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Description of chemical systems by their properties*

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Abstract: Proper handling and communication of data on chemical systems require knowledge about the mathematical characteristics of different types of property and the unambiguous representation of singular properties. Using the terminology of the International Organization for Standardization (ISO), the concept "property" is generically divided according to various statistical characteristics of property values.

The formatting of representation of dedicated kinds-of-property as elaborated by clinical chemists in the International Union of Pure and Applied Chemistry (IUPAC) and the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC) should ensure correct data transmission between laboratory dialects in any chemical discipline.

Keywords: examination; nomenclature; object; property; system.

INTRODUCTION

A perceivable or conceivable object can only be described by defining and examining its properties and obtaining their property values. Then, it is useful to distinguish between different types of property, characterized by the respective statistical procedures that can be meaningfully applied to the property values.

The unambiguous communication of the outcome requires several elements, and these are preferably presented in an agreed format for the appellation of an individual concept, i.e., a singular property corresponding to one instance.

OBJECT AND SYSTEM

It is doubtful, especially in chemistry, that non-composite objects exist. In laboratory medicine, a composite system is considered to be a "**system**", defined as "part or phenomenon of the perceivable or conceivable world consisting of a demarcated arrangement of a set of elements and a set of relationships or processes between these elements" [2-3.3]. It is seen that "system" can be partitively divided into its subordinate concepts, namely, "element", "relation", and "process", but in chemistry another partitive division is much used, namely, "component" and "matrix", where "**component**" (or "analyte") is defined as "part of a system" [2-3.4].

A component can comprise one or more elements, e.g., cholesterol + cholesterol ester in the system high-density lipoprotein; a relation, e.g., albumin/globulin in the system blood plasma; or a process, e.g., cobalamin absorption from the system small intestine.

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PROPERTY AND QUANTITY

Any system is described by its properties, where the superordinate generic concept "**property**" is defined as "inherent state- or process-descriptive feature of a system including any pertinent components" [2-5.5].

Singular properties—each corresponding to one instance—that have a common characteristic can be subsumed under a general generic concept "**kind-of-property**", defined as "common defining aspect of mutually comparable properties" [2-6.19], e.g., color, pH, and amount-of-substance fraction.

The concept "property" can be generically divided in many different ways, but a customary set of subordinate concepts is "qualitative property", "semiquantitative property", and "quantitative property". Unfortunately, the perceived delineation of these concepts varies and, therefore, in this text, the algebraic characteristics of the property values of singular properties will determine the division as proposed by Stevens in 1946 [3] and 1959 [4], see Table 1, using slightly modified terms.

Table 1 Mathematical characteristics of subordinate coordinate concepts under the generic concept "**property value**" [2,3].

Property value	Algebraic comparison	Salient statistics	Example of kind-of-property
nominal	a = or ≠ b	mode chi-square	specified chemical compound
ordinal	a < or = or > b	fractiles sign test	octane number
differential	$\lvert a - b \rvert$ = or ≠ $\lvert c - d \rvert$	average variance t-test	Celsius temperature
logarithmic differential	as previous on logarithmic values	as previous on logarithmic values	pH
rational	$a = nb$	geometric average coefficient of variation	mass concentration

Presenting these concepts as a generic concept diagram is complicated by Maxwell's introduction about 1870 of the concept "quantity" [5,6], where a given (singular) quantity is said to be expressed by two factors, namely, a numerical value and a measurement unit of the same kind(-of-quantity) as the quantity in question. The characteristic of involving a measurement unit excluded nominal and ordinal properties from being quantities.

Modern metrology by definition is concerned with measurement of all quantities with magnitude and therefore includes ordinal properties—perhaps with moderate enthusiasm—in the concept "**quantity**", newly redefined as "property of a phenomenon, body, or substance, where the property has a magnitude that can be expressed as a number and a reference" [7-1.1].

A "reference" can be a measurement unit, a measurement procedure, a reference material, or any relevant combination of such.

Omitting the concept of logarithmic differential property for simplicity, there are now at least two possible main ways of generically dividing the top superordinate concept "property" (Fig. 1). The concept "unitary quantity" [2-12.17] is optional.

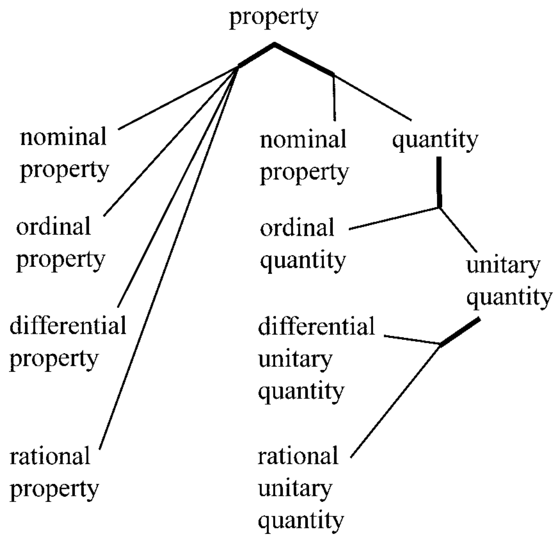

Fig. 1 Generic division of the concept "**property**" without (left-hand side) and with (right-hand side) involvement of the concept "**quantity**" (Fig. 12.21 in ref. [2]).

The structure of this two-part concept system with superordinate "property" and without "quantity" (at the left) and with subordinate "quantity" (at the right) can serve as a template for related concept systems. Important examples have the following superordinate concepts:

"examinand" ("measurand"),

"examination procedure" ("measurement procedure"),

"examining system" ("measuring system"),

"examination" ("measurement"),

"property value" ("quantity value"), and

"property value scale" ("quantity value scale"),

all necessary in sequence to obtain an

"examination result" ("measurement result").

It is seen that it has been necessary in each case to define a generic superordinate concept for the well-known (parenthetic) metrological concept. The root chosen for the respective terms was "examin" [2] as adopted by several International Standards, e.g., [8-3.6, 3.7].

All of these concepts may be said to belong to "examinology", which includes "metrology" [9].

DESIGNATION OF DEDICATED KIND-OF-PROPERTY

Clinical chemists within IFCC and IUPAC have done terminology work on the designation of properties for half a century as evidenced by the IUPAC-IFCC "Silver Book" [10] and a still growing database of about 15 000 entries [11] defined by the IUPAC-IFCC Subcommittee on Nomenclatue, Properties and Units, (S)C-NPU. Each entry constitutes a "**dedicated kind-of-property**" defined as "kind-of-property with given sort of system and any pertinent sort of component" [2-20.6] and is given a unique five-digit code value, prefaced by "NPU". Such entries are primarily meant as intermediaries between different laboratory dialects and IT systems to ensure correct transmission of data in various specialities of laboratory medicine, but should also serve as guides for designations in laboratory requests and reports.

The general format of an entry is given in Table 2.

Table 2 Format for designation of the concept "**dedicated kind-of-property**" as used in the IUPAC-IFCC database [11].

Element of designation	Example
System(specification)—	Plasma(arterial Blood)—
Component(specification);	Base excess(H^+binding group);
kind-of-property(specification)	amount-of-substance concentration (actual - norm)
measurement unit[1]	millimole per litre
code value	NPU12518
abbreviated form	P(aB)—Base excess(H^+binding group); subst.c.(actual - norm) = ? mmol/l

[1]Only for unitary property (unitary quantity)

The IUPAC-IFCC database shows this example with the component left-shifted for alphabetization and ease of sorting and the term for kind-of-property is shortened to "substance concentration", which is a convention in clinical chemistry. Most entries have no need of any specifications. Many entries have further information about calibrators, other terms, and authority for component term.

The appellation of a singular property in laboratory medicine always requires as specifications to system an identifier for the person being investigated and date/time of sampling.

CONCLUSIONS

The well-known terminology of metrology, where "quantity" and "measurement" are salient concepts, is insufficient for the overall description of many systems and their components in physics, chemistry, and biology where magnitude may not always be involved. In such cases, it becomes necessary to define the corresponding superordinate concepts "property" and "examination".

The top concept "property" can be divided advantageously according to important algebraic characteristics (Table 1, Fig. 1) determining to which subordinate concept a given singular property belongs and consequently which statistics the property values may be subjected to.

The representation of a singular property and its property value in an unambiguous way becomes especially important during transmission between different laboratory cultures and to outside services. The format elaborated for laboratory medicine has proven its value in national health systems, and the principles and format could easily be adopted in other disciplines.

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