, [volume, [num_value,[2]],
                                           [unit,   [ml]]]]]],
        [output, [$SAMPLE_1, [link, [$MILK1,$SOL1]]]]].

[add,   [id,    [$ADD1]],
        [object, [H2O,   [id,    [$H2O1]],
                         [class,  [solution]]]],

        [recipient, [$SAMPLE_1]],
        [to,    [volume, [id,    [$VOL1]],
                         [num_value, [25]],
                         [unit,   [ml]]]],
        [output, [$SAMPLE_2, [link, [$SAMPLE_1,$H2O1]],
                         [attrib, [$VOL1]]]]].
```

Figure 1. An example using the nested-list representation. The strings starting with $ are the unique identifiers of each concept.

Simultaneous determination of retinol, retinyl palmitate and α-tocopherol in serum or plasma by reversed-phase high-performance liquid chromatography.

```
[determine,
    [output, [collective_set, [id, [$RESULT_2]],
                [and,   [concentration, [attrib_of, [retinol]]]],
                [and,   [concentration, [attrib_of, ['retinyl palmitate']]]],
                [and,   [concentration, [attrib_of, [α-tocopherol]]]]]],
    [source, [disj,  [or,    [serum]],
                [or,    [plasma]],
                [id,    [$SAMPLE_1]]]],
    [method, ['reversed phase HPLC', [id,  [$HPLC_1]]]],
    [means, [$SAMPLE_PREP1]],
    [scheme, [$SAMPLE_PREP1, $FACTUAL_ANAL1]]].
```

Plasma or serum (0.2 ml) was mixed with 0.2 ml of ethanol, containing 500 μg l.minus.1 of retinyl acetate (as internal standard), and 1 ml of hexane, followed by vortex mixing for >30 s and centrifugation to remove pptd. protein.

```
['sample preparation',
    [id,    [$SAMPLE_PREP_1]],
    [object, [disj,  [id,    [$SAMPLE_1]],
                [or,    [serum,
                            [attrib, [volume, [num_value, [0.2]],
                                        [unit,  [ml]]]]]],
                [or,    [plasma,
                            [attrib, [volume, [num_value, [0.2]],
                                        [unit,  [ml]]]]]]]],
    [means, [$MIX_1]],
    [scheme, [$MIX_1, $MIX_2, $CENTRIFUGE_1, $TAKE_1, $EVAPORATE_1, $DISSOLVE_1]],
    [output, [$SAMPLE_7]]].

[mix,   [id,    [$MIX_1]],
    [object, [$SAMPLE_1]],
    [object, [ethanol, [id,    [$SOL_1]],
                [class,  [solution]],
                [contains, ['retinyl acetate', [class, [chemical]],
                            [attrib, [concentration, [num_value, [500]],
                                        [unit,  [mg/l]]]],
                            [role,  ['internal standard']]]],
                [attrib,  [volume, [num_value, [0.2]],
                            [unit,  [ml]]]]],
    [object, [hexane, [id,    [$SOL_2]],
                [class,  [solution]],
                [attrib,  [volume, [num_value, [1]],
                            [unit,  [ml]]]]],
    [output, [$SAMPLE_2, [link, [$SAMPLE_1, $SOL_1, $SOL_2]]]]].

[vortex, [id,    [$MIX_2]],
    [object, [$SAMPLE_2]],
    [duration, [sec,  [min_number, [30]]]],
    [output, [$SAMPLE_3, [link, [$SAMPLE_2]]]]].

[centrifuge, [id, [$CENTRIFUGE_1]],
    [object, [$SAMPLE_3]],
    [purpose, [remove, [object, ['pptd. protein']]]],
    [output, [$SAMPLE_4, [link, [$SAMPLE_3]]]]].

[take,  [id,    [$TAKE_1]],
    [source, [$SAMPLE_4]],
    [leaving_output, ['hexane layer',
                [id,    [$SAMPLE_5]],
                [link,  [$SAMPLE_4]]]]].
```

Figure 2 (continued)

The hexane layer was evaporated, and the residue was dissolved in 0.2 ml of ethanol plus 20 μl of H2O.

```
[evaporate, [id,  [$EVAPORATE_1]],
        [object, [$SAMPLE_5]],
        [output, [residue, [id,    [$SAMPLE_6]],
                        [link,   [$SAMPLE_5]]]]].

[dissolve, [id,   [$DISSOLVE_1]],
        [object, [$SAMPLE_6]],
        [recipient, [mixture,
                        [id,     [$SOL_4]],
                        [contains, [ethanol,
                                        [attrib,  [volume,
                                                        [num_value, [0.2]],
                                                        [unit,   [ml]]]]]],
                        [contains, [H2O,
                                        [attrib, [volume,
                                                        [num_value, [20]],
                                                        [unit,   [ul]]]]]]]],
        [output, [$SAMPLE_7, [link, [$SAMPLE_6, $SOL_4]]]]].
```

Analysis was by HPLC on a column (25 cm .times. 4.6 mm) of Zorbax C18 (5 μm), with gradient elution (1.5 ml min.minus.1) from 100% of aq. 90% methanol to 100% of ethyl acetate - propan-2-ol (9:1) over 4 min, then held for 8 min, and detection at 300 nm. (Remaining text on performance of the method.)

```
['factual analysis',
        [id,     [$FACTUAL_ANAL1]],
        [object, [solution, [id,   [$SAMPLE_7]],
        [means, [$HPLC_1]],
        [scheme, [$HPLC_1, $QUANTIFY_1]],
        [output, [$RESULT_2]]].

[$HPLC_1,
        [object, [$SAMPLE_7]],
        [instrument, [column, [id, [$COLUMN_1]],
                        [attrib, [dimension, [attrib, [length, [num_value, [25]],
                                                        [unit,   [cm]]]],
                                        [attrib, [diameter, [num_value, [4.6]],
                                                        [unit,   [mm]]]]]],
                        [contains, ['Zorbax C18',
                                        [attrib, [diameter, [num_value, [5]],
                                                        [unit,   [um]]]]]]]],
        [means, [$ELUTE_1]],
        [scheme, [$ELUTE_1, $ELUTE_2]]].

[elute,  [id,     [$ELUTE_1]],
        [object, [$SAMPLE_7]],
        [applied, [eluent, [id,    [$ELUENT_1]],
                        [attrib, [$GRADIENT_1]]]],
        [manner, [$GRADIENT_1]]
        [manner, [flow, [num_value, [1.5]],
                        [unit,   [ml/min]],
        [output, [$ELUENT_2, [link, [$SAMPLE_7, $ELUENT_1]]]]].

[gradient, [id,   [$GRADIENT_1]],
        [duration, [min,          [number, [4]]]],
        [from,  [concentration, [num_value, [100]],
                        [unit,   [%]],
                        [attrib_of, [H2O,
                                        [contains, [methanol, [attrib,
                                                        [concentration,
                                                                [num_value, [90]],
                                                                [unit,   [%]]]]]]]]]],
```

Figure 2 (continued)

```
[to,    [concentration, [num_value, [100]],
            [unit,   [%]],
            [attrib_of, [mixture,
                        [id,    [$MIXTURE_1]],
                        [contains, ['ethyl acetate', [attrib, [rel_volume,
                                                    [num_value, [9]]]]]],
                                [contains, [propan-2-ol, [attrib, [rel_volume,
                                                    [num_value, [1]]]]]]]]]].

[elute, [id,    [$ELUTE_2]],
        [input, [$ELUENT_2]],
        [applied, [$MIXTURE_2, [type, [$MIXTURE_1]]]],
        [duration, [min,        [number, [8]]]],
        [output, [eluent, [contains, [analytes,
                                [id,    [$ANALYTES_1]],
                                [modification, [separated]],
                                [interpretation,[collective_set]]]]]]].

[quantify, [id,  [$QUANTIFY_1]],
        [object, [$ANALYTES_1]],
        [means, [$DETECT_1]],
        [scheme, [$DETECT_1, $COMPUTE_1]],
        [output, [$RESULT_2]]].

[detect, [id,    [$DETECT_1]],
        [object, [analyte, [id,    [$ANALYTE_1]],
                        [element_of, [$ANALYTES_1]]]],
        [output, [$SIGNAL_1, [link, [$ANALYTE_1]]]]].

['compute concentration', [id, [$COMPUTE_1]],
        [source, [$SIGNAL_1]],
        [output, [concentration, [id, [$RESULT_1]],
                        [link,   [$SIGNAL_1]],
                        [element_of, [$RESULT_2]]]]].
```

Figure 2. First example of a method description using the representation formalism.

etc. Using these cases and relations, the recursive nested list representation is

$frame_i$	:- [$concept_i$, [id, [frame-id$_i$]], [rel_{i1}, $value_{i1}$],...[rel_{ij}, $value_{ij}$],...[rel_{in}, $value_{in}$]].
$frame_i$	:- [frame-id$_i$, [rel_{i1}, $value_{i1}$],...[rel_{ij}, $value_{ij}$],...[rel_{in}, $value_{in}$]].
$value_{ij}$	:- $frame_k$
$value_{ij}$	:- [$string_{ij}$]
if rel_{ij} =	'scheme' ∨ 'link' then ($1 \le j \le o$, $lj \in \{i \mid 1 \le i \le m\}$):
$value_{ij}$	:- [frame-id$_{l1}$,...frame-id$_{lj}$,...frame-id$_{lo}$]

in which

$concept_i$	= a string representing a concept given in the text (mainly verbs or nouns)
id	= the frame identifier indicating relation
frame-id$_i$	= unique identifier of $frame_i$
rel_{ij}	= the jth case or relation of $frame_i$
$string_{ij}$	= the value of rel_{ij} being words or numeric values of the text

This nested list representation can be transformed into a set of frames i (i: $1 - m$):

frame'$_i$	:- [frame-id$_i$, [name, [$concept_i$]], [rel_{i1}, value'$_{i1}$],...[rel_{ij}, value'$_{ij}$],...[rel_{in}, value'$_{in}$]].
value'$_{ij}$	:- frame-id$_k$
value'$_{ij}$	:- [$string_{ij}$]
if rel_{ij} =	'scheme' ∨ 'link' then ($1 \le j \le o$, $lj \in \{i \mid 1 \le i \le m\}$):
value'$_{ij}$	:- [frame-id$_{l1}$,...frame-id$_{lj}$,...frame-id$_{lo}$]

in which

name	= relation indicating the concept string represented by $frame_i$
frame-id$_k$	= unique identifier of frame'$_k$

The unique frame identifiers are used not only for the transformation of the nested-list representation to a set of frames but also for identification of each concept for referencing. Some (unspecified) output of one action can be the input of the next action and can be referred to by these identifiers. Each concept that changes regarding state (e.g. because of some action) is referred to by a new identifier. The link to its previous state is identified with the 'link' relation. This way, the temporariness of the state of a concept is tackled.

An example of the use of the nested-list representation is the mix action ($MIX1) in Figure 1. The class information is optional, but it can assist in the reasoning on mass flow. Indentation is applied to make the bracketing more readable. The identifier strings can be chosen arbitrarily, but they are chosen to represent, more or less, the concepts they identify.

Using the representation, it is possible to represent action sequences that are (to be) executed in parallel and which products/output is gathered in one next action. Also, it is possible to split one action sequence into more than one action sequence because of the differentiation in output streams.

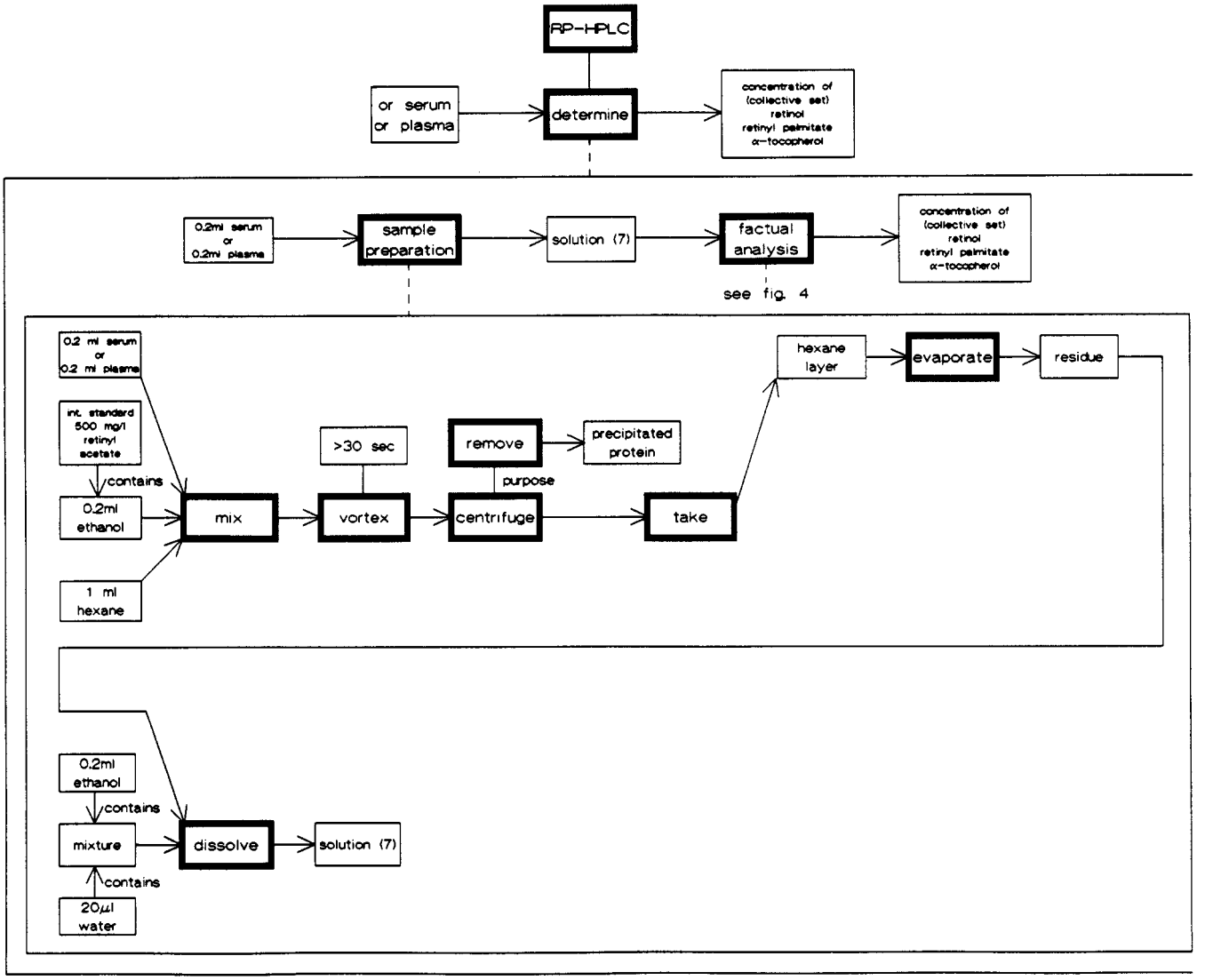

Figure 3. First part of the graphical representation of the method description given in Figure 2: the sample preparation.

Actions (processes) consisting of a number of actions will be called method actions. They are described by their participating actions using the scheme case in which their identifiers are listed. The initial action is also mentioned in the means case. The order of the actions is specified by the in- and output cases. This is more or less similar to the representation in text. Take, for example, the following passage: "The sample is etched by adding a solution of HNO_3. The solution is heated for ... and the etching is stopped by adding a solution of...". In these sentences "etch" is the method action and the first "add" and "heat" are the participating actions. The next "add" follows the "etch" process. The input of these method actions is, at the same time, one of the inputs of the initial participating action; their output is the output of the last participating action, and it is used in following actions. Input and output of the participating actions that are not mentioned in the sentence of the method action in relation to this method action (verb) will not be specified in the frame representation of the method action. An exception is the output of participating actions that is used later on in actions that follow the method action. The same holds for input of participating actions that is output of actions preceding the method action. This representation conforms more or less to a definition using λ abstractions as described by Sowa,[11] in which the in- and output conform to formal parameters of the method action and the participating actions, together with all their case values, form the body. It differs from the structures defined by Sowa, because the number and type of participating actions can vary.

An example of the representation of a method action is given in Figure 1 (which presents a sample preparation that consists of a mixing and an addition).

In method descriptions, information on the common glassware that is used (such as sample tubes and flasks) is frequently lacking and the choice is left to the user. This means that the in- and output of analytical actions are the most frequent in terms of solutions and chemicals. It may sometimes be the case that the next action has a container as input, and the link between the specified container and the material it is assumed to contain (and which is assumed to be output of the previous action) is implicit. If this is the case, the link between the container and the containment is added with the 'contains' relation using the identifiers used in the previous output.

Beside a syntax the developed representation should have a semantics. In accordance with Sowa[12] and Kamp and Reyle,[13] we have chosen an existential interpretation which means that we assume that there are objects in a model (the world) for which the specified description holds.

The quantifiers, plurals (together with their number) and sets of concepts that are used in method descriptions, should be represented in accordance with their original interpretation.

Normally, a method description starts with "a sample ..." implying existential quantification: $\exists x$ (sample(x), ...). The method has been tested using samples, chemicals, and

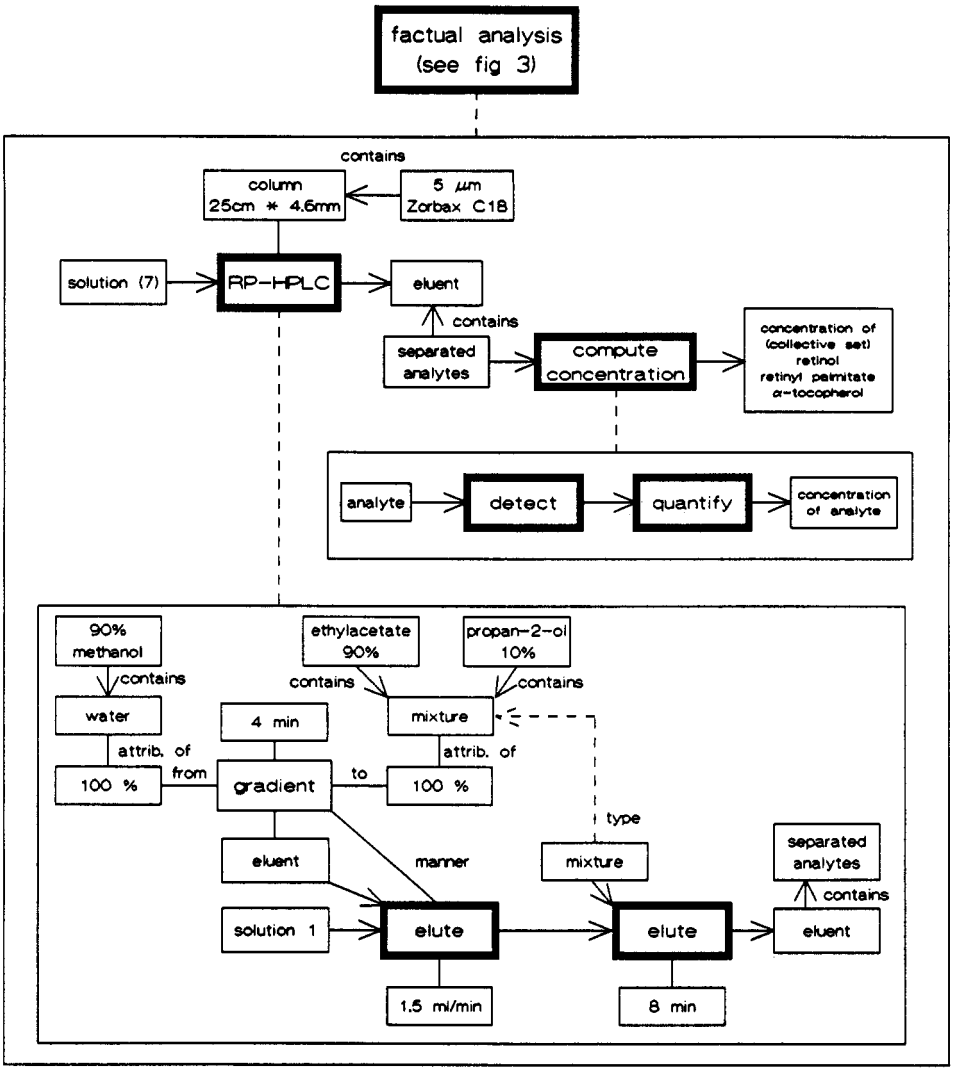

Figure 4. Second part of the graphical representation of the method description given in Figure 2: the factual analysis.

apparatus which conform their stated descriptions, and it has (should have) led to the presented performance characteristics. The method description (and the authors) however suggests a universal quantification: $\forall x \forall y$... (sample(x), instrument-(y), ...).

Still, a new method has to be validated before its use, and, if necessary, it should be adjusted. Therefore, we will assume that all input of the method is existentially quantified. The output and the input of participating actions that are outputs of previous (participating) actions are completely described and identified by these actions, their input, and circumstances. Because of this, all output is quantified by the 'definite descriptor', which is indicated by the iota-operator ι.[14] Using these quantifiers, the representations can be transformed into their logic equivalent by the method described by Sowa.[15]

Plural objects and actions in combination with numbers signify sets of objects and actions. But their interpretation can lead to ambiguities. For instance, the sentence "Three analytes have to be analyzed with three solutions" (theoretically) has a number of interpretations depending on the readings of the sets of the quantificational scopes.[16] The sets of analytes and solutions can have distributive and/or collective readings, and the analytes can have 'wider scope' over the solutions implying that nine solutions are used for the analyses of the three analytes. The solutions can also have wider scope over the analytes as is more or less exemplified by "with each of these three solutions three analytes can be analyzed". The factual interpretation, however, depends on the exact wording of the sentence, on the meaning of the sentence components, and on the background knowledge of analytical methods. For instance, in the sentence "These two reference samples have to be analyzed on 2 days", only two readings exist: distributive or collective with respect to the two reference samples. In order to make the representation unambiguous and independent of background knowledge on the sentence components, rules and markers are added that indicate the correct interpretation. These rules and markers are mainly applied to the input and output objects of an action. Normally, the reading of plurals in analytical method descriptions is distributive, and we will assume this as default reading in the interpretation. If a set of unspecified objects is to be interpreted collectively, this is indicated by the value 'collective_set' of the relation 'interpretation'; a set of specified objects is grouped within the concept 'collective_set'. A set of objects can have wider scope over the other input and output objects of an action or set of actions. This means that the actions are carried out for each member of the set of objects that has wide scope and each time with new instances of the other input and output objects. The set that has wider scope is given as case value in some method action that groups the actions. Depending on whether the set is input or output, the first or the last participating action contains an input or an output case that has as its value (a general description of) an element of that set. This element refers to the set with the relation 'element_-of' which has as value the identifier of the set. The identifier referring to the set can also occur in an action that is not the first or last participating action. The other input and output that is to be used for the repeated execution of the action(s),

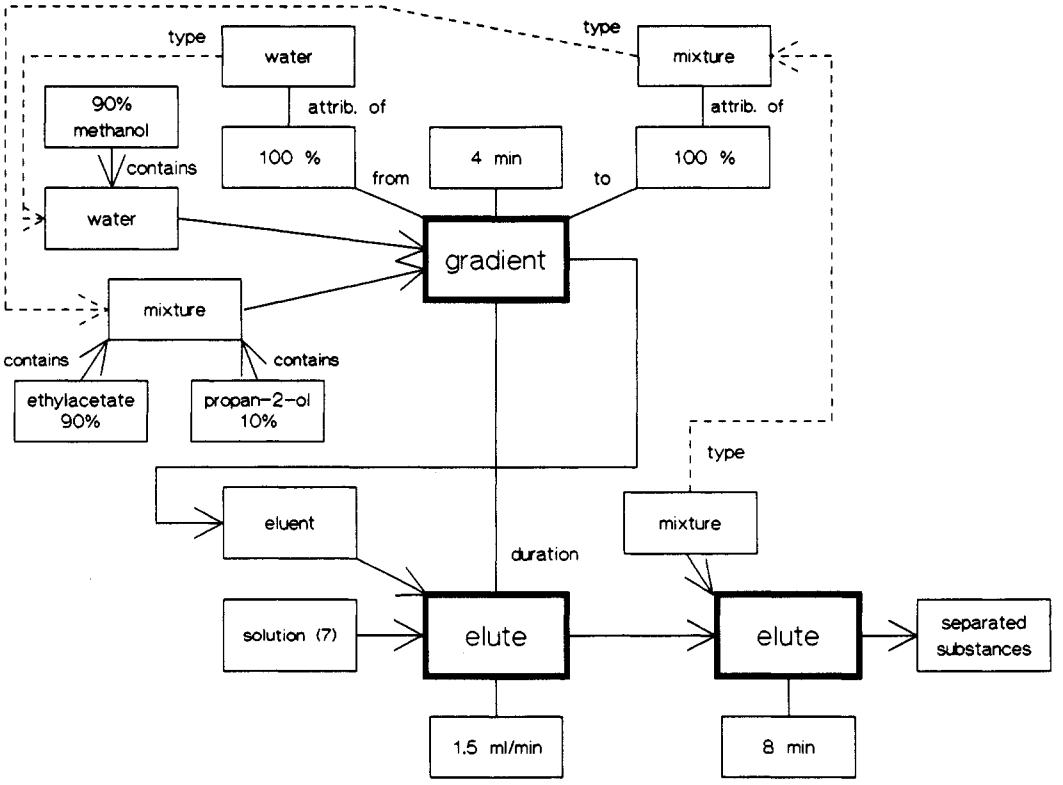

Figure 5. Alternative graph of a part of the graphical representation of Figure 4.

and that results from previous actions, or that is to be used in later actions is given in the method action as well. They are given together with their number necessary for the repeated execution of the participating actions. In the participating actions, they are referred to with the relation 'element_of'. According to these rules the representation will become like

```
[method_action, [id, ...],
   [input, ['set of objects', [id, [$INPUT_SET_1]],
        [element, [$ELEMENT_IN]],
   [means, [$FIRST_ACTION]],
   [scheme, [$FIRST_ACTION, ..., $LAST_ACTION]],
   [output, ['set of output objects', [id,
     [$OUTPUT_SET_1]]
        [element, [$ELEMENT_OUT]]]]].
['first action', [id, [$FIRST_ACTION]],
   [object, ['input object', [id, [$ELEMENT_IN]],
        [element_of, [$INPUT_SET_1]]]],
...].
['last action', [id, [$LAST_ACTION]],
...
   [output, ['output object', [id, [$ELEMENT_OUT]]]],
        [element_of, [$OUTPUT_SET_1]]]]].
```

An implicit assumption is that each input element is related to only one output element, and that each output element is related to only one input element (and that the set of input elements has the same cardinality as the set of output elements). If some participating action produces more than one kind of output, these outputs are collected in the method action in different output cases. This way, the method action serves as a context that determines the quantificational scope of sets like the propositions defined by Sowa.[17]

Examples of this representation can be found in Figures 2 ($QUANTIFY_1) and 6 (e.g. $ANALYSE_1 and $ANALYSE_2). Translation of this representation into logical formulas implies that for each distributive set in the method action a variable is introduced together with its description (members, number). For the elements of the set (referred to by the 'element' relation) another variable is introduced, and this variable is universally quantified over the set. The variable that indicates the elements is used in the logical translation of the participating actions.

It can occur that some object in one of the participating actions is to be used for all executions of the action (i.e., it is without quantificational scope). Then, this object should also occur in the method action as a single value of some appropriate case. The object in the participating action can be marked with the value 'independent' of the relation 'interpretation' as extra indication of such a situation.

In situations in which a set of objects determines the number of executions of some sequence of actions (each repetition of the actions for each element of the set), but in which this set does not occur as case value in the method action and participating actions, it is given as value of the caselike relation 'quantifier'. Within the set description the relation 'element' with an identifier as its value is supplied. This identifier serves as a variable for each element of the set. It can be used in concept descriptions within the participating actions to indicate concepts that depend on the identity of the element for which the actions are executed. An example is the sequential instrumental analysis of a prepared sample (or set of samples) on a number of analytes. In such a situation the analytes serve as quantifier. This can be seen in Figure 6, $INSTRUM_ANAL_2.

If some action has to be repeated, using its output (or one of its outputs) as input for the next execution of the action, this can be indicated by a 'number' relation that has as its value the number of repetitions. The output should represent the output of the last repetition and/or the set of outputs that is produced by each repetition of the action, but it is not used as input of the next repetition. Other input, which is not output of the previous repetition, should be given for the total number of repetitions. An example is "Heat the solution twice to 60 °C" which is represented by

```
[heat, [id, [$HEAT_1]],
     [object, [solution, [id, [$SOL_1]]]],
     [number, [2]],
     [output, [$SOL_2, [link, [$SOL_1]]]]].
```

Experimental

Materials and standard solutions. Degreased silicon slices, provided by Philips Research Laboratories, were rinsed thoroughly in 1.5 M nitric acid to remove any particulate surface material and etched as follows.

```
[determine, [id, [$DETERMINE_1]],
        [output, [$CONC4]],
        [means, [$SAMPLE_PREP_1]],
        [source, ['silicon slices', [id, [$SAMPLE_SET_1]],
                        [number, [set]]]],
        [scheme, [$SAMPLE_PREP_1, $PREPARE_0, $INSTRUM_ANAL_1]]].

['sample preparation', [id, [$SAMPLE_PREP_1]],
        [object, [$SAMPLE_SET_1, [element, [$SAMPLE_1]]]],
        [means, [$DEGREASE_1]],
        [scheme, [$DEGREASE_1,$RINSE_IN_1,$ETCH_1,$ADD_2,
                        $WASH_IN_1,$DRY_1,$SHATTER_1,$STORE_1]],
        [output, ['prepared samples', [id, [$PREP_SAMPLE_SET_1]],
                        [number, [set]],
                        [element, [$SAMPLE_10]]]]].

[degrease, [id,  [$DEGREASE_1]],
        [object, ['silicon slice', [id, [$SAMPLE_1]]
                        [element_of, [$SAMPLE_SET_1]],
        [output, ['silicon slice', [id, [$SAMPLE_2]],
                        [link,  [$SAMPLE_1]]]]].

[rinse,  [id,  [$RINSE_IN_1]],
        [object, [$SAMPLE_2]],
        [manner, [thorough]],
        [recipient, ['nitric acid', [attrib, [concentration, [num_value, [1.5]],
                                        [unit,  ['M']]]]]],
        [purpose, [remove, [object, ['particulate surface material']]]],
        [leaving_output, ['silicon slice', [id, [$SAMPLE_3]],
                        [link,  [$SAMPLE_2]],
                        [modification, [rinsed]]]]].

[etch,  [id,  [$ETCH_1]],
        [object, [$SAMPLE_3]],
        [means, [$IMMERSE_1]],
        [scheme, [$IMMERSE_1,$IMMERSE_2,$ADD_1,$REPLACE_1,
                        $LEAVE_1]],
        [applied, [$HNO3_0]],
        [output, [$SAMPLE_7]],
        [output, [$HNO3_4]]].
```

A slice was immersed in concentrated nitric acid for 2 min and in hydrofluoric acid for a further 2 min. It was replaced in the nitric acid, to which hydrofluoric acid was added slowly until effervescence occurred, and left for 30 s in this etching mixture. The etching was stopped by adding deionized water and the slice was washed ten times in water.

```
[immerse, [id,  [$IMMERSE_1]],
        [object, [$SAMPLE_3]],
        [recipient, ['concentrated nitric acid', [id, [$HNO3_0]]]],
        [duration, [time, [value, [2]],
                        [unit,  [min]]]],
        [leaving_output, ['silicon slice', [id, [$SAMPLE_4]],
                        [link,  [$SAMPLE_3]]]],
        [output, ['concentrated nitric acid', [id, [$HNO3_1]],
                        [link,  [$HNO3_0]]]]].

[immerse, [id,  [$IMMERSE_2]],
        [object, [$SAMPLE_4]],
        [recipient, ['hydrofluoric acid']],
        [duration, [time, [value, [2]],
                        [unit,  [min]]]],
        [leaving_output, ['silicon slice', [id, [$SAMPLE_5]],
                        [link,  [$SAMPLE_4]]]]].

[add,  [id,  [$ADD_1]],
        [object, ['hydrofluoric acid', [id, [$HF_1]]]],
        [recipient, [$HNO3_1]],
        [termination, [occurence, [object, [effervescence]]]],
        [manner, [slowly]],
        [output, [$HNO3_2, [link, [$HNO3_1,$HF_1]]]]].

[place,  [id,  [$REPLACE_1]],
        [object, [$SAMPLE_5]],
        [location_goal, [$HNO3_2]],
        [output, ['silicon slice', [id, [$SAMPLE_6]],
                        [link,  [$SAMPLE_5]]]],
        [output, [$HNO3_3, [link, [$HNO3_2]]]]].

[leave,  [id,  [$LEAVE_1]],
        [object, [$SAMPLE_6]],
        [location, ['etching mixture', [id, [$HNO3_3]]]],
        [duration, [time, [value, [30]],
                        [unit,  [s]]]],
        [output, ['silicon slice', [id, [$SAMPLE_7]],
                        [link,  [$SAMPLE_6]]]],
        [output, [$HNO3_4, [link, [$HNO3_3]]]]].


[add,  [id,  [$ADD_2]],
        [object, ['deionized water', [id, [$H2O_1]]]],
        [recipient, [$HNO3_4]],
        [purpose, [stop, [object, [$ETCH_1]]]],
        [output, [$HNO3_5, [link, [$HNO3_4,$H2O_1]],
                        [locates, [$SAMPLE_8, [link, $SAMPLE_7]]]]]].

# some kind of "take $SAMPLE_8 out of $HNO3_5" can be added.

[wash,  [id,  [$WASH_IN_1]],
        [object, [$SAMPLE_8]],
        [recipient, ['deionized water', [id, [$H2O_2]]]],
        [number, [10]],
        [leaving_output, ['silicon slice', [id, [$SAMPLE_9]],
                        [link,  [$SAMPLE_8]]]]].
```

It was left to dry between filter papers. A slice as shattered, as described previously [7], until the tiny fragments obtained were suitable for solid-sample insertion. The samples were stored in clean sample tubes to prevent contamination.

```
['dry between', [id, [$DRY_1]],
        [object, [$SAMPLE_9]],
        [location_goal, ['filter papers']],
        [leaving_output, ['silicon slice', [id, [$SAMPLE_10]],
                        [link,  [$SAMPLE_9]]]]].

[shatter, [id,  [$SHATTER_1]],
        [object, [$SAMPLE_10]],
        [means, [described, [time, [previously]]]],
        [termination, ['are suitable', [object, [$FRAGMENTS_1]],
                        [purpose, ['solid-sample insertion']]]],
        [output, ['tiny fragments', [id, [$FRAGMENTS_1]],
                        [link,  [$SAMPLE_10]]]]].

[store, [id,  [$STORE_1]],
        [object, [$FRAGMENTS_1]],
        [location_goal, ['sample tubes', [id, [$TUBE_1]],
                        [attrib,  [clean]],
```

Figure 6 (continued)

```
        [purpose, [prevent, [object, [contamination]]]],
        [output, [$FRAGMENTS_2, [link, [$FRAGMENTS_1]],
                        [location, [$TUBE2, [link, [$TUBE_1]]]],
                        [element_of, [$PREP_SAMPLE_SET_1]]]]].

# also possible:
#       [output, [$TUBE_2, [link, [$TUBE_1]]
#                       [contains, [$FRAGMENTS_2,
#                                       [link, [$FRAGMENTS_1]]]]]]].
```

Deionized water was used throughout. Stock standard solutions (1 mg ml-1) of antimony(III), lead, manganese(II), iron(III), silver, zinc and cadmium were prepared from potassium antimony tartrate hemihydrate and hydrated cadmium chloride in water, iron sponge and manganese flake dissolved in the minimum volume of 8 M nitric acid, lead and silver nitrates dissolved in 1% (v/v) nitric acid, and zinc shot dissolved in the minimum volume of 6 M hydrochloric acid. These solutions were diluted to volume with water (Sb, Cd, Fe), 1% nitric acid (Pb, Mn, Ag) or 1% hydrochloric acid (Zn).

```
[prepare, [id,    [$PREPARE_0]],
        [output, [conj,  [id,     [ST_SOL_SET_1]],
                         [and,    [$ST_SOL_1]],
                         [and,    [$ST_SOL_2]],
                         [and,    [$ST_SOL_3]],
                         [and,    [$ST_SOL_4]],
                         [and,    [$ST_SOL_5]],
                         [and,    [$ST_SOL_6]],
                         [and,    [$ST_SOL_7]],
                         [and,    [$ST_SOL_8]]]],
        [means, [$PREPARE_1]],
        [scheme, [$PREPARE1,$PREPARE_2,$PREPARE_3,$PREPARE_4,
                $PREPARE_5,$PREPARE_6,$PREPARE_7,$DILUTE_9]]].

[prepare, [id,    [$PREPARE_1]],
        [output, ['stock standard solution', [id, [$STOCK_1]],
                        [contains, ['Sb',
                                [attrib, [valence, [num_value, [3]],
                                                [sign,   [+]]]],
                                [attrib, [concentration,
                                                [num_value, [1]],
                                                [unit,   ['mg/ml']]]]]],
        [source, [water, [id,     [$H2O_3]],
                        [contains,
                                ['potassium antimony tartrate hemihydrate']]]],
        [means, [$DILUTE_1]],
        [scheme, [$DILUTE_1]]].
# A 'dissolve' could be added that produces $H2O_3 as output.

[dilute, [id,     [$DILUTE_1]],
        [object, [$H2O_3]],
        [to,     [volume]],
        [applied, ['deionized water', [id, [$H2O_5]]]],
        [output, ['stock standard solution', [id, [$STOCK_1]],
                        [link,   [$H2O_3,$H2O_5]]]]].


[prepare, [id,    [$PREPARE_2]],
        [output, ['stock standard solution', [id, [$STOCK_2]],
                        [contains, ['Pb',
                                [attrib, [concentration,
                                                [num_value, [1]],
                                                [unit,   ['mg/ml']]]]]]],
        [source, [$PbNO3]],
        [means,          [$DISSOLVE_1]],
                [scheme, [$DISSOLVE_1,$DILUTE_2]]].

[dissolve, [id,   [$DISSOLVE_1]],
        [object, ['lead nitrate', [id, [$PbNO3]]]],
        [recipient, ['nitric acid', [id, [$HNO3_10]],
                        [type,   [$HNO3_100]]]],
        [output, [$HNO3_11, [link, [$HNO3_10,$PbNO3]]]]].

['nitric acid', [id, [$HNO3_100]],
        [contains, ['HNO3',
                        [attrib, [concentration,
                                        [num_value, [1]],
                                        [unit,   ['v/v %']]]]]]].

[dilute, [id,     [$DILUTE_2]],
        [object, [$HNO3_11]],
        [to,     [volume]],
        [applied, [$HNO3_101, [type, [$HNO3_100]]]],
        [output, ['stock standard solution', [id, [$STOCK_2]],
                        [link,   [$HNO3_11,$HNO3_101]]]].

# etc. Likewise the other stock solutions.
```

More dilute standard solutions were produced daily by appropriate dilution.

```
[dilute, [id,     [$DILUTE_9]],
        [object, ['stock standard solution portions', [number, [N]],
                        [and,    [$STOCK_8, [type, [$STOCK_1]]]],
                        [and,    [$STOCK_9, [type, [$STOCK_2]]]],
                        [and,    [$STOCK_10, [type, [$STOCK_3]]]],
                        [and,    [$STOCK_11, [type, [$STOCK_4]]]],
                        [and,    [$STOCK_12, [type, [$STOCK_5]]]],
                        [and,    [$STOCK_13, [type, [$STOCK_6]]]],
                        [and,    [$STOCK_14, [type, [$STOCK_7]]]]]],
        [interval, [day,  [number, [1]]]],
        [applied, ['nitric acid', [number, [O]],
                        [contains, ['HNO3', [attrib, [concentration,
                                                [num_value, [1]],
                                                [unit,   ['v/v %']]]]]]]],
        [scheme, [?]],
        [output_from_object, ['standard solutions',
                        [and,    [$ST_SOL7, [link, [$STOCK_8]]]],
                        [and,    [$ST_SOL8, [link, [$STOCK_8]]]],
                        [and,    [$ST_SOL1, [link, [$STOCK_9]]]],
                        [and,    [$ST_SOL2, [link, [$STOCK_10]]]],
                        [and,    [$ST_SOL3, [link, [$STOCK_11]]]],
                        [and,    [$ST_SOL4, [link, [$STOCK_12]]]],
                        [and,    [$ST_SOL5, [link, [$STOCK_13]]]],
                        [and,    [$ST_SOL6, [link, [$STOCK_14]]]]]]].
```

The concentrations used for preparing the calibration graphs were (in ug ml-1): lead, .01; manganese, 0.01; iron, 0.05-0.2; silver, 0.1; zinc, 0.01; cadmium, 0.01; antimony, 2-7 (for solid samples), and 0.2-0.75 (for dissolved samples). In all cases, these solutions were 1% (v/v) in nitric acid.

```
['standard solution', [id, [$ST_SOL1]],
        [contains, ['Pb',       [attrib, [concentration, [num_value, [0.01]],
                                        [unit,   ['ug/ml']]]]]],
        [purpose, [prepare, [object, ['calibration graph']]]]].

['standard solution', [id, [$ST_SOL7]],
        [number, [set]],
        [contains, ['Sb', [attrib, [concentration, [min_number, [2]],
                                        [max_number, [7]],
                                        [unit,   ['ug/ml']]]]]],
        [purpose, [prepare, [object, ['calibration graph']]]],
```

Figure 6 (continued)

```
        [purpose, ['solid samples']],
        [contains, [$HNO3_16]]].

# etc.; likewise for the other standard solutions.
```

Apparatus. A Varian Techtron AA6 atomic absorption spectrometer was used with an Instrumentation Laboratory controlled-temperature furnace atomizer, and the sample was inserted in a pyrolytically-coated graphite microboat, exactly as described previously [7].

Determination of trace elements in solid silicon samples. Set up the atomic absorption spectrometer and furnace as in the instruction manual, using the most sensitive resonance line for each element being determined except for antimony where a less sensitive line at 231.2 nm is preferable.

```
# because of scope of analytes:
['instrumental analysis', [id, [$INSTRUM_ANAL_1]],
        [object, [$PREP_SAMPLE_SET_1]],
        [quantifier, ['trace elements', [id, [$TRACE_SET_1]],
                        [and,   ['Sb',  [id,    [$Sb1]]]],
                        [and,   ['Pb',  [id,    [$Pb1]]]],
                        [and,   ['Mn',  [id,    [$Mn1]]]],
                        [and,   ['Fe',  [id,    [$Fe1]]]],
                        [and,   ['Ag',  [id,    [$Ag1]]]],
                        [and,   ['Zn',  [id,    [$Zn1]]]],
                        [and,   ['Cd',  [id,    [$Cd1]]]],
                        [element, [analyte, [id,  [$ANALYTE_0]]]]]],
        [applied,['resonance lines', [id, [$LINES_1]],
                        [element, ['resonance line', [id, [$LINE_1]],
                                        [of,    [$ANALYTE_0]]]],
                        [and,   ['most sensitive resonance line', [of, [$Pb1]]]],
                        [and,   ['most sensitive resonance line', [of, [$Mn1]]]],
                        [and,   ['most sensitive resonance line', [of, [$Fe1]]]],
                        [and,   ['most sensitive resonance line', [of, [$Ag1]]]],
                        [and,   ['most sensitive resonance line', [of, [$Zn1]]]],
                        [and,   ['most sensitive resonance line', [of, [$Cd1]]]],
                        [and,   ['less sensitive line', [attrib, [wavelength,
                                                [num_value, [231.1]],
                                                [unit,  [nm]]]],
                                        [of,    [$Sb1]]]]]],
        [scheme, [$INSTRUM_PREP_1, $CALIBRATE_1, $FACT_ANAL_1]],
        [output,[$CONC_4]]].

['instrument preparation', [id, [$INSTRUM_PREP_1]],
        [object, [conj,  [and,  ['atomic absorption spectrometer',
                                        [id,    [$AAS_1]]]],
                        [and,   ['furnace atomizer',
                                        [id,    [$FURNACE_1]]]],
                        [and,   [microboat,
                                        [id,    [$BOAT_1]]]]]],
        [means, [$SETUP_1]],
        [scheme, [$SETUP_1, $SETUP_2, $SETUP_3, $HEAT_1]],
        [output, [conj,  [and,  [$AAS_2]],
                        [and,   [$FURNACE_3]],
                        [and,   [$BOAT_2]]]],
        [output, [$BLANK_1]]].

['set up', [id,   [$SETUP_1]],
        [object, [$AAS_1]],
        [means, [instructions, [location, ['instruction manual']]]],
        [applied, ['resonance line', [id, [&LINE_1]],
                        [element_of, [$LINES_1]]]],
        [output, [$AAS_2, [link,        [$AAS_1]]]]].

        ['set up', [id,   [$SETUP_2]],
                [object, [$FURNACE_1]],
                [means, [instructions, [location, ['instruction manual']]]],
                [output, [$FURNACE_2, [link, [$FURNACE_1]]]]].
```

Set the heating programme for the element under study to the conditions given in Table 1.

```
[set,   [id,    [$SETUP_3]],
        [object, ['heating programme', [id, [$HEAT_PROG_1]],
                        [of,    [$FURNACE_2]]]],
        [to,    [conditions, [location, ['Table 1']]]]],
        [output, ['heating programme', [id, [$HEAT_PROG_2]],
                        [link,  [$HEAT_PROG_1]],
                        [of,    [$FURNACE_3, [link, [$FURNACE_2]]]]]]].
```

Subject an empty microboat to the heating programme repeatedly til there is no element blank or until the blank is reasonably small and constant.

```
[heat,  [id,    [$HEAT_1]],
        [object, [microboat, [id, [$BOAT_1]],
                        [attrib,  [empty]],
# implicit:
                        [location, [$TUBE_1, [location, [$FURNACE_3]]]]],
        [manner, [$HEAT_PROG_2]],
        [number, [M]],
        [termination, [disj, [or,  [blank, [id,    [$BLANK_1]],
                                        [attrib, [absent]]]],
                        [or,    [blank, [id,    [$BLANK_1]]
                                        [attrib, [small]],
                                        [attrib, [constant]]]]]],
        [output, [blank, [id,    [$BLANK_1]]]],
        [output, [$BOAT_2, [link, [$BOAT_1]]]]].

[construct, [id,  [$CALIBRATE_1]],
        [applied, [$ST_SOL_9, [element_of, [$ST_SOL_SET_1]],
                        [contains, [$ANALYTE_1, [type, [$ANALYTE_0]]]]]],
# etc, like 'factual analysis'.
        [output, ['calibration graph', [id, [$GRAPH_1]]]]].
```

Add a small sample of silicon (see Table 1), weighed to the nearest 0.01 mg, to the microboat and run the heating programme. Repeat this operation a further six times.

```
['factual analysis', [id, [$FACT_ANAL_1]],
        [object, [$PREP_SAMPLE_SET_1]],
        [applied, [$BLANK_1]],
        [applied, [$GRAPH_1]],
        [instrument, [$AAS_2]],
        [instrument, [$FURNACE_3]],
        [instrument, [$BOAT_2]],
        [means, [$TAKE_1]],
        [scheme, [$TAKE_1, $ANALYSE_1, $AVERAGE_1, $REPLACE_1,
                                                $HEAT_3]],
        [output, [$CONC_4, [element, [$CONC_3]]]]].

[take,  [id,    [$TAKE_1]],
        [source, ['prepared sample', [id, [$PREP_SAMPLE_1]],
                        [element_of, [$PREP_SAMPLE_SET_1]]]],
        [leaving_output, [sample, [id, [$PREP_SAMPLE_2]],
                        [link,  [$PREP_SAMPLE_1]],
                        [number, [7]],
                        [attrib,  [small]],
                        [attrib,  [weight, [obj_reverse, [given,
                                                [location, ['Table 1']]
        ]]]]]]].
```

If the quality of the absorbance peaks deteriorates, replace the microboat. Obtain the mass of element producing each peak area, corrected for any blank, from the

Figure 6 (continued)

appropriate calibration graph and calculate the concentration of trace element in the sample in ug g-1. Average the seven concentrations and calculate their standard deviation. Convert the concentration to ppm (atomic) from ppm (atomic) = (ug g-1) * (M/m), where M and m are the relative atomic masses for silicon and the trace element, respectively.

```
[analyse, [id,    [$ANALYSE_1]],
        [object, [$PREP_SAMPLE_2]],
        [means, [$WEIGH_1]],
        [scheme, [$WEIGH_1, $ADD_1, $INSERT_1, $HEAT_2, $DETECT_1,
                        $CHECK_1, $MEASURE_1, $CORRECT_1,
                        $QUANTIFY_1, $CALCULATE_1]],
        [termination, [deterioration, [object, [$PEAK_QUAL_1]]]],
        [output, [$BOAT_5]],
        [output, [concentrations, [id, [$CONC_2]],
                        [element, [$CONC_1]]]]].

[weigh, [id,    [$WEIGH_1]],
        [object, [$PREP_SAMPLE_3, [element_of, [$PREP_SAMPLE_2]]]],
        [manner, [accuracy, [num_value, [0.01]],
                        [unit,   [mg]]]],
        [output, [$PREP_SAMPLE_4, [link, [$PREP_SAMPLE_3]]]],
        [output, [weight, [id,    [$WEIGHT_1]],
                        [attrib_of, [sample, [id,  [$SAMPLE14]]]]]]].

[add,   [id,    [$ADD_1]],
        [object, [$PREP_SAMPLE_4]],
        [loc_goal, [disj, [or,    [$BOAT_2]],
                        [or,    [$BOAT_5]]]],
        [output, [$BOAT_3, [locates, [$PREP_SAMPLE_5,
                                [link, [$PREP_SAMPLE_4]]]],
                        [link,   [$BOAT_2]]]]].

# implicit:
[insert, [id,    [$INSERT_1]],
        [object, [$BOAT_3]],
        [loc_goal, ['graphite furnace', [id, [$TUBE_1]]]],
        [output, [$TUBE_2, [link, [$TUBE_1]],
                        [locates, [$BOAT_4, [link, [$BOAT_3]]]]]]].

[heat,  [id,    [$HEAT_2]],
        [object, [$TUBE_2]],
        [manner, [$HEAT_PROG_2, [of, [$FURNACE_3]]]],
        [output, ['atomized sample', [id, [$ATOM_SAMPLE_1]],
                        [link,   [$SAMPLE_15]]]],
        [output, [$TUBE_3, [link, [$TUBE_2]],
                        [locates, [$BOAT_5, [link, [$BOAT_4]]]]]].

# implicit:
[detect, [id,    [$DETECT_1]],
        [object, [$ATOM_SAMPLE1]],
        [instrument, [$AAS_2]],
        [output, ['absorbtion peak', [id, [$PEAK_1]]]]].

[check, [id,    [$CHECK_1]],
        [source, [$PEAK_1]],
        [output, [quality, [id,    [$PEAK_QUAL_1]],
                        [attrib_of, [$PEAK_2]]]],
        [output, [$PEAK_2, [link, [$PEAK_1]]]]].

[measure, [id,   [$MEASURE_1]],
        [source, [$PEAK_2]],
        [output, ['peak area', [id,        [$AREA_1]],
                        [link,   [$PEAK_2]]]]].

[correct, [id,    [$CORRECT_1]],
        [object, [$AREA_1]],
        [applied, [disj,  [id,    [$BLANK_3]],
                        [or,    [$BLANK_1]],
                        [or,    [$BLANK_2]]]],
        [output, ['peak area', [id, [$AREA_2]],
                        [link,   [$AREA_1,$BLANK_3]]]]].

[quantify, [id,   [$QUANTIF_1]],
        [object, [$AREA_2]],
        [applied, ['calibration graph', [id, [$GRAPH_1]]]],
        [output, [mass,  [id,    [$MASS_1]],
                        [link,   [$AREA_2, $GRAPH_1]]]]].

[calculate, [id,  [$CALCULATE_1]]
        [source, [$MASS_1]],
        [source, [$WEIGHT_1]],
        [output, [concentration, [id, [$CONC_1]],
                        [link,   [$WEIGHT_1,$MASS_1]],
# implicit:
                        [element_of, [$CONC_2]],
                        [attrib_of, [analyte, [id,  [$ANALYTE_2]],
                                [containment, [$PREP_SAMPLE_5]],
                                [type,   [$ANALYTE_0]]]]]]].

[average, [id,   [$AVERAGE1]],
        [object, [concentrations, [id, [$CONC_2]],
                        [interpretation, [collective_set]]]],
        [output, [$CONC_3, [link, [$CONC_2]],
                        [element_of, [$CONC_4]],
# implicit:
                        [attrib_of, [$ANALYTE_3,
                                [containment, [$PREP_SAMPLE_1]],
                                [type,   [$ANALYTE_0]]]]]]].

[replace, [id,   [$REPLACE_1]],
        [object, [$BOAT_5]],
        [applied, [$BOAT_6]],
        [condition, [deterioration, [object, [$PEAK_QUAL_1]]]],
        [output, [$BOAT_6, [type, [$BOAT_1]]]]].

# implicit:
[heat,  [id,    [$HEAT_3]],
        [object, [microboat, [id, [$BOAT_6]],
                        [attrib,  [empty]]]],
        [manner, [$HEAT_PROG_2]],
        [condition, [deterioration, [object, [$PEAK_QUAL_1]]]],
        [termination, [disj, [or,  [blank, [id,    [$BLANK_2]]
                                [attrib,  [absent]]]],
                        [or,    [blank, [id,    [$BLANK_2]]
                                [attrib,  [small]],
                                [attrib,  [constant]]]]]],
        [number, [X]],
        [output, [$BLANK_2]],
        [output, [$BOAT_7, [link, [$BOAT_6]]]]].
```

Construction of calibration graphs. Heat an empty microboat repeatedly (see Table 2) until there is no element blank or until the blank is reasonably small and constant. Pipette a suitable volume of a standard solution of the element into the microboat (see Table 1) and obtain the absorbance peak by initiating the heating programme, which is usually identical to that for solids except that a drying stage is added. Repeat the operation a further six times with various masses of the element. Measure each peak area, correct for any blank, and plot peak area vs. mass of element.

Figure 6. Second example of a method description using the representation formalism. #: Added remarks.

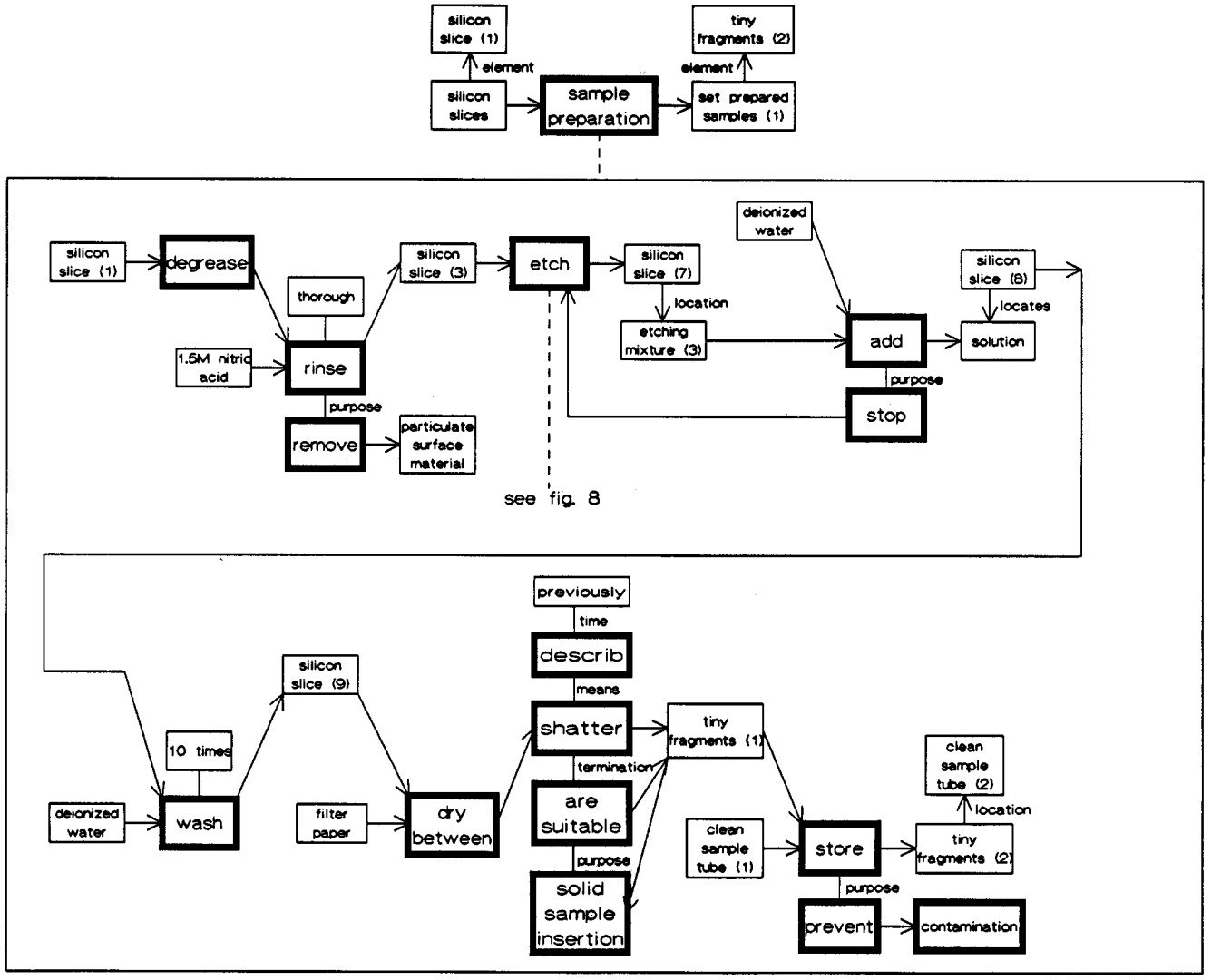

Figure 7. First part of the graphical representation of the method description given in Figure 6: the sample preparation.

In the same way "Extract the solution twice with a portion of hexane. The hexane layers ..." can be represented by

```
[extract, [id, [$EXTRACT_1]],
    [object, [solution, [id, [$SOL_1]]]],
    [number, [2]],
    [applied, [hexane, [id, [$HEXANE_1]],
            [number, [2]]]],
    [output, [$SOL_2, [link, [$SOL_1]]]],
    [output, ['hexane layer', [id, [$HEXANE_2]],
            [link, [$HEXANE_1]],
            [number, [2]]]]].
```

This representation is more complex, and the information that the solution $SOL_1, after the first extraction, is used as input for the next extraction can only be derived from the fact that this object and its related output have no number slot. The repetition can, of course, be written out as well.

Representations of actions that have to be repeated on different times (which is indicated by the 'time' case) contain all input and output necessary for all repetitions. If the action is a method action, then the participating actions are repeated for each element of the method-action input and/or output, and for each indicated time point. The same holds for analyses that have to be carried out in duplo (represented by '[manner, [duplo]]').

As a result of these representation principles, the output (given that, in the case of conjunctive sets, these sets have a distributive interpretation) or the 'number' value of each action implies the number of times the action is executed independent of the current scope, and the number of input and output objects is always explicitly represented in each action. Exceptions can occur with method actions which contain an explicit specification of all the participating actions. The total number of times an action (or an action sequence) is executed is determined by the multiplication of the various nested quantificational scopes and the aforementioned number of outputs or the 'number' value of the action.

This way, the representation can remain compact. Of course, repetitions can be written out beforehand, so that the interpretation definition can be more simple. As was partly mentioned before, sets of concepts with a description of each member can be described with a concept describing the type of set (disj, conj, collective_set), the 'or' or 'and' relation, and the set members as their values. Disjunctions of actions also contain a specification of the input and output. The input is the input of the actions in the disjunction that is linked to the output of the previous action, and the output is the output of the actions in the disjunction that is the input of the next action. According to these rules the representation will become like

```
[disjunction,
        [input, ['some object',
                [id, [$INPUT_OBJECT_1]]]],
        [or, [$FIRST_ACTION]],
        [or, [$SECOND_ACTION]],
        [output, [$OUTPUT_OBJECT_1]]].
['first action', [id, [$FIRST_ACTION]],
```

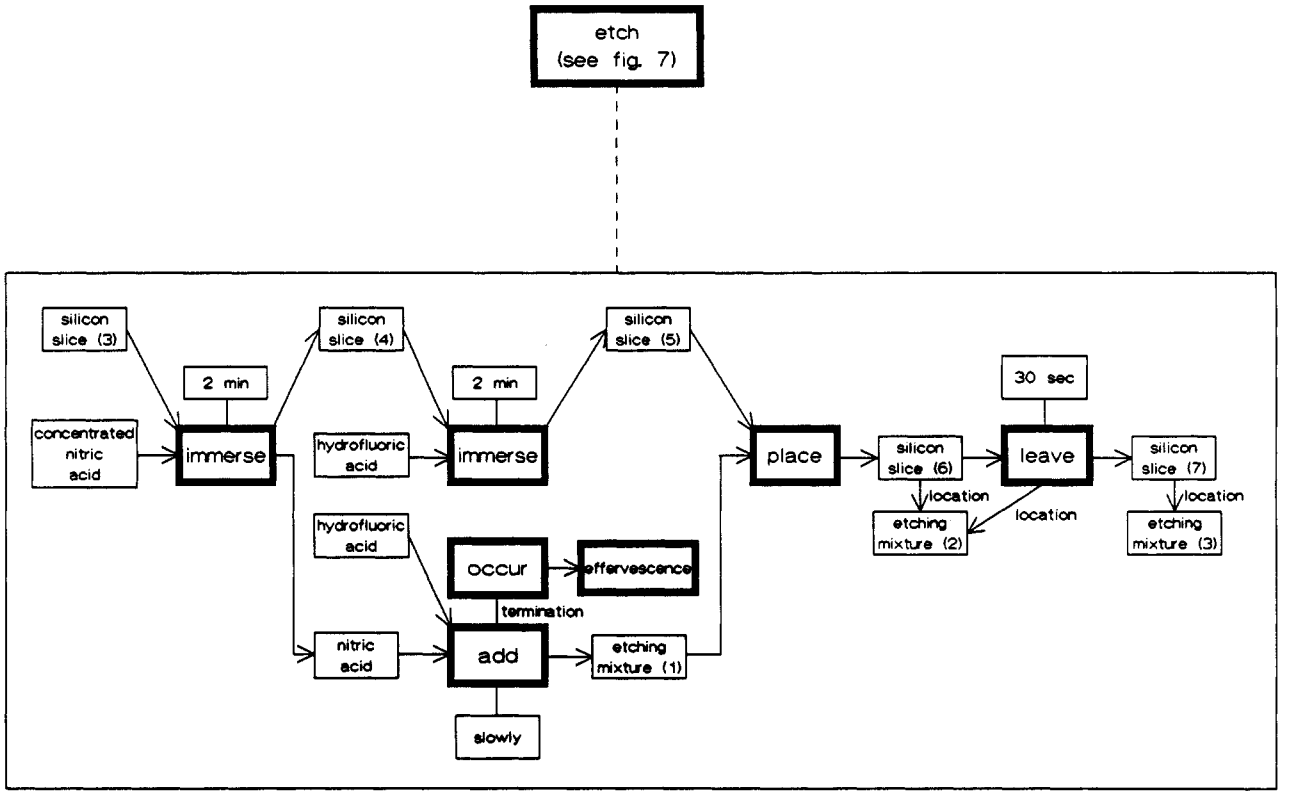

Figure 8. Second part of the graphical representation of the method description given in Figure 6: the etching procedure of the sample preparation.

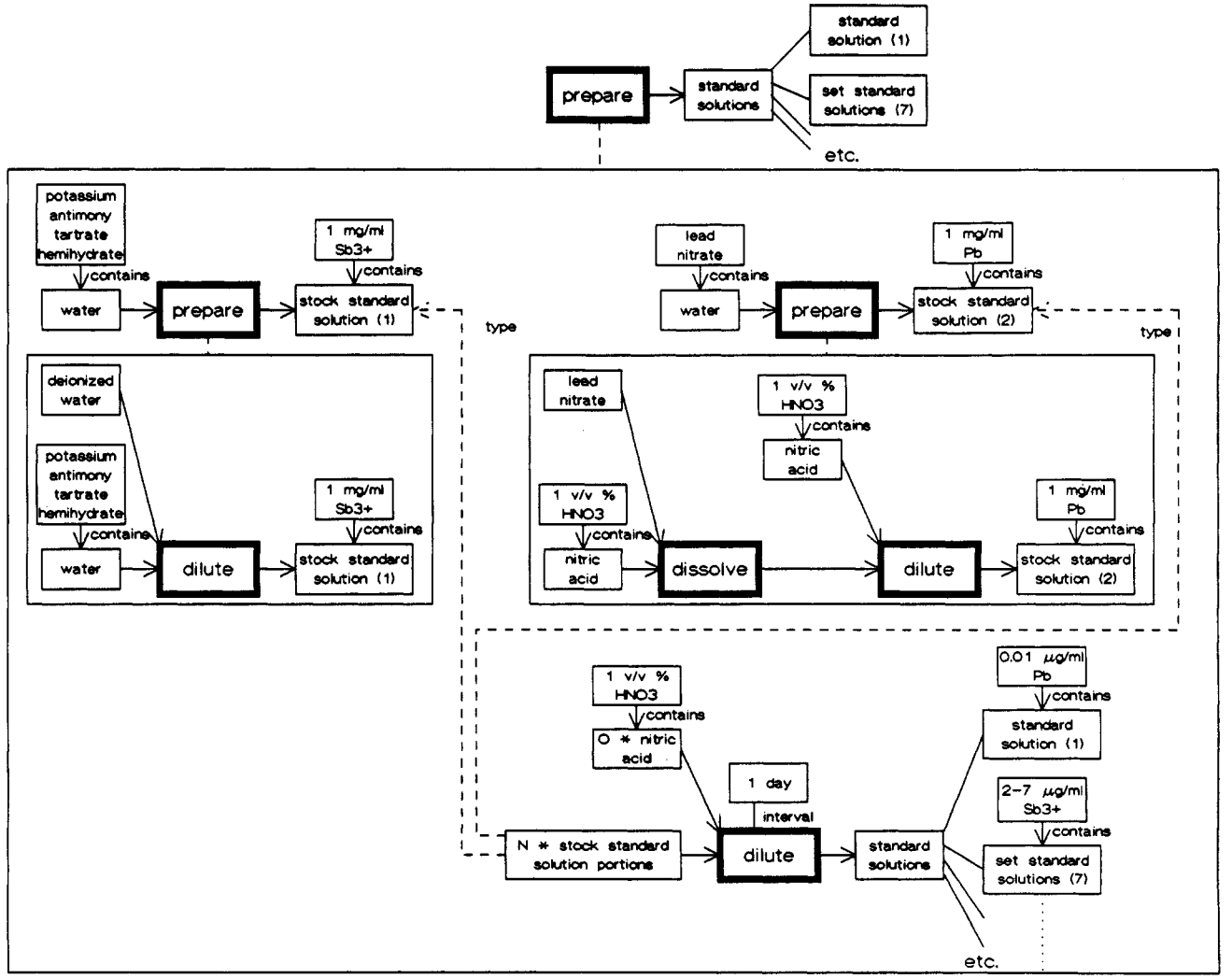

Figure 9. Third part of the graphical representation of the method description given in Figure 6: the preparation of the standard solutions.

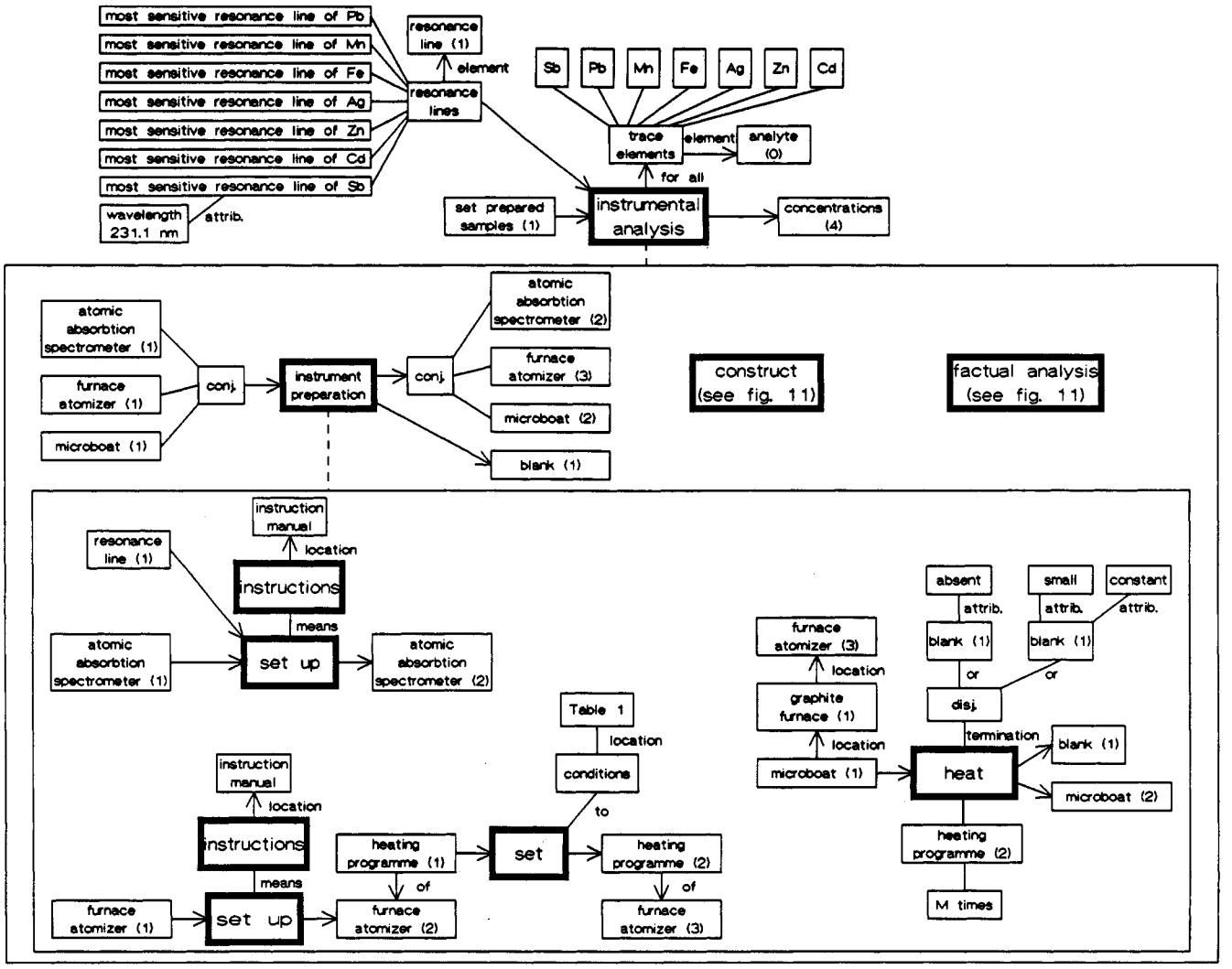

Figure 10. Fourth part of the graphical representation of the method description given in Figure 6: (part of) the instrumental analysis.

```
    [object, [$INPUT_OBJECT_1]],
    ...
    [output, ['some output',
        [id, [$OUTPUT_OBJECT_1]],
        [link, [$INPUT_OBJECT_1]]]]].
['second action', [id, [$SECOND_ACTION]],
    [object, [$INPUT_OBJECT_1]],
    ...
    [output, ['some output',
        [id, [$OUTPUT_OBJECT_1]],
        [link, [$INPUT_OBJECT_1]]]]].
```

The purpose of the input and output specification is to facilitate a simple graphical representation algorithm.

GRAPHICAL REPRESENTATION

Using the developed formalism, the method description can be represented graphically (Figures 3 and 4). The basis of the graphical representation is a horizontal line, along which one action sequence is represented in sequences of input–action–output from left to right. The output is the input of the next action. If a recipient, location_goal, or source case exists, its value is represented on the horizontal line and linked to the action with an arrow directed to that action. Other input (object, applied) is presented above the recipient (and if it is output of another action sequence, this sequence is represented parallel to the line containing the recipient) with an arrow representing the link to the next action.

If there is no recipient, location_goal or source, the object (or, in the absence of these cases, the input-case value) is presented on the current horizontal line (with an applied case value above it if present). The output directly related to the horizontal input is also positioned on the horizontal line and linked to the action with an arrow directed to the output. 'Leaving_output' is represented above the horizontal line and linked with an arrow from the action.

The cases indicating the conditions of the action are presented directly above and/or below the current action with a line linked to it. This way, no information on the type of link (i.e. case) is necessary: what has to be added to what and what is taken out from what is clearly visualized by the slanting lines, and the conditional information is separated from the in- and output specifying information. The type of link/case of the conditional information is largely implicitly determined by the class of the information. Exceptions are the time related information: then the link has to be labeled by the case or, if more convenient (because of the shorter stringlength), by the case related preposition. Also, the links representing the 'from' and 'to' case, the location case, and the condition and purpose case have to be labeled. The number case together with its value can be represented by "x times" (x = value). The quantifier case can be represented with the string "for all". Type information of a concept (object or action) is represented by a broken line to its type. The scheme information is represented by a link of the method action to an outlined graph containing its participating actions. This way, the method actions provide a quick overview of the method; the details can then be found in the outlined graphs.

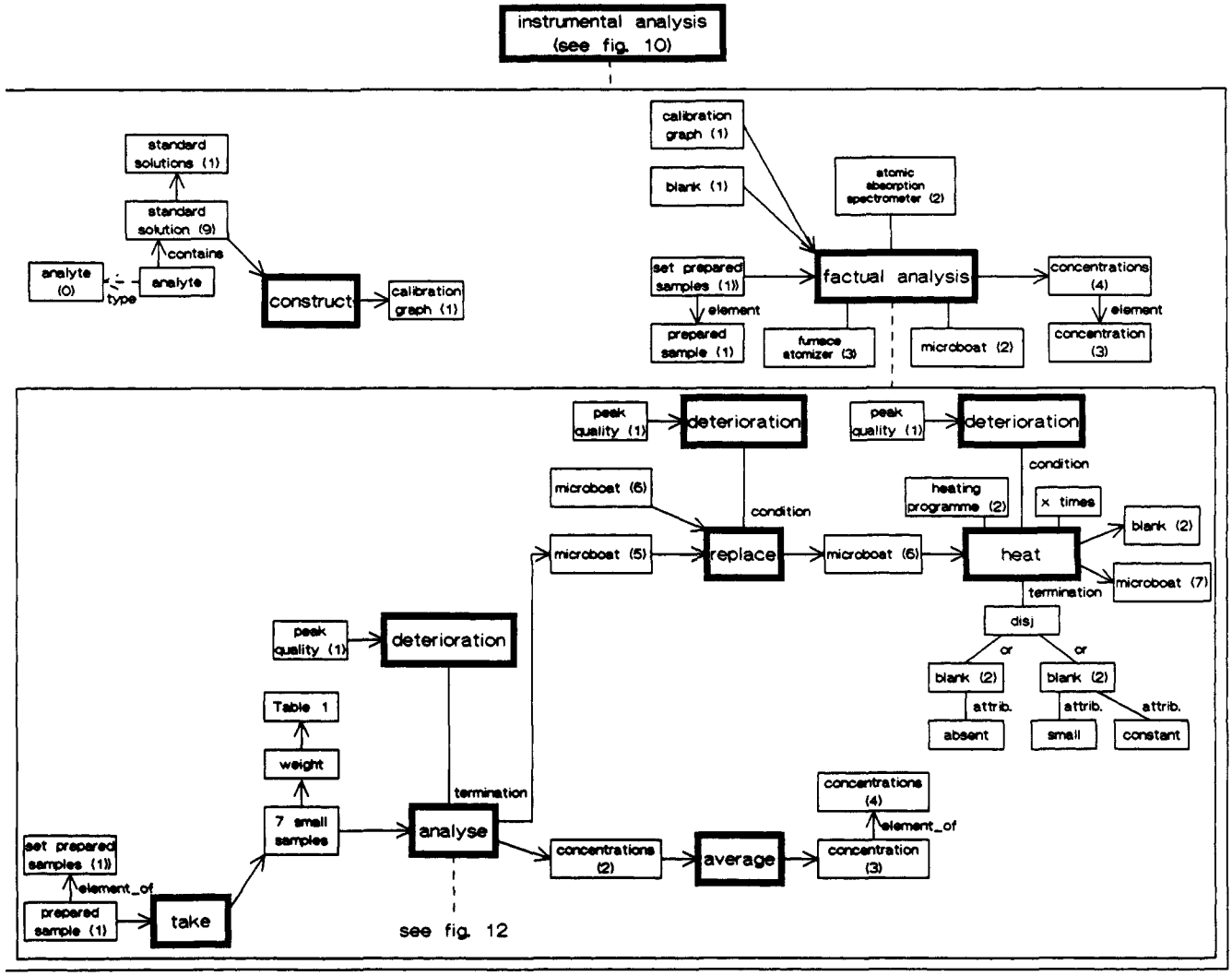

Figure 11. Fifth part of the graphical representation of the method description given in Figure 6: second part of the instrumental analysis.

The attributive information (such as concentration or volume) has to be parsed back to the textual representation and can be presented within the boxes that outline the objects. The procedures necessary for this parsing are simple and straightforward. Another possibility within computer environments is to receive detailed information on objects in separate windows which appear after clicking with a mouse on these objects. The 'contains' relation is represented by labeled arrows. In order to stress the actions, their boxes can be drawn with thicker lines. Disjunctions of actions have their input and the disjunction concept on the current horizontal line. The actions of the disjunction are drawn on the right of the disjunction concept above each other, and they are linked to the disjunction with arrows directed to them. The output of the disjunction is, again, located on the same level as the disjunction concept, and it is linked with arrows coming from the actions of the disjunction.

EXAMPLES AND DISCUSSION

The strength of the representation can be exemplified by the two usages of "rinse" in "rinse the sample in nitric acid" and "rinse the sample into a flask with nitric acid". The first example will become

[rinse, [object, [sample, [id, [$SAMPLE_1]]]],
[recipient, [HNO3, [id, [$HNO3_1]], ...]],
[leaving_output, [$SAMPLE_2, [link, [$SAMPLE_1]]]]].

and the second

[rinse, [object, [sample, [id, [$SAMPLE_1]]]],
[location_goal, [flask]],
[applied, [HNO3, [id, [$HNO3_1]], ...]],
[output, [$HNO3_2, [link, [$HNO3_1, $SAMPLE_1]]]]].

A complete short method description[18] is given in Figure 2, and is represented graphically in Figures 3 and 4. These representations (as well as those of the other figures) are made by hand: programs for the automation of this process are being developed.

Also, the factual analysis step is represented to exemplify the possibilities of the representation: it need not be restricted to the sample preparation.

As can be seen from the examples, some information, such as 'sample preparation' and 'factual analysis', is added to group and mark out related information (actions). General background information (detect, compute, and "determination of ..." = "determination of the concentration of ...") is added to complete the method description and graph in order to have a complete description from initial (sample) input to final (concentration) output. The link between 'detect' and 'compute concentration' is information instead of material, as is the final output of the procedure. The gradient applied during the elution is interpreted as a changing property (concentration), and it is linked to both the eluent and the elute action. An interpretation in which the gradient is interpreted as a gradient forming action is given in Figure 5. This interpretation has as a drawback that the graph is more complex and not easy to understand. The actions 'detect' and 'compute

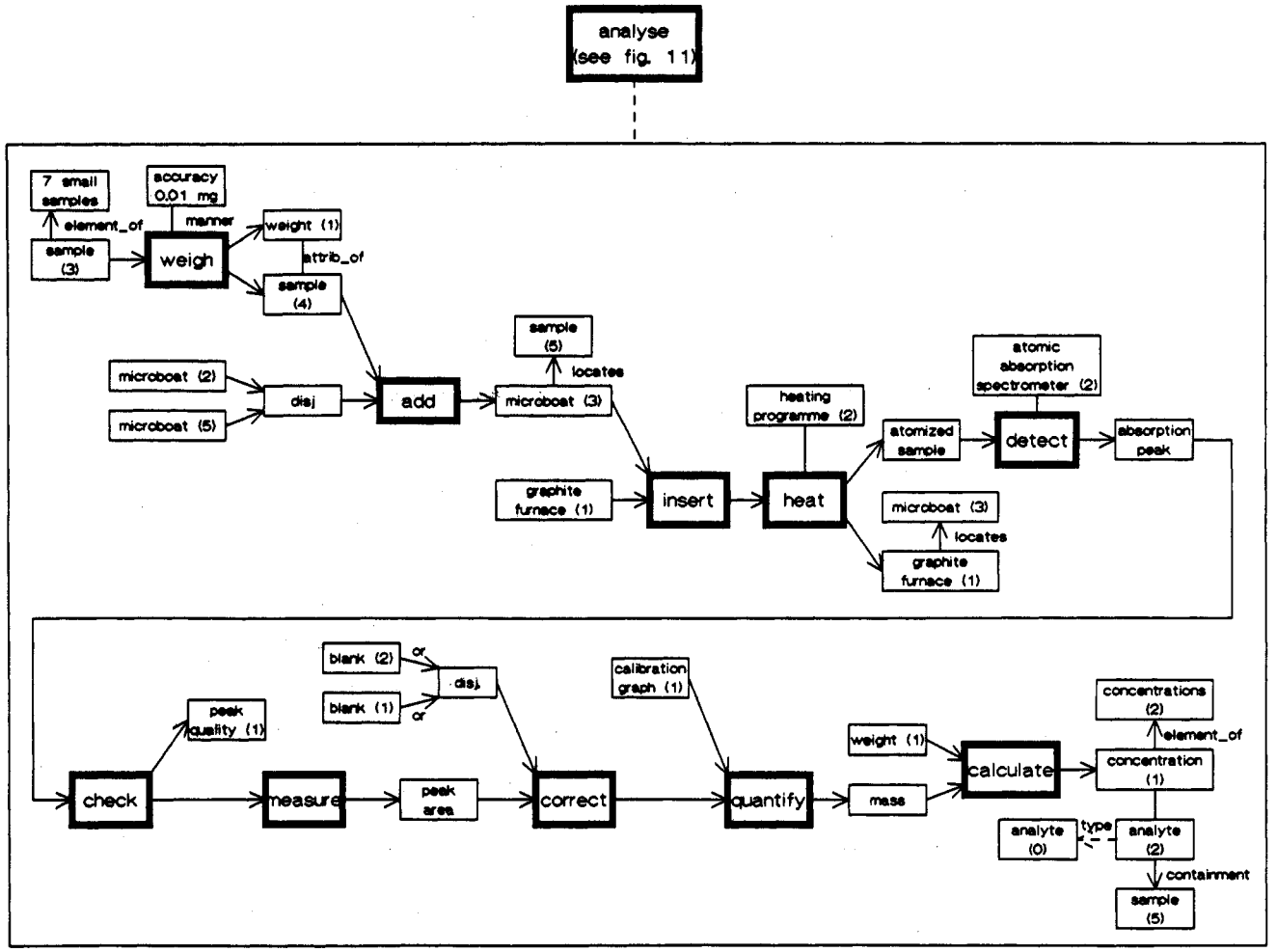

Figure 12. Sixth part of the graphical representation of the method description given in Figure 6: third part of the instrumental analysis.

concentration' are grouped within 'quantify', using the set of separated substances as scope, because in $ELUTE_2 the output is a collective set of separated substances, but in 'detect' these cannot be collectively detected (producing only one signal).

In Figure 6, an almost complete method description is given. The description is the method description using solid sample introduction for the given trace elements, and it is published in ref 19. The different parts, being the sample preparation, the preparation of the standard solutions, the instrument preparation, and the factual instrumental analysis, are graphically represented in Figures 7–12.

Also, in these representations, general background knowledge is added such as $DETERMINE_1 with its output concentrations. Information on the identity of the analytes is retrieved from elsewhere in the publication. The representation illustrates the possibilities of the formalism using the so called method actions as context for scope indication. $DETERMINE_1 has as input a set of samples, each of which seven concentrations (of the seven trace elements respectively) are determined from. This set of samples is the input of the sample preparation, and the resulting set of prepared samples is the output. The 'scheme' case of the sample preparation lists the actions that are to be executed for each sample. The instrumental analysis $INSTRUM_ANAL_1 is to be executed for each trace element, and its participating action 'factual analysis' is to be executed for each element on each sample with seven replications. The conversion from one sample input to seven (sub)samples, which are used for the replications, is given by the take action ($TAKE_1, see 'factual analysis' $ANALYSE_1), implicitly present in the original method description. Another use of a method action is illustrated by $PREPARE_0, which groups the preparations of the stock standard solutions. Now the scheme case lists the individual preparations of the stock solutions for each analyte. In this situation the 'means' case is hardly necessary, because the actions are not consecutive (or, in such a situation, it should be allowed to contain all starting actions).

The 'factual analysis' represents a mixed situation of repeated actions on input, that is new each time, and on input that is the output of its previous execution. The latter situation holds, e.g., for the microboat that is used in $ADD_1 (see $ANALYSE_1) as the location goal: only the first analysis after the instrument preparation can refer to the output $BOAT_2 of the instrument preparation $INSTRUM_PREP_1, but the later analyses use the microboat that is the output of their previous analysis. The only correct way to represent this would be to write out all the actions for all the samples. To circumvent this, the location goal of $ADD_1 refers to either $BOAT_2 or $BOAT_5. Still, the representation does not contain information on which of these has to be taken in which situation. Also, the output $BOAT_5 of $ANALYSIS_1 is not the correct identifier. This situation holds for most objects that are used as the instrument, and for the values of this case a rule could be added that takes care of this exception. The number of applied portions of nitric acid for the daily preparation of the standard solutions in $DILUTE_9 depends on the unknown number of standard solutions and the number of dilution steps. The number of stock standard solution portions is unknown as well (some of their identifiers can refer to sets). Because of this, the variables N and O are introduced.

The order of the weigh and add action ($WEIGH_1 and $ADD_1) should possibly be interchanged.

The conditional sentence "If the quality of the absorption peak..." implies some continuous check of the absorption peak ($CHECK_1). The condition itself is represented using the 'condition' case in $REPLACE_1, and in the implicit $SUBJECT_2 and the 'termination' case in $ANALYSIS_1. In fact, something like a negation of this condition should be added to $AVERAGE_1. The result is a new blank that should be used in the next analysis.

If the representation formalism is used for more than the sample preparation, then the definition of the 'applied' case should be extended to indicate things other than the physical material. This can be seen in, e.g., $CORRECT_1 and $QUANTIFY_1. This entails that, for reasoning along the material streams, the class information of the case values should also be provided. Another less attractive possibility is to subdivide the 'applied' case.

Ther verb 'prepare' has different usages and should be represented correctly. In "sample preparation", the sample has the object case and is input of the prepare action (see $SAMPLE_PREP_1). In "preparation of stock standard solutions" mentioned in the 'Materials' part of a method description, the stock standard solution should also get the object case, but it is now the output of the action series. In this case, the stock standard solution is labeled as the output (see also $PREPARE_0–$PREPARE_2).

On various locations in Figure 6 (e.g. $DILUTE_2 and $DILUTE_3), the use of the 'type' relation can be seen. It prevents the description of, e.g., a solution to be repeated each time it is needed. In fact, it implies some action like "take a portion (or a certain size) from this solution".

One drawback of the current representation is that choices have to be made with respect to scope and interpretations of sets. Sometimes these choices cannot (completely) be motivated by textual information or by background knowledge on analytical methods. This situation may occur if there is more than one way to perform (part of) a method (depending on, e.g., local circumstances), but it can also be the result of imperfections of the method description. In the former case, a possible way out may be to develop a semantics where such ambiguities remain in a controlled way (e.g. by using so called pseudopartitions[20]). Further investigation has to show whether these semantics can indeed be implemented.

It is possible to differentiate between the various types of conditional information that need explicit information on the type of link by color or line-type. This will save space in the graph, but it requires extra background information and hinders a direct visual interpretation by the potential user.

Most of the requirements of analytical method representations defined by Kateman[3] are, in our opinion, satisfied. Although possible, the hardware units are not fully described within the representation, because of the existence of shorter representations. The energy flow is not described either, because this information is hardly present within normal method descriptions. Textual descriptions of specialized instrumental setups including wiring are possible using the representation, because there is no restriction on the verbs that can be used. If necessary, dedicated relations such as 'connect_to' instead of the phrase "A is connected to B" can be added. Besides, graphical representations of the instrumental setup are more efficient. Calculation procedures have a mathematical language of their own.

Another possible use of the developed representation can be the (automatic) control of analytical method descriptions, which could then assist in improving the quality of published method descriptions. That such an improvement is necessary is shown in ref 21.

ACKNOWLEDGMENT

The authors wish to thank Dr. P. A. J. M. Coppen of the Department of Language and Speech and I. S. M. de Jong for their contributions.

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