On *mole* and *amount of substance*

A study of the dynamics of concept formation and concept attainment

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ABSTRACT

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At the 14th meeting of the General Conference on Weights and Measures (Conférence Générale des Poids et Mesures, GCPM) in 1971 1 mol was adopted as the unit of the base physical quantity *amount of substance* within the International System of units (Le Système International d'Unités, SI).

On the other hand it is empirically found that only 3 among 54 chemistry educators, acting on different levels of the Swedish educational system in the late 1980's, recognise 1 mol as an SI unit for the base physical quantity *amount of substance*.

This thesis aims to provide an answer to the question: Why have the educators not attained the 1971 convention?

Two main routes have been followed to grasp the conceptual situation. One empirical and synchronic manifested in the overt statements individuals have made concerning the actual concepts, and one theoretical and diachronic, coincident with the formation of the scientific concepts.

The first route deals with semi-structured open-ended individual interviews comprising a theoretical sample of 54 Swedish Chemistry educators on different levels in the Swedish educational system from upper secondary school to university level. A contextual analysis of the transcribed interviews has generated results mainly in the format of *categories of descriptions* accounting for the variation of conceptions among the respondents. This kind of qualitative research approach is denoted *phenomenography*.

The second route comprises a historical account of the formation of the concepts 'the mole' and *amount of substance* and a conceptual analysis of the contemporary scientific convention.

In the encounter between the two routes a theory is elaborated to model the process of concept attainment.

Via the theory it is shown that the defaulting attainment of the 1971 convention among the educators is a consequence of a non-apprehension of the base physical quantity *amount of substance*, and thereby the conceptual habitat of the SI unit 1 mol. A vast majority of the educators comprehend 1 mol as the unit measure of number of elementary entities (atoms, molecules, ions, etc.) in portions of matter. This conception belongs to discontinuum physics. However, the 1971 definition of 1 mol belongs to continuum physics since *amount of substance* is a continuous physical quantity. This is not generally noticed by the educators acting and interpreting within the frames of the grand theory of matter, the atomic theory, which is foundational in explaining chemical events. The non-attainment of *amount of substance* and its unit 1 mol is an example of the fact that concepts are theory-laden and can only be attained within the theories to which they belong.

The accounted conceptual situation also reflects an ongoing scientific controversy about the nature of the physical quantity *amount of substance* and whether *number* should be used instead of *amount of substance*. This is a matter of didactical choice and convention. The decision ought to be made under conceptual transparency. Hence, the representatives of the International Union of Pure and Applied Chemistry (IUPAC) are addressed to reconsider the commentary on *amount of substance* and the unit 1 mol in the IUPAC manual, inter alia in view of the results of the present investigation.

Some educational implications of the conceptual situation are discussed.

To
Per and Carolina

CONTENTS

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Helge Strömdahl

CHAPTER 1

INTRODUCTION

Since 1971 the international system of units and physical quantities (SI[1]) includes the base unit 1 mol (CGPM,[2] 1971) with *amount of substance* as the concordant base physical quantity. In a series of consecutive empirical studies it was found that the SI definition of the mole and the physical quantity *amount of substance* has not been generally attained and made a central component of teaching and learning in chemistry education in the Swedish educational system (Lybeck, Strömdahl & Tullberg, 1985a, 1985b, 1988, 1989, 1995; Strömdahl, Tullberg & Lybeck, 1989, 1994). These studies aimed at explaining why 'the mole'[3] is considered as conceptually difficult, among teachers and learners. The primary concern was to identify and establish the variations in conceptions of 'the mole' among students, teachers, trainee teachers, textbook-authors and university lecturers in the Swedish educational system.

This investigation is an attempt to find out some reasons for the low attainment of the 1971 definition of 1 mol and thereby the base physical quantity, *amount of substance.*

The study is focused around four main themes. First, the identification of the variation in conceptions of the actual scientific concepts involved, based on the empirical studies. Second, a historical reconstruction of the concept formation process, including a theoretical conceptual analysis of the physical quantity *amount of substance* and its

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[1] Le Systéme International d'Unités, (The International System of Units).

[2] Conférence Général de Poids et Measures, CGPM (General Conference on Weights and Measures).

[3] The notion 'the mole' denotes here the various conceptions of the unit 1 mol as it is conceptualised by the respondents in the empirical investigations accounted for in this thesis.

SI-unit 1 mol as expressed and exposed in the IUPAC[4] manual of units and quantities (Mills, Cvitaš, Homann, Kallay, & Kuchitsu, 1993). Third, the modelling of a theory accounting for the process of attainment of scientific concepts. The theory has been elaborated in reciprocal and dialectic interaction with the empirical findings and the theoretical conceptual analysis. Fourth, the results of the previous themes aim at making the actual conceptual components and structures explicit for educational treatments.

From a contemporary scientific point of view, the term 'the mole concept'[5] can no longer be used. The unit 1 mol must be dealt with in the broader context of theory in the physical sciences, where the conventions of SI and quantity calculus are to the fore. It is a reasonable responsibility of science teachers on different levels of the educational system, to teach about the coherent system of physical quantities, the theory of measurement and quantity calculus across science disciplinary borders and to thematize *amount of substance* and its SI unit 1 mol in that context.[6]

1.1 The knowledge-content domain

Stoichiometry (Greek, στοιχειον = element, first principle; μετρεω (μετρον) = a measure; element measuring; Richter, 1792) is the subsection of chemistry dealing with the quantitative aspect of chemical reactions. It is a phenomenal, empirical observation that substances involved in a chemical reaction do not react in an arbitrary way but in fixed mass proportions, viz. in multiples of invariant individual masses, historically denoted 'combining weights'. Masses of 'portions of substances' [7] converging at chemical reactions show a conformity to law, 'the law of constant (fixed) proportions'. As a denotation for the invariant individual masses, converging at chemical reactions, Ostwald

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[4] International Union of Pure and Applied Chemistry, IUPAC.

[5] The notion 'the mole concept' is a generic term for all conceptions of 1 mol and their conceptual surroundings before the 1971 decision of the GCPM.

[6] According to Swedish law, SI should be taught in all educational institutions. In 1965 it was decided that SI should be followed in Swedish schools. See, *Aktuellt från Skolöverstyrelsen* [The National Swedish Board of Education Newsletter] 1964/65: 13, p.193.

[7] Cf. Weninger (1959) about the use of the term 'portion of substance', referring to concrete things.

introduced the term 'Mol.' (Ostwald, 1889). Later on the capital letter M and the full-stop were dropped and the notion eventually turned into 'mol'. Ostwald's contemporary, Nernst (1890), introduced the phrase 'Gramm-Molekül' with a similar connotation. Both terms were also used as denotations of the very concrete portion (with the mass '1 mol'!) of matter involved in a chemical reaction.

Ordinary macroscopic measurement of mass show that

4.03 g	***combines***	32.01 g	***and***	36.04 g
hydrogen	***with***	oxygen	***gives***	water

expressed in moles

2 mol	***combines***	1 mol	***and***	2mol
hydrogen	***with***	oxygen	***gives***	water

When the atomic theory was experimentally verified and scientifically accepted, empirical observations of invariant masses on the macro level were interpreted as a consequence of invariant masses of individual atoms on the micro level.[8] Hence, the mole became a kind of 'bridge' between the non-visible corpuscular micro-world of atoms (elementary entities) and matter conceptualised in the every-day perspective as continuous.

$$2H_2 \circ O_2 \rightarrow 2H_2O$$ [9]

$$2 \cdot 2 \cdot m(1\ \mathrm{H}) + 2 \cdot m(1\ \mathrm{O}) = 2 \cdot (2 \cdot m(1\ \mathrm{H}) + m(1\ \mathrm{O}))$$

where $m(1\ \mathrm{H}) = 1.008$ u is the atomic mass of hydrogen and

$m(1\ \mathrm{O})=16.00$ u is the atomic mass of oxygen (atomic mass unit, 1 u [10])

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[8] This interpretation was taken as a hypothesis in Dalton's atomic theory (Dalton, 1808).

[9] Ordinarily the plus-sign is used in chemical equations. Since no mathematical (arithmetical) addition is meant, a sign of composition (°) is chosen and read as and (cf. Weninger, 1979b, p. 211).

[10] Since 1961 atomic masses have been measured in relation to the atomic mass constant $m_u = m_a(^{12}\mathrm{C}) / 12$ (SI unit; kg). In the IUPAC recommendations (Mills *et al.*, 1988, p. 19; Mills *et al.*, 1993, p.20) it is said that m_u is equal to the *unified atomic mass unit*, with the symbol u, i.e. $m_u = 1$ u. Even if it is not a part of the SI, it will continue to be used in appropriate contexts (ibid., 69). Thus, $m\ (1\ ^{12}\mathrm{C}) = 12$ u.

$$2\cdot 2\cdot 1.008\ \text{u} + 2\cdot 16.00\text{u} = 2\cdot (2\cdot 1.008\ \text{u} + 16.00\text{u})$$

$$4.03\ \text{u} + 32.00\text{u} = 36.04\ \text{u}$$

As a logical consequence of the atomic interpretation of the fixed (invariant) masses involved in macroscopic chemical reactions, 'the mole' can also be identified as equal to a fixed number, Avogadro's number or Loschmidt's number of atoms with individual invariant mean masses, (cf. e.g., Pohl, 1958; Kieffer, 1961; Lee, 1961; Westphal 1963). According to the empirical findings presented in this study this last connotation of 'the mole' is currently the most common conception among educators and students.

Through organisations in the scientific society, mainly IUPAC, IUPAP[11] and ISO[12], the 14th meeting of the General Conference on Weights and Measures (CGPM) in 1971[13] decided on introducing the physical quantity *amount of substance* and the unit 1 mol in SI accounting for the measure of substances conveyed in chemical reactions.

> Suivant les propositions de l'U.I.P.P.A., de l'U.I.C.P.A. et de l'I.S.O., le C.I.P.M. a donné en 1967 et confirmé en 1969 une définition de la mole qui a été finalement adoptée par la 14^{e} C.G.P.M. (CGPM, 1971, Résolution 3).
>
> 1° La mole est la quantité de maitière d'un système contenant autant d'entités élémentaires qu'il y a d'atomes dans 0,012 kilogramme de carbone 12.

The value of 1 u in terms of the corresponding SI unit is not exact, since it is dependent on the value of the physical constant, Avogadro constant, N_A, which is determined by experiment. The value of $N_A = 6.022\ 136\ 7\ (36) \times 10^{23}\ \text{mol}^{-1}$ gives $1\text{u} = 1{,}660\ 540\ 2\ (10) \times 10^{-27}$ kg (Cohen & Taylor, 1986). Avogadro constant could be denoted by the alternative symbols L, and N_A (ibid., 35) (IUPAP(3) and ISO(4.i)).

The numerical value of the Avogadro constant N_A, in this thesis denoted N_0, is the conversion factor between the two units of mass the kilogram (1 kg) and the atomic mass unit (1 u). Hence, N_0 could also be interpreted as the exact number of atoms in 0.012 kg carbon 12, viz. approximately $6.\ 022\ 136\ 7\ (36) \times 10^{23}$.

1 Da (one Dalton), as synonym of 1 u is sometimes used in biochemistry but is not approved by CGPM.

[11] International Union of Pure and Applied Physics, IUPAP.

[12] International Organization for Standardization, ISO.

[13] Bureu international de poids et mesures, Le Système International d'Unités, 2^{e} Edition, Paris 1973, p. 8.

> 2° Lorsqu'on emploie la mole, les entités élémentaires doivent être spécifiées et peuvent être des atomes, des molécules, des ions, des électrons, d'autres particules ou des groupements spécifiés de telles particules.
>
> Cette définition de la mole précise en même temps la nature de la grandeur dont la mole est l'unité.

The definition translated[14]:

> The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12.
>
> When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.
>
> This definition of mole determines at the same time the nature of the physical quantity of which the mole is the unit.

To avoid common misinterpretations of the definition some facts must be emphasised.

According to the coherence of base physical quantities and quantity calculus, *amount of substance* is a mathematically continuous variable measuring a property framed by the theory of continuum physics.

According to the definition it is essential to notice that it is the *system* that contains "...as many elementary entities as..." and not 1 mol that contains these elementary entities. 1 mol is an abstract entity, a unit, of the physical quantity *amount of substance* and could not contain anything.

The last sentence in the definition states the fact that *amount of substance* is one of the seven dimensionally independent base quantities in SI. It is not explicitly defined, but its nature is determined by the definition of the base unit 1 mol. This is in agreement with other base quantities in SI, e.g. the physical quantity *length* whose nature is not defined but determined by the definition of 1 m. However, the natural referent (phenomenal referent) of *length* is the property of one-dimensional spatial extension. According to the inherent logic of physical quantities, *amount of substance* ought to have physical significance as well. *Amount of substance* is a property of a physical system.

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[14] *The International System of Units*. Translation approved by the BIPM, Page, C.H.; Vigoureux, P.: Editors. Her Majesty's Stationery Office: London, 1977.

Prior to the contemporary meaning of *amount of substance* (Ger. Stoffmenge, Fr. quantite de maitiere, Sw. substansmängd), the phrase connoted a concrete portion of matter, a mass, or sometimes, especially regarding gases, a number of molecules (Burger, 1983, p. 75). Its contemporary physical significance or reference is discussed below.

Originally the International System of units (SI) was adopted by the 11th CGPM in 1960. The general characteristics of SI is found in the IUPAC recommendations:

> It is a coherent system of units built from seven *SI base units*, one for each of the seven dimensionally independent base quantities (...) : they are the metre, kilogram, second, ampere, kelvin, mole and candela, for the dimensions length, mass, time, electric current, thermodynamic temperature, amount of substance, and luminous intensity, respectively. (...) The *SI derived units* are expressed as products of powers of the base units, analogous to the corresponding relations between physical quantities but with numerical factors equal to unity (...).
>
> In the International System there is only one SI unit for each physical quantity. This is either the appropriate SI base unit itself (...) or the appropriate SI derived unit (...). However, any of the approved decimal prefix, called *SI prefixes*, may be used to construct decimal multiples or submultiples of SI units (...).
>
> It is recommended that only SI units be used in science and technology (with SI prefixes where appropriate). Where there are special reasons for making an exception to this rule, it is recommended always to define the units used in terms of SI units. (Mills *et al*., 1993, p. 69)

1.2 The adherent educational domain

Problems in teaching and learning connected to stoichiometry have partly been linked to difficulties in grasping 'the mole' and partly to problems with the mathematics involved, especially proportionality. Also the format, the number of steps, and the general complexity of stoichiometric tasks, has been considered as major factors contributing to the experienced problems. Several attempts have been made to identify, describe and eliminate these sources of troubles, as have suggestions to facilitate the teaching of 'the mole' (for a brief review, see, Lybeck, Strömdahl & Tullberg 1985b, pp. 3-5;).[15]

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[15] A distinct route was followed in the late DDR, as reflected in textbooks (Autorenkollektiv, 1977) and in the journal *Chemie in der Schule* (Arndt, 1973; Osterwald, 1973; Osterwald, 1975; Schellenberg, 1974; Buschmann, 1975;

As regards the foundations of the mole and *amount of substance,* Dierks (1981) reviewed about 300 journal articles especially concerning problems emerging in connection to the 1971 definition. Dierk's review is also a condensed historical survey of the domain up to 1980, starting with the discussions in FR Germany in the early 1950's. A most intense discussion was about whether it was necessary to furnish the 'unit' 1 mol with a physical quantity, '*Stoffmenge*' (*amount of substance*). The aim was evident:

> It is plain from the questions raised and the comments made that the issue stems from the desire that 'quantity calculus' [...] be used in scientific calculations. (Dierks, 1981, p. 146)

A most radical claim has been put forward by Weninger (e.g., 1982b). Based on extensive theoretical studies, it is Weninger's conviction that *number* is the only appropriate quantity to use in stoichiometric calculations[16]:

> Wenn Stoffmenge und Anzahl einander immer und überall proportional sind, ist eine der beiden Größen, und zwar - aus den angefürten Gründen - die Stoffmenge, überflüssig und sollte daher aus dem Größensystem eliminiert werden. Daß man mit der Stoffmenge rechnen kann, besagt nicht, daß sie eine sinnvolle Größe ist. (Weninger, 1982b, p. 30)

Amount of substance is conceptualised as a 'construction', without any reference to reality,

> Ich möchte darauf aufmerksam machen, daß der Name "Stoffmenge" (...) keine physikalische Größe bezeichnet, sondern ein Konstrukt, dem in der Realität nichts entspricht. (Weninger, 1982b, p. 30)

Wegner, 1978; Leitz, 1979). The status of *amount of substance* as a physical quantity and 1 mol as a unit as well as the use of quantity calculus in alignment with SI was unreservedly applied. Before the emergence of the SI definition of 1 mol Wenzel & Krystoph (1969) presented, besides the traditional identification of 1 mol as individual masses, the possibility of using 1 mol as a unit for the base physical quantity amount of substance (Ger. Stoffmenge) based on the decision of IUPAP 1957 and the acceptance of that decision by IUPAC 1967. Their article took its point of departure in Dürselen (1964) and Wenzel (1967) who had accounted for different definitions of the mole. The educational result of the DDR approach is not known.

[16] This quotation and following quotations in the German language are chiefly confirmatory statements in addition to the current text. Those who are not familiar with German could leave them without loosing the main thread of the text.

According to Weninger, *amount of substance* is redundant and should be deleted from SI (on Weninger's detailed criticism of *amount of substance* see, chapter 6).

However, as discussed below, *amount of substance* can be well-founded as a mathematical idealisation of the particulate nature of matter on the microlevel to make the metric of the variable *amount of substance* mathematically continuous ($n \in \mathbf{R}_+$) on the macrolevel. Whether this is scientifically sound, beneficial, or convenient must be a question for the decisionmakers of the scientific community. A stipulative definition is never right or wrong, its acceptance is a question of negotiated agreement.

The introduction of *amount of substance* as a physical quantity, to adjust the historical 'mole' to the base SI-unit 1 mol, although obeying the demands of the theory of physical quantities, did not satisfactorily solve the conceptual problems united with 'the mole'. No conceptual agreement has been reached in praxis. Still, there are different conceptions and opinions about the meaning of the mole and *amount of substance*. The long-lasting and ongoing discussion is further reflected in a broad review of the German and American discussion by Lybeck, Strömdahl and Tullberg (1991).

In-depth studies on the mole and *amount of substance* have been made by Weninger (e.g., 1970, 1977, 1979a, b, 1980, 1981, 1982a, b, 1983, 1985, 1990), Dierks (1980a, b, 1981) and Rang (e.g. 1985, 1987a, 1987b, 1988). Weninger has approached the domain from a multidimensional point of view including educational, historical, philosophical and physical quantity theoretical aspects.

1.3 A methodological separation of the knowledge content and educational domains

Most studies concerning 'the mole' (*amount of substance* is marginally studied, except by Weninger, Dieks and Rang) have been done in an educational perspective concerning students' 'misconceptions'. However, the researcher's own conception of 'the mole' is often loosely thematized. It seems to be implicitly taken for granted as 'the prevailing scientific' or the educationally 'correct' one. With such an approach there are some methodological problems introduced. If the taken for granted conception is made a base for forming a judgement of students (mis)conceptions there are risks that mistakes can be done. Expressions

used in research reports such as 'mole concept', 'number of moles', 'mole contains Avogadro's number of particles', 'mol represents a big number of atoms or molecules' represent certain standpoints which are not consistent with the legitimate scientific definition of 1971.

To get a solid base about 'the mole' and *amount of substance* in an educational perspective presupposes a thorough analysis of the intended scientific meaning of these concepts.

The difficulties in separating the scientific and educational domains are obvious, even when good intentions are present. For example Allsop (1977), a researcher with an educational approach, explicitly intended to create conceptual clarity about the SI definition but fell back into traditional conceptions of 'the mole':

> ... the mole is simply the official unit of amount, and if there is a concept involved it is that of amount of substance. In a pedantic world we would have to amend our phrase to 'the concept of amount of substance whose unit is the mole', but this seems unlikely to occur in everyday usage. (Allsop, 1977, p. 286)

Is conceptual clarity pedantic? Why not an everyday usage of the statement "..*amount of substance* whose unit is the mole,..."? (cf. the base physical quantity *mass* whose unit is the kilogram and *length* whose unit is the metre). Besides, scientific clarity is not improved by denoting *amount of substance* as 'a concept' and not a physical quantity. Especially when 'a concept', as defined by Allsop (1977, p. 286), is a "generalisation or name of a class of objects with common features". Further, the expression 'the mole concept' is used throughout the whole article maintaining conceptions of mole prior to the 1971 definition. This is notable in view of Allsop's intentions:

> Above all, the mole concept gives a coherent pattern to the teaching of elementary chemical theory, providing a powerful structure for later development whilst removing diffuse and difficult historical ideas which formerly frequently confused. (Allsop, 1977, p. 288)

In the prevailing situation several parties, both educational and subject-scientific, have dealt with the complexity regarding 'mole' and *amount of substance* as pointed out by Dierks (1981).

However, even in two recent educational studies on 'the mole' by Staver and Lumpe (1993; 1995) the conceptual situation is fuzzy. For instance, they use the expression 'the mole concept' in spite of the fact that their explicit intention is to follow SI and IUPAC. These two studies will be briefly analysed in chapter 8 (section 8. 6) via the results of the present conceptual analysis and the proposed theory of concept attainment.

Hence, it seems likely that a clear methodological distinction of research must be maintained between, on the one hand, the legal scientific concept and its intrinsic conceptual features and structure, and on the other hand, the educational problems and demands in connection to that scientific concept. Such a distinction makes it possible to clarify and specify the scientific concept on its own terms and the educational claims and demands on theirs.

The methodological separation is not a position denying an interchange between educational demands and the formation of scientific concepts, but a distinction adopted to make the components of the research area salient and explicit.

The empirical findings show that there are different general beliefs among the educators about general teaching and learning as well as what is necessary, possible and desirable to teach to students. Moreover, different conceptions of science and a scientific approach among educators call for an urgent need of the applied methodological distinction.

Educational adjustments of scientific concepts often mean simplifications and sometimes distortions of the original meaning. If subject matter in teaching and learning should be in agreement with science and scientific conventions the point of departure must be taken in the entire scientific domain.

The prevailing scientific standpoint can be discussed, but it is another issue to discuss different pedagogical approaches concerning how to teach a scientific concept. In the present case the scientific society has, through international organisations, decided on a convention (CGPM, 1971). From this scientific convention there is scope for pedagogical creativity in designing appropriate teaching and learning strategies, but no room for distorting the meaning of the scientific concept, without being explicit about such deviations.

In view of the applied methodological distinction, the traditional expert-novice distinctions must be handled with care. Should expertise be based on criteria of knowledge of the scientific domain or the educational domain, or to both? Assume a teacher's conceptual

behaviour is classified, in educational stoichiometric problem-solving, as corresponding to an 'expert' by meeting certain criteria accounting for an algorithmic, straightforward and successful outcome. Does this necessarily mean that the educator has got 'expert' knowledge of the underlying conventional scientific concepts? No, there is no logical relationship between a successful algorithmic approach and a scientific comprehension (cf. Niaz, 1989, p. 424).

Thus, even if the problem-solving is judged as 'effective in praxis' and the teacher could be taken as a skilful performer, s/he could not be labelled as an 'expert' according to criteria accounting for a 'scientific conceptual approach'. Due to these circumstances, categorisation in the 'expert-novice' perspective does not seem to be either appropriate or fertile in the present research approach.

The scientific domain under investigation, quantity calculus and the SI conventions, are intrinsically scientific. No direct connection to everyday phenomena is present concerning the mole and *amount of substance*. No conceptions about the mole and *amount of substance* is to be expected before the individual has met the domain in formal education. Revealed conceptions of ‘the mole’ and *amount of substance* are artefacts of education. Hence, conceptions held by educators and text-book authors about 'mole' and *amount of substance* are considered to be of primary concern, because students' conceptions rest on educators' conceptions and conceptions of text-book authors, manifested in text-books and transferred to the students via the educational process. On a collective level, this connection is confirmed in the empirical data. On the other hand, concepts used in connection to 'the mole' such as 'particle', 'amount', 'dozen' and 'substance' are biased by everyday language comprehension.

1.4 Aims

In accordance with the methodological distinction made about scientific knowledge content interest and educational knowledge interest, two main tracks are followed in this investigation. On the one hand, the rise, development, nature and relevance of empirically found conception(s) of the scientific concepts, as they are communicated by individuals in the Swedish educational system. On the other hand, the rise, development, nature and relevance of the persistent scientific convention on *amount of substance* and 1 mol. This approach makes it possible to articulate and make explicit the tension in the encounter between educational 'praxis' and scientific 'theory', viz. how 'the mole' is virtually used by individuals contrasted to the scientific definition.

Considering the components of that encounter, a theory of attainment of scientific concepts is elaborated. It aims at making the process of concept attainment explicit, thus contributing to an explanation of the low attainment of the SI definition among the educators.

The aim of the thesis can be stated more precisely as the effort to answer the following three questions:

* How are the actual scientific concepts attained?

* Why have educators not attained the SI-definition?

* What educational implications can be concluded from the answers to these two questions?

1.5 Disposition

Chapter 2 is a brief survey regarding the general research traditions on conceptions of scientific concepts compared to the approach in this thesis. Especially the notions 'misconceptions' and 'conceptual change' are discussed. Some notes about terminology used in the thesis are made.

The empirical results presented in chapter 3 is the point of departure of the research problem discerned. The main emphasis is put on the results of the interviews with 54 chemistry educators. However, the general perspective is the broader context concerning both educators, trainee teachers and students, vertically through the educational system in Sweden. Hence, the data and results from studies on students and trainee teachers are included throughout the entire investigation. This approach makes it possible not only to see conceptions isolated for each group of subjects, but also to ascertain the mechanism of the dynamic transfer of knowledge traditions from teacher to student. A rationale for the qualitative research methodology on individuals' conceptions is also included in chapter 3.

The formation of the mole and *amount of substance* within the scientific community resulting in the 1971 SI decision are reconstructed out of historical data (chapter 4). This is followed by a conceptual analysis of *amount of substance* as it is treated in the present IUPAC manual *Quantities, Units and Symbols in Physical Chemistry* (Mills *et al.*, 1988; 1993) (chapter 5). In chapter 6 the critical position of Weninger regarding the physical quantity, *amount of substance*, is accounted for. Preparatory to the elaboration of a theory of concept attainment, some assumptions of concepts are established in relation to an exposition and commentary of some actual theories of concepts and conceptual change. (chapter 7). Via the proposed theory the actual concepts and conceptual processes of the domain are made explicit (chapter 8). Finally the thesis is completed with a chapter on educational implications (chapter 9) followed by a general discussion (chapter 10).

As noted in footnote 16, quotations in German are briefly confirmatory statements in addition to the current text. Those who are not familiar with German could ignore them without loosing the main thread of the text.

CHAPTER 2

A COMMENTARY ON SCIENCE EDUCATION RESEARCH

Educational research on conceptions of different phenomena dealt with in science have mostly been restricted to children, pupils and undergraduate students. Early contributions concerning physics are e.g. Hall and Brown (1903), Banholzer (1936) and Zietz (1938). Oakes' (1947) bibliography lists about 110 publications on children's explanations of natural phenomena.

In the early 1970's this type of research increased immensely. General reviews on research on scientific concepts are e.g. Driver and Easley (1978), Driver and Erickson (1983). Mc Dermott (1983) has in his review focused research reports on dynamics and kinematics, and Driver (1989) and Tiberghien (1983) heat, temperature, light and electricity. Pfund and Duit (1994) is an extensive bibliography of reports regarding students conceptions of phenomena within the natural sciences, updated at regular intervals. The latest edition (1994, 4th edition) encloses around 3500 references.

In Sweden, Andersson (1976) has studied science education and the development of thinking in a piagetian perspective, Kärrkvist (1985) has investigated conceptions of electric circuits among 13-16 year old pupils, Renström (1988) conceptions of matter among 13-16 years old pupils, Neuman (1987) conceptions of elementary arithmetic among primary school pupils, Halldén (1988) pupil and school perspectives on the evolution of species, Bergqvist (1990) about learning by pupil-centred experimentation, and Pedersen (1992) how student understandings of complex biological concepts (evolution by means of natural selection) develop during the later compulsory school (grade 7-9, age 13-16). Helldén (1992) has focused primary school pupils' (grade 2 to 5) conceptions of ecological processes.

The investigations done by Lybeck (see e.g., 1981) on density and proportionality among 16-19 years old students have also led to the generation and development of a pedagogical content knowledge research model.

At the university level, technology students' conceptions of force and motion have been investigated (Johansson, 1981; Svensson, 1989) .

Educators' (teachers, authors of textbooks, lecturers at the university) conceptions of concepts and phenomena in science have been less investigated. Among the growing number of reports are e.g. Ameh and Gunstone (1986), Arzi, White and Fensham (1987). Some recent studies include primary school teachers' conceptions of energy (Kruger, 1990), force and energy (Kruger, Palacio & Summers, 1990), electric current (Webb, 1992) and the earth's place in the universe (Summers & Mant, 1995). Chin (1992) has investigated preservice science teacher conceptions of proportionality.

Extensive studies have been made about expert-novice behaviour concerning problem-solving, including various scientific domains enclosing both students and teachers (e.g. Larkin & Reif 1979; Larkin, McDermott, Simon & Simon, 1980). Several studies on teachers' and trainee teachers' conceptions of teaching and class-room activities specifically linked to the expert-novice perspective have also been accomplished (deGroot, 1965; Chi, Feltovich & Glaser, 1981; Fredricsen 1984; Berliner, 1987, 1988; Calderhead, 1983; Carter *et al.*, 1987, 1988; Leinhardt and Greno, 1986). Associated to the last approach, Lybeck (1981) and Schulman (1986) have stressed the need for research dealing with subject-pedagogical content knowledge.

Implications of research on teachers' belief structures has been exposed by Kagan (1992) and a critical review of the domain has been delivered by Pajares (1992).

Educational research on concepts and conceptions is linked to the classic philosophical (ontological and epistemological) and psychological research about concepts, concept-formation and conceptual change. Several epistemological and psychological theories and methods have been adopted. Constructivism in different versions seem to be the dominant epistemology (cf. e.g., Driver,1985; von Glasersfeld, 1989; Novak, 1987; Solomon, 1987; Ernest, 1990, 1991). Solomon and Ernest stress the socio-cultural aspect of knowledge construction in science and mathematics.

Driver, Asoko, Leach, Mortimer and Scott (1994) have explicated their view of learning science as involving both individual and socio-cultural processes.

The multi-disciplinary approach of the domain is typically manifested in the classical studies by Piaget through his comprehensive research effort to elaborate a genetic epistemology, based on extensive empirical research on conceptions held by individuals (Piaget, 1970).

In his work Piaget was guided by the striking similarities recognised between children's conceptions of different phenomena and the conceptions of the same phenomena described by the history of science. The analogy of the embryological development dogma that ontogenesis is a repetition of phylogenesis is explicitly stated by Piaget (1930, p. 309).

A substantial portion of educational research on scientific concepts have been carried out within the frames of the Piagetan 'stage theory'. Especially the 'formal stage' has been in focus, since it has been seen as a necessary stage to reach in order to manage abstract scientific concepts. The 'stage theory' has been criticised since no individually stable stage has ever been identified (the problem of 'horizontal décalage'). 'Stages' have turned out to be context-dependent and domain or task-specific (cf. Hundeide, 1977; Donaldson, 1978; Wood, 1988).

Hitherto the most dominant theory of conceptual learning has been the theory of conceptual change elaborated by Hewson (1981), Posner, Strike, Hewson and Gertzog (1982b) and Strike and Posner (1985), which owes a lot to Piagetian theory and the paradigm theory of Kuhn (1962/70). However, criticism has been levelled against this theory (see section 7.6).

2.1 About 'misconceptions'

Contrary to the extensive traditional empirical educational research of concepts and phenomena in science resulting in a categorisation of 'misconceptions', the present research interest is, in accordance with the phenomenographic approach (Marton, 1981) and appointed epistemological standpoints, to find the total variation of conceptions of a specified content domain, phenomenon or concept, without any predetermined valuation of their veracity.

The empirically found variation in conceptions of a concept or phenomenon, together with documented historical data and a critical analysis of the scientific concepts involved, make up a base for generating theories to elicit conceptual ambiguity, indeterminacy and vagueness and to identify educational traps.

In view of the explicit knowledge interest, the use of the terms misconception, naive conception, preconception, children's conceptions, etc. is obsolete. Gauld (1987) has identified more than 20 different such combinations of "basic terms" (e.g., conceptions, ideas, science structures, frameworks) and "qualifiers" (e.g., alternative, children's, personal, mis-). Logically the word 'misconception' is used relative to something that is manifested as a 'correct conception' or 'true conception'. Hence, 'misconception' is used in science education studies as a denotation of a conception which is in disagreement with the prevailing scientific concept. The naming of the research activity evidently reflect a certain standpoint, an ideology or epistemological commitment. Nussbaum (1989) has addressed the term 'misconception' to an empiricist point of view, Gilbert (1983) as a 'realist' view, with its claim of science as *the truth*, verified by careful observations and formal logic. According to that interpretation it is remarkable that the term or its equivalents are sometimes used by researchers committed to constructivism. If a version of constructivism is based on the idea that 'truth' is revealed by plain perception it rests on empiricism or naive realism. However, a view of scientific theories as historically rooted traditions precludes such versions of constructivism (cf. Matthews, 1992a).

Traditional 'misconception research' seems not yet to have paid enough attention to the paradigmatic break with Aristotelism/empiricism in modern science initiated by the Galilean/Newtonian approach of mathematical idealisation to natural phenomena. This is e. g. discussed by Matthews (1992b):

> The philosophical issues associated with idealisation and abstraction in science has of course implications for the massive misconceptions (Helm 1980) or alternative conceptions (Driver and Easly) or naive conceptions literature in science education. To go back to del Monte:[[17]my footnote] he

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[17] del Monte was Galileo's patron, described as the greatest mechanican of the 16th century, insisted that the pendulums he tested was not isochronic contrary to the theory of Galileo. Galileo replied that ideal pendulums was. del Monte was impressed by the mathematics of the ideal pendulum elaborated by Galileo but he

> had no misconceptions about pendulum motion, he only had misconceptions about the new science's view of pendulum motion. It is commonly said that Aristotelians had misconceptions about the real world; it would be more accurate to say that they had misconceptions about the contrived and constructed world of Galileo and Newton, that is the theoretical objects of the new science, not material objects around them. The philosophical issue also has implications for the Piagetian cognitive conflict that is supposedly the motor of conceptual change. To repeat what has been said: experience is very Aristotelian. So much so that one prominent historian of the Scientific Revolution remarked that 'observation and experience...had a very small part in the edification of modern science; one could say that they constituted the chief obstacles that it encountered on its way' (Koyré 1968, p. 90). The recognition of scientific idealisation gives rise to many questions in this area; what is a misconception? is the real world the touchstone against which we judge our conceptions or is the touchstone just another conceptualisation of the world? (Matthews, 1992b, p. 27)

The question could be raised whether the results of 'misconceptions'-research could be interpreted as having revealed 'excluded teaching' about the ontology of modern physics among pupils and students (idealisations, mathematical models, etc.). What seems to be revealed in 'misconceptions-research' is expressions of common-sense theories or theories in 'every-day life world language' (cf. Hills, 1989).

Further, the present type of research and epistemological point of view does not consider the prevailing scientific conception as a basis for forming an absolute judgement, but rather as one among other empirically found conceptions of a defined domain among people. A conception is a conception embedded in an implicit or explicit theory, whether it is called a 'misconception' or not. It is another point that the prevailing scientific conception occupies a place apart in contemporary science, a target to defend and strive at in teaching, if it is in alignment with the teaching intentions.

Another term used is 'mixconception' (Nussbaum, 1989)[18] denoting a retention of old conceptual elements during gradual conceptual change:

> The records of each study's conceptual change suggest that it forms an evolutionary pattern in which the student maintains substantial elements of the old conception while gradually incorporating individual elements from the new one. (Nussbaum, 1989, p. 538)

Nussbaum is here referring to studies made by Nussbaum (1979), Nussbaum and Sharoni-Dagan (1983) and Nussbaum (1985 a,b).

In the empirical investigations the existence of mixconceptions are confirmed (Chapter 3).

2.2 Some preliminaries on the notions concept, conception and conceptualisation

Since this study is dealing both with concepts which are stipulatively defined in science, and individual conceptions of these concepts, it is necessary to make some notes on the semantic and linguistic terms used.

The distinction between concept, conception, conceptualisation and definition in this study is made in the following way:

Scientific concepts are taken in their classical conventional, logical and stringent meaning as denoting a class of phenomena connected by certain determined common properties. The scientific concept is characterised by its range and content. The scientific concept highlights, cultivates and sometimes makes mathematical idealisations of some specific properties, out of the experiential basis of a delimited domain (cf., e.g., Vaihinger, 1920; Nyman, 1951). This is equivalent to defining concepts by giving necessary and sufficient conditions for their application.

In science, concepts are fixed by definitions (conventions, agreements) to be invariant according to sense and reference. This is a necessity in order to make them applicable in logically consistent theories. Hence, most definitions in science are *stipulative* (or *notional*), meaning an explicit prescription of range and content. The range is the set of all phenomena enclosed by the class. The content is the common properties. Range and content is inversely dependent. The wider the range the lesser content and vice versa. The delineated range and content (unequivocal features) of scientific concepts are decisive.

A concept stipulatively defined can not be true or false, only suitable or not suitable for its intentions. The definitions of physical quantities and units in science are of this kind. The stipulative definition is therefore

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did not classified it as physics, which was dealing with phenomena in the real world. Not only del Monte but also Huygens disbelieved Galileo's claim.

[18] This is an educational parallel to Toulmin's (1972) standpoint in the philosophy of science that conceptions gradually change

of special interest in the present investigation of *the mole* and *amount of substance*.

Other types of definitions discussed in this study are lexical, operational and ostensive definitions.

The *lexical* (descriptive or dictionary) definition is a description of how a concept-word is used in praxis within a specified speech community. A lexical definition can be true or false. Common errors of the lexical definitions are that they are inadequate viz. too wide or too narrow or are circular. Two important properties of lexically defined concepts are *ambiguity* and *vagueness*. Classical philosophical studies of vagueness have been made by Russel (1923, p. 85), Körner (e.g. 1960; 1975), Black (1937) and Hempel (1939). A critical analysis of the classical studies of vagueness as well as a development of a new theory of vagueness has been elaborated by Rolf (1981).

The empirically revealed categories of description in the present investigation could be regarded as qualitatively separated lexical definitions of the concepts of 'the mole' and *amount of substance*.

The distinction of lexical and stipulative definitions rests on the early elaboration made by Pascal during the 17th century and Arnauld and Nicole (1662).

An *operational* definition of a term is a prescription of the concrete operations, procedures or methods used to establish and measure a special phenomena denoted by the term, e.g. intelligence, creativity, etc. (cf. Bridgman, 1927 about operational definitions in physics).

Making an *ostensive* definition means actually to point out the phenomenon (an instance) which is denoted by the term. Strictly speaking, it is not a definition in conventional meaning but a relation between a word and reality (cf. Wittgenstein, 1967).

A *conception* is an individual's communicated experience of a delimited domain in connection to a defined scientific concept and related phenomena. The features and the open-ended character of conceptions are further developed below.

Conceptualisation is the process of the constitution of a conception.

In this investigation concepts are studied as structured by the semantic terms *concept-word, sense* and *reference* . These terms are not used in an orthodox Fregean sense (Frege, 1892a) but as pragmatic tools in the concept(ual) analysis.

Irrespective of a concept's definition it is an empirical fact that superordinate concept categories are graded structures (cf. e.g., Rosch & Mervis, 1975). For instance in the category *base physical quantities*, *length* is supposed to be a more representative instance of the category than say, *luminous intensity*, providing more information about all category members. Accordingly *length* exhibits a prototype status.

Future details about properties of concepts are found in chapter 7.

CHAPTER 3

THE EMPIRICAL INVESTIGATIONS

What is presented in this chapter constitutes the empirical findings of the conceptions of 1 mol, the physical quantity *amount of substance* and related concepts as they are comprehended and conceptualised by strategically chosen samples (theoretical samples) of educators, trainee teachers and students. Theoretical sampling is chosen to get maximal variation of the conceptions of the actual concepts. The respondents have participated in audiotaped in-depth interviews. The verbatim transcribed interviews are subjected to qualitative analysis. The empirical findings regarding 1 mol have the form of qualitatively distinct categories of descriptions. The chapter starts with an exposition of qualitative method.

3.1 An exposition on methodology

Five methodological issues are considered in the following discussion related to the empirical part of this investigation:

*The general nature of qualitative research
*The applied subject didactic model
*The pheomenographic approach
*The interview and the analysis of the interview
*Validity and reliability

3.2.1 The general nature of qualitative research

The question of the scientific status of results gained by qualitative research methods is under constant discussion. While "objective truth" produced by quantitative research methods in humanistic and social sciences, with natural science as a pattern, has usually been taken as self-evident, severe criticism has often been raised against qualitative research. The main target of criticism is the alleged subjectivity

involved in data collection/production and analysis, meaning validity and reliability problems.

Among the warrants for "truth" in quantitative studies are the well-defined conditions for data collection/production. Data is generated by measuring a quantity (a defined measurable property, trait, construct) with a measuring device (an instrument) resting on a measurement and a predetermined scale. Data is digital, or made digital in the subsequent statistical treatment.

These conditions are presupposed as objective, true and safe for scientific inferences. Validity and reliability tests can be made within the frames of their statistical definitions as warrants for "truth", objectivity and replicability.

What is less stressed is the qualitative foundation forming the measurement theory, which enables the construction of a measuring device and a measuring scale (addressing numerical values to the actual variable (trait, property, etc.). The fact is, qualitative statements precede quantitative measurements, as noted by Cook and Campbell (1979):

> Naive social quantifiers continue to overlook the presumptive, qualitatively judgmental nature of all science. (Cook & Campbell, 1979, p. 93)

In discussing the function of measurement in modern physical science Kuhn (1977b [1961]) argues from the point of history of science

> ...that large amounts of qualitative work have usually been prerequisite to fruitful quantification in the physical sciences. (Kuhn, 1977b, p. 180)

Patton (1990) establishes that:

> Social scientists are exhorted to eschew subjectivity and make sure that their work is "objective". The conventional means for controlling subjectivity and maintaining objectivity are the methods of quantitative social science: distance from the setting and people being studied, formal operationalism and quantitative measurement; manipulation of isolated variables, and experimental designs. (...) Numbers do not protect against bias; they merely disguise it. All statistical data are based on *someone's* definition of what to measure and how to measure it. (Patton, 1990, p. 479)

Scriven (1972) has discussed objectivity and subjectivity in relation to quantitative and qualitative research at some length and shows among other things that objectivity has been mixed up with consensual validation.

Dealing with foundational judgements, the qualitative investigation is not a measuring procedure, but an explorative enterprise, aiming at discovering properties and structures, to reveal meaning and create understanding of the domain under investigation.

In qualitative investigations both quantities and traditional measuring instruments are lacking. For instance, qualitative data collection by the clinical interview method is not a data collection in the meaning of a measurement. Instead, interview data makes up a 'landscape' (a topology) of statements for exploration and discovery with the goal of generating a theory or model of the actual domain.

Qualitatively gained findings sometimes have properties that are salient and quantifiable, making them suitable to the language of logic, algebra and theory of functions. Such properties are qualified to generate a measuring theory followed by the creation of 'measuring instruments'. Data gained by such instruments could then be treated within the usual frames of scientifically legitimate quantitative methods.

Hence, a qualitative investigation is prior to a quantitative investigation. The qualitative investigation is a pre-quantitative, pre-measuring enterprise. In that sense the qualitative and quantitative approaches are complementary.This view is in agreement with Cook and Campell (1979):

> In uncritical quantitative research, measurement has been viewed as an essential first step in the research process, whereas in physics the routine measures are the products of past crucial experiments and elegant theories, not the essential first steps. (Cook & Campell, 1979, p. 93)

All variables in a quantitative investigation must be defined in some way or another. Definition is a qualitative enterprise.

As said above, in qualitative research no measurements are done in a conventional meaning. The term measurement can only be metaphorically transferred to the process of data collection/production in qualitative research. *The interviewer, denoted as a 'measuring instrument', can only be looked upon as a metaphor.*

The metaphorical use of 'measurement' has undesired consequences, through the fact that the psychometric concepts validity and reliability are forced upon qualitative research in a way which obscures the knowledge claims of the qualitative research enterprise.

Data gained in a qualitative study is given in descriptive terms, unfolding salient characters (properties) and structures of the concept under scrutiny.

Establishing a theory from qualitative 'data' is an iterative process. A 'final' theory, with melioristic stability, is reached when new data is satisfactorily 'explained' within the provisional theory. The theory is taken as a 'conjecture' (cf. Popper, 1963), the fittest contemporary suggestion to describe and explain the domain under investigation (cf. Törnebohm, 1983[19]). Its supporting capacity (fitting; convincing force) must be judged out of criteria of good theories and models: e.g. explanatory power, fruitfulness, generation of new questions, ability to be falsified, elegance and not by the instruments testing good measurements.

3.1.2 A pedagogical content knowledge research model

Lybeck (1973, 1978, 1979, 1980, 1981, 1994, 1995a,b; see also Lybeck, Strömdahl, & Tullberg, 1989) has elaborated a pedagogical content knowledge research model for the study of teaching and learning in natural sciences and mathematics. The model concerns structure and level of interaction between the different actors in the educational setting. The structure generates research questions. The answers to these questions establish knowledge with bearing on the praxis of teaching and learning: i.e. knowledge, which could be used as content in e.g. teacher-training education.

The model presupposes a content-related empirical research approach and is aimed at generating authentic descriptions of teaching and learning in classrooms and lecture theatres.

The model for educational studies is developed as an analogue to a theory of scientific growth elaborated by Törnebohm (e.g., 1976, 1983) within the philosophy of science. The influence of knowledge from the humanistic and social sciences is essential. The approach to educational studies in biology, chemistry, physics and environmental studies is both integrative according to method and to results. This type of research defines a new research-field which stresses the integrative structures within the natural sciences and mathematics (cf. Lybeck, 1986, p. 188; 1995a, p. 36) with implications for the educational system. Lybeck (1978) has specified the field of research in the following way:

> Like the theory of science, our discipline (science education) studies human contexts. Using the analogy, we wish to point out that, e.g., the theory of science of physics is not a branch of physics, and that physics education is not

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[19] See Törnebohm (1983) about the LFP (Swe. 'Löpande ForskningsParadigmet'; Eng. 'the running research paradigm').

> a branch of physics. Thus scientific education has demarcation lines with other disciplines. It is of course a reasonable requirement that the researcher in, e.g., physics education has intimate knowledge of physics. Our research territory is not the scientific discipline itself but the thought content of the students in relation to them. And in fact, the content of the students' thoughts can neither be read in books nor said by teachers during lessons. (Lybeck, 1978, p. 5)

The demarcation between the scientific discipline and the study of science education of that discipline corresponds with the methodological separation between the scientific and educational demands in educational settings pointed out above (section 1.3). This distinction is basic, since this kind of research on scientific concepts is not limited to conceptions of the individuals acting in the educational domain, but to the larger context where the scientific concept has its disciplinary habitat. The contemporary scientific concept must be known in detail when contrasted to the conceptions held by both educators and students. Hence, intimate knowledge of the discipline domain is essential in this kind of research.

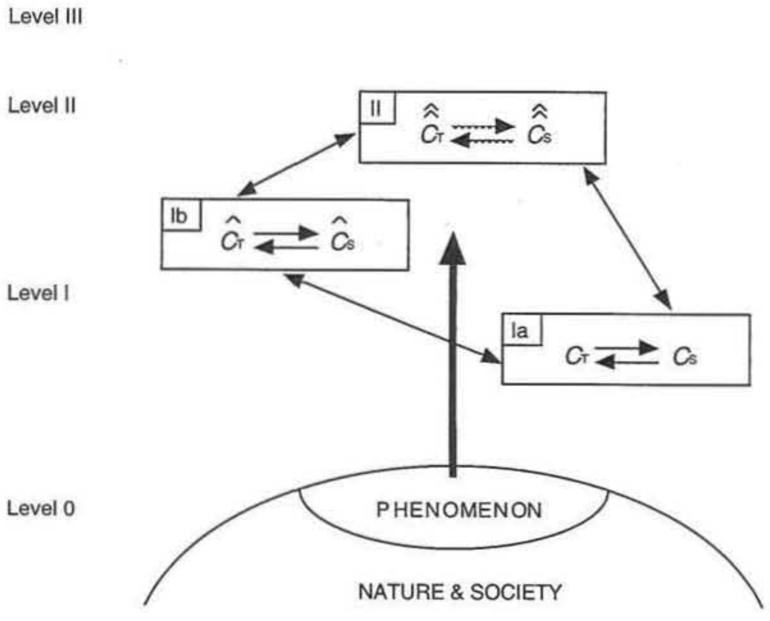

Figure 3.1 Model of subject-didactic problem areas (Lybeck, Strömdahl & Tullberg, 1989).

In the model (see figure 3.1) level Ia represents product concepts (such as density, force, pressure, *amount of substance*, etc.) and Ib process concepts or 'meta'-concepts (e.g. problem, instrument, data, experiment and theory). The arrows within the levels represent dialogue between student conceptions (C_S) and teacher conceptions (C_T). The dotted arrow represents an empirically found less developed dialogue. Only implicit dialogue is registered in this investigation since data has been gained by individual interviews. The dubblecusped arrows denote relationships between the levels. Out of this model the strategic planning of research starts in the Ia level and develops into the other levels. This is done without loosing the relation to the Ia level and the knowledge content or phenomenon (level 0). This is stressed by the bold arrow. Thus, in this and previous investigations we have studied both the teachers' and the students' conceptions (C_T and C_S) of "the mole" and related concepts.

Level II represents the metacognitive level, where educators and students reflect on the content of levels Ia and Ib. In this investigation the reflection on different conceptions of mole as well as reflective suggestions of teaching 'the mole' belong to this level.

The research model has been continuously revised. In 1989 the model was supplemented by a level 0 and a level III (Lybeck, Strömdahl & Tullberg, 1989). The former referring to the phenomenon under investigation and the latter to the implication of the integrated results of levels I and II to the contents of curricula and syllabi in the school system. A detailed description of the model in relation to this and other investigations is to be found in Lybeck, Strömdahl and Tullberg (1989).

Recently Lybeck (1995a) has revised the original model into a model of paradigms and the general structure is now in a form depicted by Fig 3.2.

The revised model is a specification of the levels II and III. Level III is the curriculum/policy level including representatives of local, regional, parliamental and governmental actors as well as actors like employers, trade unions, parents associations, and other organisations in society with interests in the educational system.

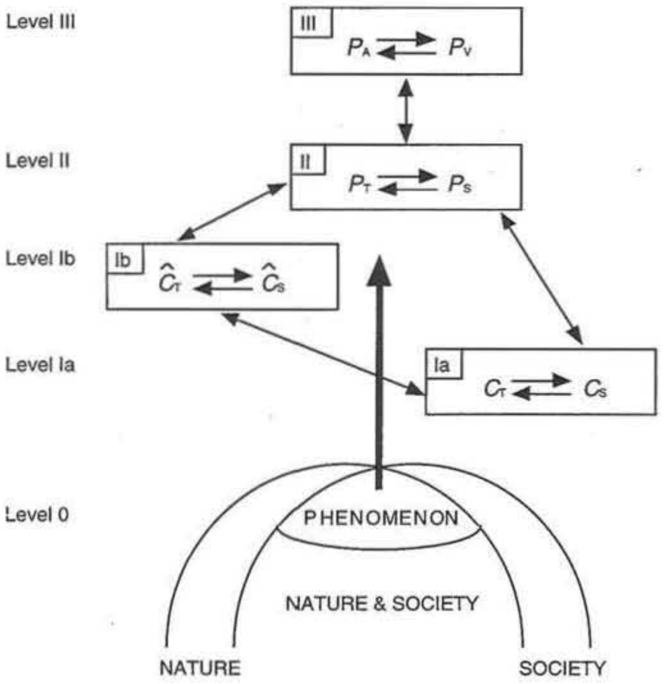

Figure 3.2 Model of subject-didactic problem areas considering paradigms of different actors inside and outside the educational system (Lybeck, 1995a).

The original model has previously been used in research on teacher-student interaction at the upper secondary school (Lybeck, 1981). By the 'mole-studies', the model has been extended to trainee teachers, lecturers teaching subject methods, textbook authors and university subject lecturers. The model has also been applied in studying the supervision of doctoral students (cf. Lybeck & Asplund-Carlsson, 1986) and can be used in other contexts where a 'teacher - student' relation is at fore. The revised model has been applied to environmental studies (e.g. Lybeck, 1994) and a case study, a biographical exposition around the development of a researching teacher (Mellgren, 1995) via a subject didactic learning situation (cf. Lybeck, 1986, pp. 170-179).

The overall research interest is to empirically reveal the total variation of conceptions of strategically chosen subject matter domains among students and teachers on different levels in the model. This is done

within the phenomenographic approach with the revised clinical interview as a data-collection/production method.

Questions raised in this investigation, structured by the model, are for instance: Should the subject content in teaching be in agreement with the prevailing scientific conventions? Which are the paradigms of the teachers on level II. What knowledge traditions are mediated in the discourse between teachers and students on level II ? How well-developed are the teachers conceptions on levels Ib and II ? Are the problems recognised at level Ia a function of the state of the levels Ib and II? What are the implications for the curriculum level (III)?

3.1.3 Phenomenography and contextual analysis

Phenomenography is a qualitative research-programme, aiming at finding out the range of variation of qualitatively distinct conceptions of a defined domain (a phenomenon or a concept). With the attempt to capture all traditional conceptions of the domain, a strategically chosen set of individuals make up the sample investigated in order to gain generality in the results. The general outlines of phenomenography are found in Marton (1981).

Concerning the aims of the phenomenographic enterprise Marton (1986) states:

> Effort is made to uncover all the understandings people have of specific phenomena and to sort them into conceptual categories.
>
> (...)... we cannot specify exact techniques for phenomenographic research. It takes some discovery to find out the qualitatively different ways in which people experience or conceptualise specific phenomena. There are no algorithms for such discoveries. (Marton, 1986, p. 32 and p. 42)

Phenomenographic studies are carried out in what Marton (1981) calls a 'second order perspective', viz. the researcher makes statements about peoples conceptions of the world (statements-about-perceived-reality) and not about the world as such (reality), the latter is called a 'first order perspective'.

This is as Marton (1981) says a pragmatic and very simple distinction, and he makes a reservation:

> The discerning of these two alternative perspectives has nothing to do with the metaphysical distinction between the real and the apparent, or with arguments for or against as to whether there is a reality as such that is accessible to us. (Marton, 1981, p.178)

In spite of this reservation there is still a source of ambiguity when using the expressions 'statements-about-reality' and 'statements-about-perceived-reality' (Marton, 1981, p. 188). Implicitly, the distinction indicates that there are two categorially different realities, a 'directly accessible reality' on the one hand and a 'perceived reality' on the other. Moreover, since all communication about reality is perceived reality, we need to ask if it possible to make statements about reality which are not 'statements-about-perceived-reality'. In short, the objects for study in a phenomenographical approach are individual 'statements of perceived reality' communicated in some context.

In order not to end up in an ontological discussion, it seems necessary to make an explicit methodological separation between the 1st and 2nd order perspectives by a distinct use of language. In the 2nd order perspective the researcher **is directed** towards **individual descriptions of the world** (may be written, drawn or orally distributed) while in the 1st order perspective the researcher is **directed** to **the world**.

This separation is in agreement with Marton (1981):

> In the first (...) we orient ourselves towards the world and make statements of it. In the second perspective we orient ourselves towards people's ideas about the world (or their experience of it) and we make statements... (Marton, 1981, p. 178)

The statements made by respondents in phenomenographic research and constituted into categories of description by phenomenographic researchers are always statements of content, viz. statements of the 'subject matter' (P). In Marton's terminology, statements in the first order perspective.

When forming the categories of description the researcher makes statements of P on the basis of peoples (students, teachers, etc.) statements of P. Thus, the 1st and 2nd perspectives are complementary.[20]

The historic dimension as well as the melioristic nature of knowledge is also noted by Marton (1981):

> New forms of thought are thus introduced from time to time and become, through being transformed to common categories of interpretation, parts of "the perceived world". This is one of the reasons why an "ultimate" description of human thinking can never be achieved. (Marton, 1981, p. 197)

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[20] The separation in two perspectives is a research methodological distinction.

Phenomenograpy has tuned out to be a multifarious (versatile) approach (cf. Uljens, 1989) but some general invariant elements are discerned: delimiting a research-domain, formulating some kind of interview-task, data-gathering (predominately by the interview-method, audio- or videotaped), 'contextual analysis' of transcribed interviews, constitution of conceptions and categories of description based on the transcribed interviews, ending up in a set of categories of description (an outcome-space).

Five foundational methodological assumptions within phenomenography will now be described:

i) the human-world relation; a non-dualistic ontological position
ii) the choice of respondents
iii) constitution of conceptions and categories of description
iv) research method
v) contextual analysis
vi) the tenability of the set of categories of description, the outcome-space

The human-world relation

Conceptions are constituted in the relationship between man (M) and a world phenomenon (P). The unique individual relation M--P emerges due to context. Thus, the conception of an individual is uniquely context-dependent[21]. However, an individual M--P is more or less stable over different contexts, a fact only accessible through empirical investigation.

In principle, there are as many conceptions as there are individuals, since every individual has a unique cognitive biography. A conception is an individual description, a delimitation and determination of a concept or phenomenon in focus. However, the respondent's 'true conception' in some absolute sense (if there is such a thing), or 'lived' conception is not possible to determine. It is the conception communicated in dialogue with the researcher (interviewer) in the actual context that is the object of the analysis. It is the redundancy, the articulation and the confirmatory statements made by the respondent in the

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[21] The 'conception of a an individual' should be taken as the individual acting and reasoning in agreement with a conception, participating in a discourse, rather than 'having' that conception.

interview that makes up a sound data base for discerning the conception.[22]

The individual conceptions contain elements and structures which transcend individuality due to their presence in the overt communication of other individuals. A fact that reflects the social dimension of cognition. At a collective level, as an expression of a common semantic linguistic community, conceptions vary within a limited range. The trans-subjectivity (or inter-subjectivity) permits a classification of the conceptions into a limited number of categories, which are separated through their semantic differences. The claim on the categories is that they should be qualitatively distinct, 'incommensurable'.

The relation between conceptions and categories of description is articulated by Marton (1981):

> A conception exists in the real world only in terms of a mental act and it is exhibited by someone who does something in a certain setting. In talking about categories of description, then we "bracket" the dynamic-activity perspective and we consider the categories almost as if they were "frozen" forms of thought. (Marton, 1981, p. 196)

From an ontological point of view, the phenomenographic description of the nature of the human-world relation is now influenced by the philosophy of modern phenomenology initially elaborated by Husserl (e.g. 1900/1901).[23] The phenomenological approach is an attempt to overcome the dichotomy of objectivism and rationalism, traditionally supported in western thought.

The concept of *intentionality* introduced by Brentano (1874) is also a key-stone in phenomenography, as well as in the philosophy of phenomenology. Consciousness is always directed towards some kind of content.

Several concepts used in phenomenography are imported from phenomenology. However their connotations are altered and given a more methodological character in the phenomenographical praxis

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[22] It is what is overtly communicated (linguistically shown) in the interview and audio- /video-taped in interviews and verbatim transcribed that is the *data*, no claim is made whether this is the *true* conception of the individual. By this approach there is some kind of behaviourism in the phenomenographical approach, a 'linguistic-semantic behaviourism'.

[23] Cf. Hegel (1807) as a forerunner.

compared to the epistemic, ontological, philosophical tenor within phenomenology. For instance, the phenomenological concept 'epoché', the 'putting into brackets' is in phenomenography given the methodological meaning 'bracketing' the researcher's presuppositions about a concept or phenomenon in focus to be open to conceptions held by the respondents, trying to understand them on their own terms. When looked upon as a method (a set of methodological rules), the ontological terminology of phenomenology seems to lack relevance to phenomenography. In a recent report about the relationship between phenomenology and phenomenography, Uljens (1992) says:

> ...phenomenography is an empirical science whereas phenomenology again is an epistemological project. (Uljens, 1992, p. 1)

The choice of respondents

Respondents in the present phenomenographical investigations are strategically chosen by theoretical sampling (cf. Glaser & Strauss, 1967), with the aim at getting maximum variation in conceptions to guarantee generality of the established results, the categories of description.

The number of respondents in a phenomenographic study varies depending on subject matter considerations.

Constitution of conceptions and categories of description[24]

Based on repeated empirical observations, the phenomenographical approach presupposes a limited number of qualitatively distinct ways of conceptualising or experiencing a defined domain These *categories of description* are summarised under the denotation *outcome-space*. The categories are never known or defined in advance, they are genuine products of the empirical and theoretical research process. This process can be characterised as an interplay between empirical data and certain thematized perspectives. Among a 'complete' set of *categories of description*, one will coincide with the scientific concept. The number of categories of description varies across different investigations. The outcome-space, together with a distribution of the respondents among the categories is the main result of the phenomenographic study.

About the applicability of the decontextualized categories of description in new contexts Marton (1986) has stated:

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[24] About a recent discussion of the status of the terms *conception* and *categories of description* see, Säljö (1994), Marton (1995) and Marton and Booth (in press).

> ...we end up with categories of description which, though originating from a contextual understanding, are decontextualized and hence may prove useful in other contexts other than the one being studied. (Marton, 1986, p. 34)

The decontexualisation is made visavi the original actual context in the interview situation documented through the transcribed interview. In fact, the categories are never decontexualised in an absolute sense, since they belong to potential contexts where they have significance. The status of the decontexualised 'category of description' is similar to a *lexical definition* (see section 2.3) of a concept or phenomenon.[25] Hence, Marton's notion "may prove useful in other contexts" is too weak, since the general applicability of the set of categories of description in new contexts is essential. Viewed as a part of a theory the general applicability is conclusive for its resistance against falsification.

The categories can be formally looked upon as discrete 'values' of the concept denoted by the concept-word or phenomenon (the linguistic or perceptual 'sign'). Formally, sense and reference (S, R) of the concept denoted by the concept-word (W) can be seen as a function with the functional relationship

$W = f(S, R)$

Thus the phenomenographic investigation ends up in a set of categories of descriptions, an outcome-space, of the following shape:

$W = f(S_1, R_i)$
$W = f(S_2, R_{ii})$
$W = f(S_3, R_{iii})$
.
.
.
$W = f(S_n, R_j)$

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[25] The categories of description resemble qualitatively separated lexical definitions (cf. Marton (1981, p. 196) characterising categories of description as *"frozen" forms of thought*). Originally their status could be any type of definition. The fact that the phenomenographic enterprise is directed to the collective variation in conceptions of concepts supports a view of the outcome-space as a set of lexical definitions.

The result of the phenomenographic investigation is a set of discrete sense and reference 'values' ('non-numerical values') of a concept.[26]

When an empirical observation is made of the variable W (concept, phenomenon) e.g. in an interview, the individual and the actual context is decisive for the 'values', (S_n, R_j).

The phenomenographical approach aims at empirically determining the variation in sense and reference of a concept expressed as distinct categories of conceptions. The approach is similar to empirical semantics (cf. Bolzano, Frege, Russel, Wittgenstein (later period), Naess and Hägerström), an investigation of sense and reference of concepts in manifest spoken and written language.

Marton (1986, p. 35) has characterised the identification of the categories of description as a discovery. Such a discovery is not a 'pure' observation, description or a measurement of some quantity. It is best described as *a prelude to a theory of the actual concept or phenomena.* This view is in alignment with Marton (1986):

> Above all, each category is a potential part of a larger structure in which the category is related to other categories of description. It is a goal of phenomenography to discover the structural framework within which various categories of understanding exist. Such structures (a complex of categories of description) should prove useful in understanding other people's understandings. (Marton, 1986, p. 34)

The tenability of the set of categories is a matter of the extent to which empirical data can be 'explained' within the set. The authorisation of the set of categories of description is analogous to the authorisation of e.g. theories in natural and social sciences.

> ... once the categories have been found, it must be possible to reach a high degree of intersubjective agreement concerning their presence or absence if other researchers are to be able to use them. (Marton, 1986, p. 35)

Similar arguments about qualitative research in general has been articulated by Cronbach (1971).

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[26] It should be stated that a phenomenological analysis of interview data ends up with the essence of a concept, not the variation in sense and reference. (cf. Hycner, 1985)

The claims of general applicability of the categories of description is a salient feature:

> The set of categories is thus stable and generalizable between situations, even if the individuals "move" from one category to another on different occasions.(...)
>
> (...) we can view the results as categories of description considered as abstract instruments to be used in the analysis of concrete cases in the future. (Marton, 1981, pp. 195-196)

Hence, the result of the phenomenographic research, the qualitatively separated categories of description, the outcome-space, could be used as a tool (instrument) in educational praxis (cf. Lybeck, 1978; 1981).

> (...) what is of immediate pedagogical interest is how students' conceptions can be changed by teachers and how better understandings can be arrived at by students (...) (Marton, 1984, p. 44)

Here phenomenography links up with the educational knowledge interest of the pedagogical content knowledge model (see section 3.2.2). This is the didactics of phenomenography (cf. Kroksmark,1988).

In the present study findings in the format of categories of description make up an empirical base to elaborate a theory of concept attainment.

Research method
According to the actual research interest appropriate methods are chosen to gain data.

> (...) we should bring together findings arrived at by highly differing methods. Phenomenography is thus more or less neutral from the point of view of specific research methods. (Johansson, Marton & Svensson, 1985, p. 255)

Interviewing is hitherto the primary method. Data production is resting on the assumption that conceptions are orally and verbally communicable. Verbatim transcribed audiotaped interviews make up the raw-data. Individual conceptions are uncovered from this data. Imaginative ability and aware interventions (conversational tactics) by the interviewer (the researcher) during the course of the interview are crucial for the quality of the data. Wide knowledge of the subject matter (knowledge content domain) as well as knowledge of philosophy of science and history of science of the actual domain are vital ingredients in such an interview approach.

Contextual analysis
Analysis of the respondents' statements in the transcribed interviews are made in the full context in which they are stated in order to make tenable interpretations. This is the essence of contextual analysis. It is an iterative process interchanging between the wholes and the parts. Contextual analysis has analytic, explorative, interpretative and synthetic elements.

Svensson has summarised contextual analysis in the following schema (Svensson, 1985, p.13):

Methods	1. Delimitation of wholes (phenomena) 2. Differentiation of whole qualities representing the nature of the phenomena
Results	1. Description of similarities and differences in meaning of whole qualities in the form of categories and relations between categories 2. Generality in the form of decontextualisation and analogies

The most prominent guideline of the analysis is the searching for differences, similarities (comparative elements) and complementarities (synthetic elements).

> (...) we are looking for structurally significant differences that clarify how people define some specific portion of the world. (Marton, 1986, p. 34).[27]

In the research process the demand of openness, flexibility and creativity is decisive. As well as in the interview phase wide knowledge of the subject matter and knowledge of philosophy of science and history of science of the actual domain are vital ingredients in this phase of the research enterprise. Such knowledge endows the researcher with powerful interpretative tools.

The tenability of the set of categories of description
The uncovering of the conceptions from the verbally transcribed interview and the synthesis of the categories of descriptions are done in a perspective chosen by the researcher. This situation calls upon an

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[27] Note that Marton uses the term 'define' in this quotation, which is additional evidence, or a signal for an interpretation of categories of descriptions as lexical definitions.

explicit account for the applied perspective. Inter-subjective judgement must be possible about the raison d'être and tenability of the perspective.

The tenability of the results depends on:

a) the ability of the interviewer to get the respondent to communicate his/her conception of the concept or phenomenon under investigation (quality of data)

b) the ability of the analyser to uncover the conception (or conceptions) of the respondent from the verbally transcribed interview (quality of analysis).

c) the ability of the analyser to constitute generalised categories of description (quality of synthesis).

3.1.4 The clinical interview

As mentioned above the dominating method of data collection/ production in the phenomenographic research approach is the clinical interview. In the early 1920's, working with Simon in the Binet laboratory in Paris, Piaget adopted the clinical interview. The clinical interview was Piaget's methodological answer to what standardised tests failed to measure about children's' cognitive structures (Piaget, 1929, pp. 3-4).

Though it was the main method of gathering data in his entire research, Piaget only gave his fullest account of the clinical interview as a method, in the introduction to *The Child's Conception of the World* (Piaget, 1929). In the preface to Piaget's first book *The Languge and Thought of the Child* (1926) E. Claparède, a forerunner and collegue at the Geneva Institute, describes Piagets method as an art:

> The clinical method, which is also an art, the art of questioning, does not confine itself to superficial observations, but aims at capturing what is hidden behind the immediate appearance of things. It analyses down to its ultimate constituents the least little remark made by the young subjects. (Piaget, 1926, p. xiv)

The methods of clinical interviewing can be adapted to suit some different goals. Since the research interest is to find out the various conceptions of a defined domain the clinical interview is used *in situ* to make discoveries. This kind of interview is similar to what has been called 'focused interview' (Merton & Kendall, 1946) and 'elite interview' (Dexter, 1970). Two of the characteristic features of an 'elite interview' (as well as some forms of the clinical interview) are letting the respondent introduce his notions of what s/he regards as relevant and to treat registered conceptual deviations as highly valuable in developing the approach to the studied domain.

The clinical interview as a method for making discoveries has some distinct features in the actual studies. Three components are salient: a) a task b) open ended interview c) and contingent questions are asked.

The respondent is presented to a task, aiming at channelling him/her towards the target domain. The initiative to structure and solve the task is given to the respondent. It is crucial to avoid bias, both by setting the introductory questions and the following up questions on the respondents answers. The latter questions are contingent, since they are determined by unpredictable statements made by the respondent.

This semi-structured interview is a technique appropriate to minimise disturbances of the respondent's genuine way of communicating his/her conception of the domain under examination.

What is required from the respondent in the interview is, on the one hand a direct oral account of what is done or thought (thinking aloud), on the other hand a reflection of what was done or thought.

The clinical interview allows a flexible presentation of the task. If this task initially misunderstood it could be posed in an alternative way to avoid failure due to task construction which otherwise could have obscured factual competence.

What is brought up in the interview is heavily dependent on the task presented and questions asked. However, open-ended questions as an invitation to the respondent to unload his/her own dimensions of the focused domain are essential.

The reason for a flexible and open-ended interview is the intention to 'tap off' the conceptions of the respondent to find key meanings and provide a substantial ground covering the collective variation of conceptions. No measurement is done. The activity is pre-measurement, and thus foundational.

Once some discovery is made, the interview method can be used to identify and elaborate it by rich verbalisation to underpin a given answer. This is done by: a) checking reports b) clarifying ambiguous statements c) testing hypotheses.

A sort of experimentation could be made during this phase of the interview by holding some variables constant while others are deliberately varied.

To determine strength of belief, counter-suggestion could be used to challenge the respondents response, however, in a considerate way.

The interviews are verbatim transcribed. Information which is inherent with speech (prosody) is mainly deleted during the transcriptions. However, longer pauses, laughs, and exceptional behaviours, as well as expressions like 'ah', 'eh', 'mmh', etc. are noted down in the transcripts.

The transcripts make up the data (information), 'landscapes' (topologies) which are contextually analysed ('explored') individually and collectively to find out previously unknown 'formations'.

The course of the very special interview regarding 'the mole' is accounted for in section 3.3.

The nodes of the interview

During the clinical interview there is a mutual interchange between the actors.

> Communicating with each other, the interviewer and respondent negotiate an understanding of the subject matter in question, each performing preliminary interpretations of the responses and offering commentary as well as additional questions. (Bruhn Jensen, 1989, p. 96)

Data collection/production is accomplished through language (dialogue), where the researcher, the interviewer, focuses a territory with the intention to release the respondents' verbal cognitive activity of that territory in order to make it overt.

The clinical interview is an iterative process where the data (information) collected reaches a stable state, a kind of saturation point.

> The interaction during an interview between interviewer and respondent(s) is an essentially communicative process. Both parties introduce, re-introduce and develop particular themes while closing off other aspects of the discursive universe. The participants ideally negotiate a form of common understanding, and the process of negotiation becomes accessible to analysis through tapes and transcripts. (Bruhn Jensen, 1989, p. 102)

Every statement made by the respondent is an argumentation for a special perspective or position. However, perspectives and positions

could change during the interview, e.g. due to changes in the contextual situation.

In the relationship subject (S) phenomenon (P) a meaning is emerging, communicated by S in a set of utterances , $u_s(P)$, about P:

$u_s(P) = \{u_1(P), u_2(P), u_3(P) \dots u_n(P)\}$.

In the individual case the relation S-P is provisional, however *temporally contextually stable.*

The communication between the respondent (S) and the researcher (R) is an interchange. The quality of the communication between S and R is decisive for the outcome of the interview. Awareness of the possibility that mutual opaque meanings appear even if genuine communication is intended must be accounted for.

Due to the fact that our respondents are adults and the nature of the research object, the response errors reported by Piaget (1929, pp. 10-11) at interviews with children are negligible. The power-balance between S and R is pointed out by e.g. Theman (1983) as an important factor to observe and control.

Further, R must control his/her latent statements about P, $u_{R,l}(P)$, potentially present, governing current preliminary interpretations of the elements in $u_s(P)$ and his/her explicit questioning and overt statements (comments) about $u_s(P)$. The ambition is that the researcher's overt statements about (P), $u_{R,o}(P)$, shall be minimised, 'put into brackets', and that $u_s(P)$ shall be qualitatively optimised. S shall be 'tapped off' of statements about P, in order to make it possible for R in the phase of analysis to constitute S's conception of P, $C_S(P)$.

Sensitivity and intuition is needed by R, to make the respondent's aspects (determination) of P overt. Dexter (1970, p. 61) has metaphorically stressed that the interviewer "must be able to shift gears rapidly". Posner and Gertzog (1982a) have expressed a similar point of view.

> (...) the clinical interviewer must be continually alert - ready for the unexpected and able to respond to it - for it is that very response which may lead to something unique and essential in the thought of the subject. (Posner & Gertzog, 1982a, p. 198)

R does not have complete control of the meanings of the elements in $u_s(P)$ during the interview. Instant opaqueness is present. Hence, it is utterly important to optimise the number of elements in $u_s(P)$, their quality and their originality. The latter demand is partly reached by surpressing R's overt interpretation of the elements in $u_s(P)$ during the interview. An overt interpretative intervention can distort the respondent's following utterances about P and make them less usable.

In following up phases of the interview, R's interpretation of the elements in $u_s(P)$ must be consciously controlled and used with caution only when other possibilities to clarify the respondents statements are exhausted and R cannot follow the respondent. This is a balancing act, which R must be fully aware of.

3.1.5 Analysis and interpretation of transcribed interviews

Context free literal meaning is a modern myth (Rommetveit, 1988). If knowledge of the world were immediately given, theories would be redundant (cf. naïve realism and empiricism). Scientific problems would be reduced to trivialities. Interpretation and meaning is provisional, bound to time and a social context. Scientific analysis is always interpretative and contestable. Analysis could not be performed without some predisposition and done under a certain perspective. Analysis is made under conceptual 'refraction' (Vološinov, 1973). In contextual analysis raw-data is allowed to structure the analysis (a posteriori-analysis).

The individual conception is embedded in the statements in the actual transcript. The analysis starts with a critical reading of the transcribed interviews, individually and collectively and a comparison of similarities and differences around chosen and cultivated themes. Found variation in the transcripts is the ground for making hypotheses about qualitatively distinct conceptions. In this phase of the analysis subject matter knowledge, knowledge of history of science and theory of science about the delimited domain under investigation is decisive for the synthesis of generating possible categories of description. The generated hypothesis (a hypothetical 'pro'- or pre-category) is re-entered into the empirical data, and it is modified or rejected. This process is repeated a number of times. The categories of description grow out from this iterative process.

The interpretation of the individual interview is concluded in R's utterances about the categorial habitat of S's conception's. This could be partly validated by a confirmatory statement of the respondent when confronted with the result of the research. This kind of validation process has been applied to some of the respondents.

A conclusive review of the phases of analysis
i) All interviews are read through to create a well-arranged impression of the total collection of interviews

ii) Selection and registration of utterances according to contextual meaning on the bases of relevance to the specified domain from all interviews. The quotes obtain their meaning from their interview context as well as from the context of the collected quotes.

The analytical rigor of the method of *contextual analysis* is a crucial point (Svensson, 1976; 1985; 1989; Svensson & Theman, 1983; Marton & Säljö, 1984; Theman, 1985). Individual conceptions are constituted on the basis of internal contextual relations in the individual transcripts.

iii) On the collective level, comparisons are made iteratively between the interpretations of utterances from different individuals. Utterances are brought together into categories on the basis of their meaning similarities, and are separated by identification of significant differences.

Gradually or instantly (there is no explicit time-schedule for this process) a pattern is discerned and constituted, which ends up in the set of qualitatively distinct (incommensurable) categories of description, the outcome-space.

3.1.6 A discussion of validity and reliability

The validity questions in focus in the empirical part of this investigation are: Are there any unidentified categories of descriptions outside the outcome-space? Are the categories of descriptions communicating tenable and qualitatively distinct conceptions? Do they reflect the conceptions "in action" in a scientific and tenable way? Do they reflect the meaning of the respondents statements?

Validity
Within traditional social sciences, validity accounts for the question

> ... are we measuring what we think we are measuring? (Kerlinger, 1973, p. 457)

Validity problems are connected to the uncertainty in the definition of the actual 'quantity' measured. What is going to be measured in social sciences is seldom captured in an unequivocal stipulative definition. 'Measurements' are often a registration of the "on/off" value of dichotomised indicators of a 'construct' (e. g. political power, anxiety, intelligence), which only in a metaphorical way share the well-defined properties of a physical quantity. In research where this metaphor is not accounted for, the result is doubtful. The mis-interpretation of the role of measurement in physics applied to social quantitative research is mentioned above (section 3.1.1).

Cronbach (1971) has explicitly pointed to the necessity of a theoretical ground of measurements gained in what he calls *prior research*, including a theory:

> Construction of a test itself starts from a theory about behaviour or mental organisation, derived from prior research, that suggests the ground plan for the test. (Cronbach, 1971, p. 443)

Validity of the results within the empirical part of this investigation is focused to the tenability of the set of categories of description, taken as a proto-theory of senses and references of the actual concept. It is a question of the 'truth'-status of the set of categories of description.

Traditional demands on 'truth' are:

a) *coherence* (logical truth, alt. deductive, probabilistic, semantic, explanatory truth (cf. Thagard 1992, p. 64)

b) *correspondence* (semantic "truth") arrived at through intersubjective negotiation (cf. intersubjective reliability)

c) *pragmatism* (purpose, predicative "truth") The fertility of the categories of description and their power of prediction are decisive.

Violation of coherence (logical truth, deductive truth) is 'easily' discovered and corrected. However, the "truth"- problem in scientific theories concerning modelling of natural phenomena cannot be determined by formal logic. What is essential to the scientific theory is the empirical demands b) and c), the "truth-resemblance" or "depictive fidelity"[28] (Swed. 'avbildningstrohet'; cf. Törnebohm, 1983, p. 10) and potentiality of prediction, respectively. It is the efficacy of the theory, what it can 'do', that matters.

As long as the scientific theory remains invariant in encounting new phenomena with sustaining power it has depictive fidelity. In other words the kind of validation argued for in the present investigation is a

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[28] Fidelity is used as a term connoting the preciseness of a model's (theory's) representation of a phenomenon.

process where attempts are made to falsify a theory. As long as it resists the attempts to be falsified and proves to be fertile, it is regarded as scientifically satisfying. No further claims on 'truth' are made here.

Even if the categories is firmly established in empirical data, the tenability and generality of them are only confirmed when they are confronted with new contexts, such as new interviews and texts. The set of categories must be constantly exposed to attempts of falsification. In that respect Kvale's (1989, p. 77) statement "to validate is to investigate" is applicable. New interviews could be made with new respondents as well as with former respondents.

The validation of the elaborated theory of concept attainment is similar to theory validation in physical sciences:

> Physical scientists, one notes, speak not of validating a measuring procedure but of validation of scientific theories, as in the title of Frank's (1956) symposium volume [*my note*. Frank, P. (1956). (Ed) The validation of scientific theories. Boston: Beacon]. Since each experiment checking upon a theory is an opportunity to modify or extend the theory, validation is more than corroboration; it is a process for developing sounder interpretations of observations. (Cronbach, 1971, p. 443).

Another form of validity test is respondent validity, which has been performed with some lecturers from teacher education colleges and text-book authors.

Reliability

Reliability is a quantitative measure of the accuracy of a measuring instrument, a measure of the consistency or replicability of measurement accounting for contingent as well as systematic errors. When there are considerable validity problems high reliability is a chimera.

Reliability tests are applicable when quantitative elements emerge beyond the qualitative phase of the investigation. Reliability tests taken as replicability are possible via a detailed account of the procedures and the intention of the actual investigation. This is a prerequisite for an independent researcher to replicate the measurement.

If the set of categories of description is regarded as a 'measuring instrument' and the single categories as discrete values on a measuring scale, the reliability could be measured by letting an independent researcher distribute the single respondents over the established categories of description based on their utterances in the verbatim transcribed interviews. The extent of agreement (in percent) between this researcher and the original researcher is a measure of reliability (inter-rater reliability). The procedure reflects how precise the categories fit or communicate conceptions expressed by the respondents.

In this original piece of research reliability has been negotiated between the members of the research team, consisting of Lybeck, Strömdahl and Tullberg, to reach intersubjective agreement.

Moreover respondent validity has been tested. The results were presented to chemistry teachers at in-service training and to university lecturers at seminars. In taped sessions they have confirmed the categories of description.

Our standpoint is that our results are valid and reliable as long as they resist attempts to be falsified.

3.2 An account of the empirical investigations and participating respondents

The empirical studies were preceded by a pilot study comprising 30 interviews with students following the natural sciences (N) and technology (T) programmes at two upper secondary schools in southern Sweden about 200 km from each other. This was done in October 1981. After some minor improvements, the task and foundational structure of the interview has been used in studies with different actors in the Swedish educational system.

In total 102 respondents have been individually interviewed. All interviews have been verbatim transcribed. Also seminars, adjacent to the individual interviews, with educators have been recorded, verbatim transcribed and analysed.

Distribution of the studies and respondents:

* 30 individual interviews with students on the N-programme in one upper secondary school in southern Sweden in April and June 1982, reported in Lybeck, Strömdahl, and Tullberg (1985). Code names are used for the individual respondents in the following way. Names beginning with an A are referring to students in the 10th grade, B in the 11th grade and E in the 12th grade, ages 16-19. Out of the 30 interviews 29 were available for analysis, as one interview was lost due to a technical failure.

* 18 individual interviews with trainee teachers in May 1984 at one teacher training college in southern Sweden, followed by a recorded seminar including 17 of the trainee teachers, preliminary reported in Lybeck, Strömdahl, & Tullberg (1995).

The respondents are labelled TT (Trainee Teachers) followed by a number (TT1 - TT18).

* 28 individual interviews with educators in 1985 at three different teacher training colleges in Sweden, followed by recorded seminars. Some of these educators were interviewed in a second round, followed by recorded seminars. Results from these interviews are partly reported in this thesis and by Strömdahl, Tullberg and Lybeck (1994); Tullberg, Strömdahl and Lybeck (1994) and Tullberg (forthcoming).

Individual respondents are labelled T1-T13 for teachers at upper secondary schools, M1-M12 for lecturers of method in chemistry at teacher training colleges, some of these are also textbook authors and U1-U3 for university lecturers in Chemistry.

* 26 individual interviews with educators in two university towns in Sweden in October and November 1988 and March and April 1989. The results are reported in this thesis and by Tullberg (forthcoming).

Individual respondents are labelled in alphabetic order TA to TI and then TK, TL, TM, TN, TU and TY for teachers at upper secondary schools, MA and MS for lecturers of method in chemistry at teacher training colleges and UB, UH, UJ, UK, UL, UM, US, UX and UY for university lecturers in Chemistry.

In all studies an "I " is used as a label for the interviewer whether it be Lybeck, Strömdahl or Tullberg.

In this thesis mainly findings from the studies with the 28 and 26 educators are considered. Systematic quotations from the study with the 26 educators are reported in appendix III. Reference is also made to the investigations with the students and trainee teachers. Specific results from all studies are tabulated in appendix II.

3.3 The course of the interview

The interview procedure regarding students has been reported in Lybeck, Strömdahl and Tullberg (1985a,b). The present account regards the interviews with educators.

All subjects in our studies, students as well as educators, have been confronted with the same task and foundational interview structure during the audiotaped interview, supplemented by questions especially designed for each category of respondents.

The questionnaire used in the interviews with the educators is found in Appendix I.

The interview adapted to the educators can be divided into seven phases.

1) Introduction
2) Task
3) Elucidation
4) Reflection on how students and trainee teachers might have solved the task
5) Personal teaching
6) Personal development
7) About the methodical and didactical debate in Sweden

All phases are directed towards making the respondents' conceptions of 'the mole' overt, revealing conceptual changes regarding 'the mole' and conceptions of how to teach 'the mole'. The notion 'the mole' is here used as a superordinate denotation including *amount of substance*, amount and molar quantities.

Each interview had its own individual course. The interview is loosely structured, within the frames of the phases and the individual run is governed by the statements made by the respondent. In this kind of interview it is more important to follow up the respondent's statements than sustain the order or literal formulations of the interview questions. The phases are the stable elements of the interview rather than the order of the questions and the formulation of the question. A brief survey of the phases is presented below. The descriptions of the phases is accompanied by quotations from the interviews with the 28 educators. They are typically illustrations to the phases but not systematically chosen. Notes made by the author within quotations are enclosed by brackets.

Introduction

The aim of the first phase is an attempt to make the respondent acquainted with the task-configuration and used to the interviewer and the interview situation. The respondent sat next to the interviewer with the configuration connected to the task right in front of him/her. The respondent is supplied with one extra plastic cylinder, one blank paper and a pencil. Small plastic cups were also available, if the respondent wanted to have a close look at the substances by pouring out the content

from the cylinders. The configuration connected to the task is an arrangement of three groups of transparent plastic cylinders (diameter: 34 mm height: 200 mm) containing filings of tin, granules of aluminium and flours of sulfur respectively. The original idea of the configuration is to be found in Novick and Menis (1976).

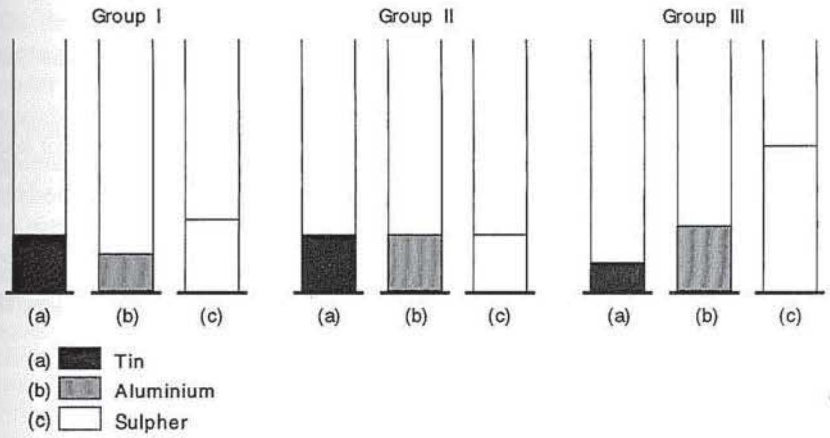

Fig. 3.3 The task configuration

The respondent is invited to make a description of the configuration, by the question: What do you see in front of you? Please, make a description!

M8: Well, I can see ... nine, ten cylinders, one is empty, they have got stop corks, and are filled with... or there is ... evidently some amount (Swed. 'mängd') decided in advance of elements in nine of them, and as I said before one is empty.

I: Please, tell me what substances you believe are in the cylinders.

M8: Well, it looks like sulfur and aluminium in those and in that one, it could be iron, but they are very difficult to separate, those grey metals. (...) Well, because it's granulated, well, well,.... in fact, it could be tin...

M12: ... I think it's sulfur in the three c-cylinders.

I: Yes, and in these two a- and b-cylinders ?

M12: (Looks at IIIa) Metals of some kind (shakes the cylinder). Sometimes magnesium looks like that, if you get a 'dark' quality, sometimes other metals looks like that. It's a metal of some kind and that includes the b-variant as well.(...) It's too light to be tin (IIb). Perhaps, it's rather aluminium.

I: Yes, it is. Why do you think that?

M12: Simply because I compared IIa and IIb, I felt the density (M12 lifted IIa and IIb in each hand). Well, let's say aluminium (in the b- cylinders) and it was right. Then the other must be a heavy metal, well, it could be iron. (...) It can be manganese, it can even be nickel. Well it can be chromium, we have had a quality which is a bit more shiny than this, but it can be any of them.

I: It's tin!

M12: So it's tin, well...

I: Perhaps it's not usual to see tin in that shape?

M12: Well, we don't have granulated tin in that shape, we have bigger granules. Tin is often more whitish, but let it be like that...

Among the substances in the different cylinders, sulfur is the easiest to identify by its typical colour and non-metallic feature. The remaining two substances are more difficult to determine, which is exemplified by the last part of the excerpt from the interview with M12.

The introduction phase is concluded by a confirmation that the subject is certain of the substances in the cylinders. This knowledge is essential in the task - solving phase.

Data from this phase of the interview, identifying the substances, are not processed any further here since they have no direct connection to the aims of this study.

The task
The task connected to the configuration (cf. Fig. 3.3) was formulated:

Which group contains 1 mol of each substance?

The principle of the task is: in group I the *amount of substance* is constant (1 mol of each substance in each cylinder; the respondents were not informed about the elementary entities of sulfur whether it was S, S_2, S_8. None asked about this matter, all presupposed the elementary entity was S, in group II the volume is constant and in group III the mass is constant.

The essence of the task is a determination of 1 mol without any measuring means, like a balance or a graduated glass. Our concern is the manner in which the respondent tackles the task (cf. 'an exposing event', Nussbaum and Novick, 1982, p. 187). Since there is no measuring device available for 'mole', not even in the laboratory, measurements of 'mole' must as always be done indirectly. In that situation the respondents' thematizing of the task and choice of physical quantities related to 'the mole' are of focal research interest.

The physical quantities brought up by the respondents[29] and applied to the bulk portions in the cylinders are mass (m), volume (V), density (ρ), molar mass (M), molar volume (V_m), number (N), Avogadro's number, N_0 and the Avogadro constant, N_A. Since the substances in the cylinders are grains there are also statements of the sizes of the grains and their influence on the bulk properties, especially volume.

On the microscopic level, atomic mass (relative atomic mass, atomic mass, atomic weight) and atomic volume (the 'size' of the atoms) are under consideration. There are few statements of these "hidden" variables among the educators in the task-solving situation in comparison to the students and trainee teachers.

If the respondent noticed the equal volumes in group II, it was possible to estimate the relations between the densities (bulk densities) of the substances.

U1: These IIa,b and c seem to be equal volumes in all three cylinders and then one could get... some feeling... that b is obvious lighter than a, and then I suspect a cheap and light metal like magnesium.

But it is more usual that the subject tried to recall numerical values of densities from memory. This is often accompanied by archetypal conceptualisations of light and heavy elements. The choice of heavy elements is restricted to iron, lead, tin, zinc, nickel or chromium and light metals to magnesium and aluminium (cf. the quotation above).

In a situation where measuring devices are lacking, estimations must be made. When the respondent asked for atomic weights, atomic masses or molar masses, only numerical values of the physical quantities were confirmed or given by the interviewer.

M12: Aluminium is 27, I think, sulfur is 32 and tin I don't know by heart (M12 gets the numerical value 119) ... yes, it's 119. Then I must search for 119 grams. In IIIa there must be less than 119 g, I believe there is 119 g in Ia as well as in IIa. Now, I am searching for 27 g of aluminium (M12 is lifting I b and IIb simultaneously) 27g, I haven't got the sensibility to determine which of them is 27 g, and then I shall try 32 g, I can't determine that either. I'm not sensitive enough to decide...

At this point the task is reduced to a technical problem of measurement of masses, but since M12 does not have any measuring device and the hands are not sensitive enough to make measurements, M12 must try another strategy:

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[29] Whether the respondents conceptualise the physical quantities in their full scientific sense or not could not be stated.

M12: ... Aluminium is so light, aluminium is a light metal. It's so very light that the density of aluminium can't be that much bigger than of sulfur. I know that sulfur has got a density very much more than one, despite the fact that sulfur (powder) floats if you put it into water. (...) I think it's group I. The argument is that this loose (powder) sulfur has got so low density that the proportions between 27 g aluminium and 32 g sulfur most likely ought to have approximately this proportion by volume.

To make "measurements" of the relations between the masses, based on the molar masses is easier:

M1: ... 27g and 32g. These should weigh approximately the same... now I compare aluminium and sulfur with each other (I b and Ic). Look if there is big differences in the groups (compares IIb and IIc ; IIIb and IIIc). There is no big difference, because you have been smart... No significant difference here. Then, that one (tin) shall weigh about 4 times as much, approximately. Now I compare tin with aluminium in all groups. Then I sort out group II. Well I think it's one mole in group I.

Another way of solving the problem is to make a rough estimate of volumes based on known or estimated densities and "molar masses" (the mass of one mole).

M2: It's 32g, 27g ... 119g. Well, the density of aluminium is less than tin ... and least is sulfur, which is about 2, I don't know if tin can be... well, 6 and 4 (M2 writes Sn, Al and S, under them 119, 27 and 32 and under these figures 6, 4 and 2, which are the estimated densities). ...the volume per mass unit is less in a compared to b. I believe ...a and b weigh about the same... I don't think it's group III... it should be as much sulfur as aluminium in grams. ... there, it's too little sulfur (group II). I believe it's group I, that's right.

M2 has not even touched the cylinders. When the interviewer says that he is allowed to lift the cylinders he says:

M2: In fact, I didn't think one could lift them.

However the educators' responses to the task are generally directed towards the determination of those masses in grams which coincide with the numerical values of the molar masses. Even if the molar masses are highlighted, there are very few statements, in this phase of the interview, which give a key to the educator's conception of the mole. The relationship between molar mass and 'the mole' is seldom explicitly expressed (cf. above, the excerpt from the interview with M12) or very loosely expressed by statements like: "molar mass is the mass of 1 mol", even if there are exceptions:

M6: Well, in my view 1 mol is a unit of number of pieces. Thus, 1 mol is $6.02 \cdot 10^{23}$ pieces of particles and since they are elements, ... it's possible to speak of atoms in

all these cases... and... then one should try to decide if this is... for instance, 1 mol of tin, or 1 mol aluminium or 1 mol of sulfur. It's reasonable to do that by weighing them, because ... this unit of pieces, that number, is chosen so the mass in grams has the same digit [numerical value] as the formula-mass of the specified substance. Since they are elements the formula-mass is the same as atomic-mass. Then you can use what table of atomic masses you want. Sulfur is 32.06 and aluminium 23 something and tin I can't remember just now.

The majority of statements made by the educators concerning the task is a collection of different strategies to make measurements or calculations by combinations of mass, density and volume with the starting-point in the numeric values of atomic masses or molar masses.

A substantial portion of piloting is introduced by the interviewer when the subject gets stuck in the measuring and calculating process. Thus these parts of the interview are of less value.

The task solving process for all 102 respondents are diagramatically accounted for in Appendix II, Tables 1 - 4.

Elucidation
This phase of the interview commences with the question:

What comes to your mind when I say (the word) mole?

The respondent's answer is generally of a definite, sometimes definitional character.

M10: Well, primarily it's number to me. But I can't see that here (in the arrangement of cylinders) (...) for instance when one is dealing with chemical equations it's, in fact the number one is dealing with. Then you deal with a number, pieces,... we must have as many on the left hand side of the equation as on the right hand of it. It's the number of atoms. I look upon them as beads, and then you enlarge the scale. The scale $6 \cdot 10^{23}$, well, then you have got 1 mol. In my view it's something tied to a number.

U3: Then, I'm thinking of 32 grams here (...) for sulfur 27 and 119 then...

The statements from this phase of the interview are essential in determining the conceptions of 'the mole' held by the respondents.

The next question is: What does (the word) amount (Swed. 'mängd') mean to you? The answers were ambiguous. Here are some examples.

T3: One ought to associate it to amount of substance. I think it's difficult.

T10: Amount can be whatever you want...

T12: An amount doesn't tell you how much it is, (...) I think of a little heap like you have weighed up... In fact, I'm thinking of volume (in a concrete sense).

M1: Well, in fact, it's the concrete number of atoms or formula units or particles or molecules.

What is amount of substance? Do you use the expression amount of substance?

M5: I must use that at upper secondary school because it's used in the textbooks, because the textbooks are governing.

I: What does amount of substance mean to you?

M5: It's molar mass.(...) I think so... (...) Now I must think. (...) Amount of substance and mol, then you put a sign of equality,... its a basic unit in SI, in fact, it's difficult to manage... what it is, this amount of substance. Mole. Well, I would perhaps not say it's molar mass. Mole is more correct.

M6: I don't use the expression so very often.(...) If I use amount of substance. Well, I would ... I think, I would use it like I use the word mass of a substance. In grams... then I leave the chemical concept amount, I think.

T10: Mostly I use amount, though the pupils are reading amount of substance in the chemistry text-book and if I only say amount, they ask what is it ...or what is the connection between amount and amount of substance. It, it's not clear to them, so I ought to be consistent and always use amount of substance, but I don't ... I'll rather confess that if you have learnt something it's difficult to change.

In the end of this phase the 26 educators were explicitly asked questions about relationships between the physical quantities used (for statements, see Appendix III) .

Reflection on students and trainee teachers solving the task.
Most educators believed that students and trainee teachers solve the task in a similar way to themselves. Problems they experienced are transferred to the students.

M12: Well, I think the students will be disturbed by the visual impression of volumes (...)(About group III). They believe that tin is much heavier (than the other substances), have got a much bigger density (lifts IIIa and IIIb)... I close my eyes to avoid seeing... (weighs with both hands simultaneously) It can't be true that IIIa is four times heavier than IIIb. (About group II) Well, I think they have got a feeling of the mole as connected to volume. I believe. In fact, the discovery of the equal volumes (in group II) would turn them away from group II, because it would be a pure coincidence... (...) The trainee teachers represent a spectrum of thinking from a less able student on the N-line to an experienced scientist, so they land in all categories... (when solving the task)

Teaching
The following questions are posed: *How do you teach mol to your students (trainee teachers)? Why do you want to teach like that?* By these questions the educator is invited to reflect over his/her own teaching. Generally the educator's reflection on his/her own teaching seems to be correlated to his/her own educational level and experience.

The quotation below is a cut down excerpt from an interview illustrating the main steps taken by an educator to teach the mole. Key steps are the particularity of matter, mass of elementary entities, number, the specific number $6.02 \cdot 10^{23}$, the concrete portion of 1 mol, and applications including relations between physical quantities. - Statements in this phase also include general conceptions of science, learning and teaching .

T12: Well,... often but not always, we have discussed the construction of the atom and things like that. But they must know that matter is constructed of atoms or molecules... well, they must know what atomic mass and molecular mass is (...) And then I try to explain that one can take one atom, two atoms, three... and if you take 10 it weighs ten times the atomic mass, etc. And in a similar way you can take molecules, if one molecule weighs 18 u, two molecules weigh 2 x 18, and they grasp that. And they grasp that how many molecules you ever take , it's the number of molecules times the atomic mass or molecular mass. (...) But if you take one mole molecules, then it's much worse. (...) I don't grasp it. I think it's odd, but it's much worse. But if I tell them $6.02 \cdot 10^{23}$ pieces, then they grasp that it weighs $6.02 \cdot 10^{23}$ times the atomic mass. But the essence of the mole, isn't the number but that you get an amount easy to handle, and if you take $6.02 \cdot 10^{23}$ pieces of atoms then you get a mass equal to the atomic mass but expressed in grams. That's good. And I use to tell them that using that number as a conversion number from the unit u to grams, exactly as grams from kilograms, but unfortunately it's a little more uneven. It would have been nicer if it had been a little bit more even, but the idea is the same.

I: Do they grasp that?

T12: Yes, some of them do. In the end I think all of them... I don't know how they think, because it's difficult to know what people think. (...) All of them can learn it, I think. (...)... then I use to weigh one mole of different substances. I use to have, for instance, water and salt (sodium chloride) and sulfur... and perhaps an element.

I: What's the purpose of that?

T12: Well, they should see how much it is... because they get a perception of how much it is. (...) And then they can see that certain substances are voluminous but yet it isn't more particles than in a little heap of something else.(...) I use, it depends on how many students I have, but this time I had small pots containing different substances and I had written the name and the formula of the substance on the pot. And then I had weighed how many grams it was (...)... and then the intention was that they should try to calculate how many moles there were in the pots, and they managed it. It wasn't difficult, they said. (...)... and if I had had less students and some more equipment I would have let them make solutions too, with defined concentrations, but now I made it myself as a demonstration.

I: Have you thought about why you want to teach like that?

T12: I don't. I don't think so much about that, but the goal is that I want them to comprehend what it is all about. I want them to learn, and I try as far as I can, to force them to grasp what I want them to grasp. It's like that.

This phase of the interview comprises a lot of statements which articulate the conceptions held by the educator. This includes simplified scientific concepts used by the educator to facilitate the teaching of 'the mole'. Due to the statements in this phase it is possible to construct individual 'teaching models' for every educator. It's important to notice that these are idealised 'models' since they are based on educators' statements about teaching 'the mole' and not on factual teaching in the classroom.

A detailed study of this phase of the interview concerning teaching models is reported by Tullberg (in progress).

Personal development
Do you remember how you learnt the mole yourself?

We followed up this question by asking about textbooks used during the educator's own education at upper secondary school and at university, about their own teachers and about experienced conceptual changes during their vocational career. Table 3.4 and Table 3.5 schematically communicate the findings about conceptual change among the 28 and 26 educators. Other aspects of this phase is reported for the 26 educators by systematic quotations appearing in Appendix III.

About the methodical and didactical debate in Sweden
The individual interview was finished by asking: What's your opinion about the methodical (didactical, pedagogical) debate concerning chemistry education in Sweden?

The answers indicate that the debate in Sweden is regarded as undeveloped nowadays. However in the 1960´s there was a lot of articles in the journal 'Elementa', a Swedish journal for teachers about topics in mathematics, chemistry and physics. Some remembered a special issue of 'Akuellt från Skolöverstyrelsen' (Newsletters from the National Board of Education) in 1965 concerning chemistry education, connected to the broad curriculum revision that year.

Besides 'Elementa' there are journals such as 'Kemisk Tidskrift', and 'LMFK-nytt' which could be appropriate for debates, but there is a weak interest from the public. What is needed is a willingness from the public to share experiences.

M 10: It's awfully meagre, and I don't no why. Firstly, there are many where ... and it isn't only me being the only one chemistry teacher at my school, not completely alone , but one more,... there isn't work for more than one chemistry teacher at each school. (...) In fact, in the daily work, there aren't any opportunities for discussions. (...) Well, the trainee teachers colleges ought to be a forum, but my contacts with the trainee teachers college are very few nowadays. The forum is, in fact, is 'Berzeliusdagarna' [30]

Even if new textbooks have been published for the upper secondary level with an unconventional and even controversial approach in chemistry such as Dahlstrand (1984) there seems to be no public discussion going on among chemistry educators.

M10: ... it's difficult to sit down and write polemic articles, or things like that. I think that people make a lot of experiments, but it's done at home. Unfortunately it's not brought out in the light... (...) You know how the teachers are: "it's nothing to speak about or nothing to write about". They are very modest, but if you look in for instance School Science Review, there is a big section of letters to the Editor, of variable quality, goodness me!, but the debate is going on.

This phase of the interview has only an implicit connection to 'the mole'. The aim of this phase was to find out channels for debate, what issues the educators consider as important and a view of the preparedness among the educators to publicly thematize their own activity as chemistry teachers. No further reference to this phase of the interview is made in this study.

3.4 Results and discussion

Results of previous studies on the conceptions of mole are reconsidered, articulated, refined, revised as well as enlarged to adjacent concepts by analysis of new empirical findings from the original interviews, all gathered to form an empirical base in alignment with the aims of this thesis. The empirical findings are presented and discussed in subsections.

3.4.1 Solutions to the task

Results
Data from all interviews show that 1 mol is always determined via 'measurement' of some physical quantity related to 'the mole'. Hence,

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[30] 'Berzeliusdagarna' is an annual meeting arranged by 'The Swedish Chemists' Society' for selected students interested in chemistry at the Swedish Upper Secondary School, and their teachers.

physical quantities, relationships and relations between relationships of these physical quantities make up the main results of the task-solving process.

The choice of group of cylinders and arguments in favour of choice of group for the 30 students is reported in Lybeck, Strömdahl and Tullberg (1985a,b,c,d), and for the 18 trainee teachers in a preliminary report by Lybeck, Strömdahl and Tullberg (1995). The main results of the student study is expressed through individual patterns of reasoning including quotations (Lybeck, Strömdahl & Tullberg, 1985d)[31].

The feature of the individual patterns of reasoning supported a classification of the task-solving process as a (macroscopic) continuous or a (microscopic) discontinuous approach. If the student concentrated his/her efforts to continuous variables (mass, volume and density) the approach was classified as continuous (C) and if the particulate, atomic level properties of matter (e. g. atomic mass, atomic volume, number of elementary entities) were focused it was classified as a discontinuous approach (D). Some approaches were classified as hybrids (C&D, (C)&D, C&(D))[32] This categorising should not be construed as the students' exhibited different conceptions of matter. The C and D categories are features to seize the strategies applied in solving the specific task (cf. Lybeck, Strömdahl & Tullberg, 1985b, p. 24 and p. 34).

The individual patterns of reasoning, choice of group of cylinders and categorisation according to the approach of all the 102 respondents are schematically accounted for in Appendix I, Table 1-4.

Table 3.1 below shows types of individual patterns of reasoning in a condensed form of the original outcome-spaces (which also include confirmatory excerpts from the interviews). The different relationships between physical quantities are denoted by the signs: (, ∩,), \, /, | and shown in figure 3.4.

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[31] The constitution of the individual patterns of reasoning for the individual interviews as well as the collective pattern of reasoning have been critically elaborated in near co-operation between Lybeck, Strömdahl and Tullberg. This procedure is judged as conclusive for the tenability of the results.

[32] The hybrids (C and D) should be interpreted in the following way. C&D: equal weight of C and D; (C)&D: D is dominating; C&(D): C is dominating.

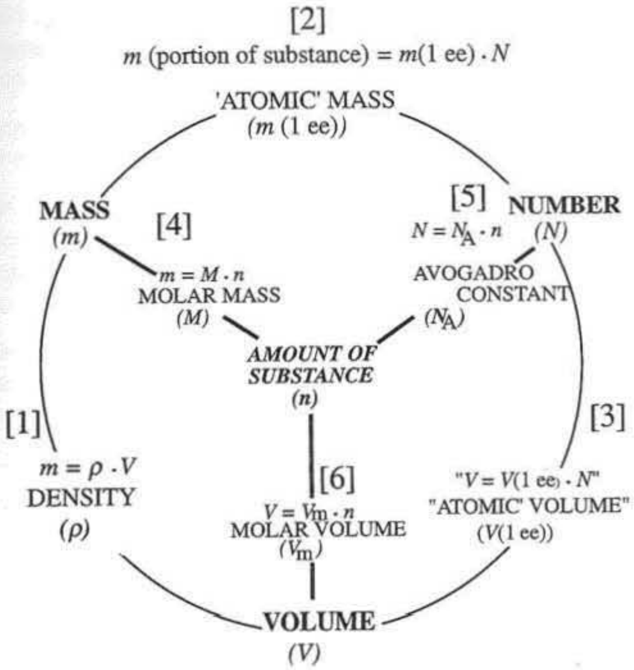

Fig. 3.4 Relationships in the individual patterns of reasoning. 1[( ], 2[∩], 3[ )], 4[\], 5[/], 6 [|]

In the 27 types of patterns of reasoning shown in table 3.1, 21 types include the relationship \ which is the relationship between mass and 'the mole', viz. the 'molar mass'.

Patterns of reasoning of the (\ -structure represent a continuous (C) approach. Such an approach mostly means procedural or algorithmic knowledge about how to determine 'the mole'. A determination of 'the mole' is equivalent to measurement of mass and considerations about volume and density (the physical quantities m, M, V, ρ is at fore). As can be seen from Table 3.1, 45[33] out of the 92 outcome-spaces follow this type of reasoning in solving the task.

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[33] The distribution of the 45 respondents are 24('28'), 9('26'), 5('18') and 9('30'). The number within brackets (' ') refers to the number of respondents in different studies, e.g. ('28') = the study with the 28 educators

Table 3.1

Distribution of 92 respondents among different types of patterns of reasoning. Arranged due to type and frequency.

Type	Frequency
01 (\	45 (cf. appendix I)
02 (\∩	6 (TT7,TT8,TT12,TÅ,UH)
03 (\ |	6 (Eva,TT9,UB,UK,UL,UX)
04 \	5 (Egon,TT16,TS,TH,MS,U3)
05 (\ /)	5 (Anders,Björn,Bosse,M6,M11)
06 \ /)	4 (Bengt,Berit,Emma,Evert)
07 (\∩ /	3 (Bror,TT17,UM)
08 \∩ /	2 (TT6,TT18)
09 ∩ /	2 (TT4,TY)
10 (\∩ /)	2 (Barbro,TT10)
11 \ |	2 (MA,US)
12 (\ |/	2 (Emil,Enok)
13 (\ /	1 (Axel)
14 (\∩)	1 (TT2)
15 (∩ /)	1 (TT5)
16 \∩ /)	1 (Adam)
17 ∩ /)	1 (TG)
18 \ | /	1 (TF)
19 \∩| /	1 (TÄ)
20 \∩|	1 (TÖ)
21 (\ | /)	1 (Ernst)
22 (\ |)	1 (Eskil)
23 \ |)	1 (UY)
24 | /)	1 (Elsa)
25 \ /	1 (Alf)
26 /	1 (Bert)
27 (∩	1 (TT3)

In the following two types of patterns of reasoning (02 and 03), the mass of the elementary entity ∩ and the molar volume | are included. Further, in type 04 density (is excluded compared to the (\-structure. These 17 patterns of reasoning are closely related to the 45 of the (\-type. All 72 individual patterns of reasoning represent a procedural approach to the task-solving (about procedural and declarative approaches see below under the headline Discussion).

Types 05 and 06 are separated from the 72 patterns of reasoning of the 01-04-type, by an additional /)-structure, viz. they are C&D-approaches.

Statements are made by the respondents about the number and the volume of elementary entities connected to 'the mol'.

In types 10 and 07-09 there is a gradual reduction of the continuous variables, (\∩ /) **----->** (\∩ / -----> \∩/ -----> ∩/, indicating a change from integrated procedural and declarative approaches of the category C&D to declarative approaches of the category C.

The structural element / in the different types of patterns of reasoning represent a declarative approach (definitional knowledge is at fore). The distribution of this structural element is

2 among the 28 educators (none with ∩)
4 among the 26 educators (3 with ∩)
6 among the 18 trainee teachers (6 with ∩)
17 among the 30 students (3 with ∩)

Patterns of reasoning comprising the | - structure mean efforts to find out molar volumes (V_m). An approach regarding molar volumes of solid substances is less developed in ordinary teaching and learning. Types 11, 12 and 18-24 include this type of reasoning but is only representing 11 respondents. Type 27 failed to give any solution to the task.

As can be seen from the Tables 1-4 in Appendix II, and Table 3.1 above the discontinuous perspective is less represented among the educators than among the students and trainee teachers.

Discussion

The task was used as a means to reveal the conceptions of 'the mole' among the respondents. Even if a right answer to the task is of primary concern to the respondent, it was not the focus of the researcher. The solution of the task was only seen as a final product of a specific reasoning. The process, the reasoning, rather than the product is of primary interest.

The task with the adjacent configuration defines a specific problem-solving context where the respondent's latent and overt cognitive and emotional communication takes place. The task context raises the concrete and pragmatic problem to choose one set out of three sets, or to rule out two sets. The respondent is confronted by the practical problem: How is 1 mol of the actual substances measured?

Since 1 mol is only measurable indirectly, the task arouses the respondent's repertoire (latent potential) of concepts related to 'the mole' and previous empirical experiences concerning measurement of 'the mole'. This is orally manifested by statements and questions posed to the interviewer about the need of a balance, the periodic system, numerical values of atomic masses, molar masses and densities. The task generates statements of quantitative concepts, physical quantities, units and relationships between these.

Statements made by the respondents reveal that they try to find solutions to questions like: Which are the suitable physical quantities related to "mole"? Which concepts should get priority? What organising principle is to be followed? Which relationships between quantities are valid? In general: What is the 'formula' that fits the situation?

An approach to the respondents behaviour using the dichotomy expert-novice or professional- unprofessional is omitted here in favour of a description of experiences and knowledge on a gradual scale, which is better suited to communicate the empirical outcome of our investigations (cf. Smith & Good, 1984). A feature of 'experience' is the "invariant recognition capability" (cf. di Sessa, 1982), the skill to generalise over different cases.

> ... because seeking an invariant in a series of different examples is the same as attempting to generalise over those examples (Hewson, 1985, p. 166)

Another feature of experience and skill is planning the problem-solving work (cf. Larkin *et al.*, 1980). The word experienced is here stressed in its qualifying connotation. Its temporal connotation is of less importance.

The approach to the task context contains two aspects:

1) the conceptualisation of the configuration and an assessment of possibilities to qualify and quantify the content in the cylinders.
2) the conceptualisation of the task and the interactive reasoning combining the task and the conceptualisation of the configuration.

These aspects are described by separating the task-solving phase in four components; problem-setting, generation of suitable quantities, measuring attempts, communicating a final solution (cf. the categories *orientation, organisation, execution and verification* used by Garofalo & Lester, 1985).

Problem-setting.
The task defines an instance, a 'case' of 'measuring' one mole of actual portions of substances. Two general approaches to the task are discerned depending on the respondent's experience on 'measurement' of mol:

a) mostly declarative knowledge is activated
b) mostly procedural knowledge is activated

Activation of procedural knowledge means process-oriented operations, while activating declarative knowledge means data-oriented operations. In other words the two kinds of knowledge reflect 'knowing how' and 'knowing that' (Ryle, 1949). Greeno (1973) uses the terms algorithmic and propositional knowledge to denote the same kind of phenomenon.

Accessibility is different for the two kinds of knowledge. Procedural knowledge is often context-dependent. But as soon as the context is recognised, procedural knowledge has the advantage of efficiency. Due to experience, by reducing the actual context to a standard context, it is possible to "handle" even the most obscure cases (odd contexts). Procedural systems fit "the situation" as soon as the contextual habitat is identified. Declarative knowledge is accessible in another way, by being of a more general kind. And it needs more of adaption to the actual context to be efficient.

Since the task is not a routine task in ordinary educational settings, it is a problem and not an exercise. That means, declarative knowledge is activated more or less in the individual depending on experience of measurements in connection to the mole. Less experienced (skilled) individuals are forced to use declarative knowledge, bringing most of what was learnt about mole to the fore. Especially definitions are in focus. Thus, the less experienced respondent, resting on mostly declarative knowledge, contemplates the task as a fairly new situation. Few experiences of 'measuring'-contexts of 'the mole' are present. This opens up a spectrum of factors, physical quantities, properties and relations between them. The multiplicity of possible variables in the problem-solving situation puts the less experienced respondents in a demanding situation where concepts must be sorted out as unproductive (unprofitable) or unnecessary when solving the task. The less experienced respondents must arrange a structure of parameters accounting for the actual context out of several possible parameters.

Further, no measuring devices are present. Different physical quantities both on the macro- and micro-level and relations between these are examined. This is done partly by 'gedanken-experiments' partly by 'quasi-measurements' (measurement with the hands). The task-solving enterprise can be characterised as a form of trial and error or even labelled 'chaotic' in the abrupt changes between different ideas (cf. Lybeck, Strömdahl & Tullberg, 1985a,b,c,d). The fact is that this approach is time-consuming, which is reflected in the interviews with the less experienced respondents. In these cases the interview makes up a learning situation.

Since 'the mole', among our respondents, is generally defined and conceptualised as a number, the discontinuous aspect of matter will play a genuine role in the task-solving situation when declarative knowledge is getting priority. This is often stressed in the beginning of the problem-solving process as some kind of an organising principle.[34]

TF: One mole, I know what it is, it contains... What was the question? You asked me in what group there is 1 mol of each...(...) Well, in fact, it shall conta.., 1 mol shall contain equal particles...

Generation of suitable quantities, parameters and relationships.
Procedural knowledge means experience of mole as calculated from molar masses and measured masses. Few statements are made by the respondent concerning general or definitional knowledge on "mole". The respondent uses mass, molar mass, volume and density, applied to matter as a continuum, thus in our terminology a continuous perspective (C) is adopted.

TM: (...) Well, it should be the proportions. (...) Sulfur, it's 32... 32... and then it was aluminium. (...) And this was tin, which is naturally a good deal heavier.

TM excludes group II because

TM: They have got equal volumes, and it would be very odd if those three... it's simply inconceivable.

After weighing the cylinders by hand his decision is group I and he motivates his choice:

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[34] However, maintaining a pure discontinuous perspective during the task-solving process is not fruitful - no student with a pure D-perspective arrived at the right solution (cf. Lybeck, Strömdahl & Tullberg, 1985b, p. 34). There is no simple relationship between Avogadro's number of elementary entities and visually perceived portions of substances.

TM: ...Ia, which is tin, ought to be a good deal heavier, because the atomic weight is much bigger than for aluminium and it is the heaviest of them, definitely heavier than, than Ib. Ib and Ic, shouldn't differ much concerning mass, and they don't either.

TY made systematic mass measurements against a background of definitional knowledge of 1 mol. He thematized the task in a hybrid (C&D) perspective. The comparisons of masses, is the decisive activity. He started lifting cylinders IIb and IIc:

TY: ... I'm led by the mass of the particle... of... the substances, or the atoms and I know that aluminium has got the particle mass... 27 and sulfur has 32.

He poured the content of IIb and IIc in two separate plastic bags and found that IIb is heavier than IIc (the portion of aluminium is heavier than the portion of sulfur). This result excluded group II.

He turned to group III and compared it visually with group I. He seemed a bit puzzled over the large volume of tin in Ia. After asking for it, he got the numerical value of the atomic mass of tin and he continued with group I:

TY: Now, I'm concentrating on the proportion 119 to 27 and I shall try to get a perception of the mass of... Ia is of the magnitude of five times the mass of Ib.

He poured the content of cylinders Ia and Ib in two separate plastic bags and compare the masses. His comment was: "It could be right". He made a similar comparison between IIIa and IIIb and said:

TY: It's absolutely not a proportion five to one, under no circumstances. It seems to be about the same. This, implies that I ...dare to say that... the amount of substances tin, aluminium and sulfur in...the same in case I. And then I have used... mol...as amount of substance, as number combined with the mass of a particle.

Since it is the volume, and proportions of volumes in the three sets, that is visually accessible in the task-solving context, densities combined with masses (molar masses) to calculate the volumes, is one strategy to solve the task.

Typical procedural knowledge is revealed by statements meaning a direct "translation" of mole to mass or "molar mass".

UM: Mhm... 1 mol, well. It's 32 grams sulfur and the other is something like 27 grams aluminium, and tin... I can't...but it's in my head... something like 140 ...(...)...I'm so bent on practical problems so I couple it directly, translate, convert it directly to mass, when I can...

Notice especially the statement "I'm so bent on practical problems so I couple it directly to mass...". This immediate coupling does not reveal the kind of the relationship between 'mole' and 'mass' (cf. "... 1 mol,... Well, It's 32 grams of sulfur..."). Hence, the relationship between 'mole' (amount of substance) and mass can be of different character. The range of quantitative (mathematical) relationships cover identity, conversion and a relationship which is correct due to the demands of quantity calculus. But a non-mathematical relationship such as 'is a kind of' is also a possibility.

An example of a declarative approach is executed by TF:

TF: I'm thinking of... the molar mass, then and how... heavy they are and how many... how much I must fill up to reach 1 mol. Well, how big... how many... particles, well how big volume I would get of it...

The conflicting concept in the task solving context is *number*. TF's conception of 1 mol as a number is confirmed later in the interview by her answer to the question of what she thinks of when mole is mentioned:

TF: I'm thinking of ... a number and I'm thinking of Avogadro's number, this 6 times 10 (last words inaudiable).

TF continued by identifying the numerical values of the molar masses with the help of the interviewer. TF chose group III by intuition. After expressing some doubts over the choice, TF began to make measurements with her hands.

Measuring attempts, calculations judgements and verification.

Identified measurements are visual estimations of volumes and tactile estimations of masses followed by various calculations. These measurements are attached to technical problems:

* inaccuracy (or inability) of visual estimation of individual volumes
* inaccuracy (or inability) of visual estimation of proportional volumes
* inaccuracy (or inability) of tactile estimation of individual masses
* inaccuracy (or inability) of tactile estimations of proportional masses

Moreover, there are some additional problems. Density is a significant quantity for the respondents since it connects the "measurable" quantities mass and volume. Even if no numerical values of density are used, there is a general conception held among the respondents that density is increasing in the order sulfur, aluminium and tin. This knowledge is of great importance for the course of the task-solving process. An additional problem is the fact that the content of the cylinders are portions of powder, filings and granulate which do not fit

with the ordinary values of densities calculated on the substances as whole bodies, but must be dealt with as 'bulk densities'.

After comparing the masses within each group by lifting one cylinder in each hand TF says:

TF: Well, now I don't know what to think, I feel totally perplexed (laughing). (...) Well, it's a matter of sorting out one's thoughts, in fact, well. What should I think and how should I think...?

TF's superordinate conception of mole as a number of particles interferes strongly with the mass measurement attempts. The conception of equal number of particles leads her to group II, but the masses do not fit.

TF: IIa and b, this... this should weigh a lot, IIa should weigh a lot more than... than b. And those two should weigh about... b and c about the same.

I: Is it so?

TF: No, I don't think so (some words inaudiable).

TF thinks that the proportions between the masses in group I fit better, but:

TF: And there, they are not about ... the amounts are not about equal, but ...

I: When you are saying amount, what does it mean?

TF: Well, the height in the cylinder ... the volume (...) But it doesn't need to mean anything ... it could be... in fact it could be equal number of particles in them anyway, I think.

The interviewer reminds TF of her arguments in favour of group II.

TF: Yes, there it was the same... Well, the heights are the same... equal numbers, so there ought to be, there... There I suppose, there ought to be... to be... I decide upon II, then we will see what...

Group III is sorted out. The choice is made by intuition:

TF: (...) it was wrong, I got it wrong. (...) tin is heavier, doesn't mean that one needs equal particles, but so isn't it, because it's the number of particles we should have.(...) I didn't that. (...) Well, in fact... if one is thinking, then one can see that... here one reaches... here one has put in... a certain number of particles, an equal number, and thus they need to reach the same height. (...) ... the particles don't need to be of equal size. Well, then... Now (...) aluminium and sulfur, ... the size of the atoms of sulfur ought to be bigger than the atoms of aluminium. In that case...

Communicating a final solution to the task

TF is pointing at group I. She does not notice any difference in weight between Ib and Ic, but she finds IIb a little heavier (than IIc) and that is wrong, since it should be the other way round, so her final conclusion is group I.

The crucial point to approach the task is to see the given case as an instance belonging to the praxis of determining 1 mol via masses and molar masses. The adherence to mass-measurement is the distinctive feature of an experienced behaviour, either if it takes place by deliberate measurements with the hands or indirectly by reasoning around approximations of volumes and densities. Even if the measuring instrument, a balance, is missing in the actual context, clinging to mass measurement, is a consistent attitude. Thus, the experienced respondent identifies the task as an instance of a stable problem-solving strategy, where measurement of mass (volume and density) is the "natural" way to handle the mole (cf. the (\ -type of reasoning). Evidence of this assertion is found by a comparison between the student study (Lybeck, Strömdahl & Tullberg, 1985a,b,c) and the trainee-teacher study (see the preliminary report Lybeck, Strömdahl & Tullberg, 1995) on the one hand and the educator studies (see Table 3.1 above and Appendix II) on the other.

A majority of the students and the trainee-teachers are case-bounded, in the sense that the task/configuration is considered in the form actually given. The task (case) is not immediately placed in a frame of reference where standard, automatized, procedural methods are applied to measure 'mole' of portions of substances.

The patterns of reasoning presented in the previous studies are results of how the respondents solve the task, only partly and implicitly revealing their conceptions of mole. However, solutions to the task contribute to the constitution of the conceptions of 'the mole' by revealing relationships between ' the mole' and other 'measures'. 'The mole' is 'concealed' in a another 'measure-gestalt' (e.g. mass, volume, number). Thus, from the individual pattern of reasoning it is possible to extract the contextual conception of the relationships between 1 mol and other quantities.

Several respondents declared that the task could be easily solved by weighing the substances in the cylinders with a balance. Those cylinders containing portions of substances with masses corresponding to the molar masses contain 1 mol. The relationship 'correspond' is seldom explicitly described in the task-solving phase of the interview.

The general conclusion of the results of the task solving process is that 1 mol is always 'measured' via some other physical quantity. The stress of the relationships between 'the mole' and some physical quantity varies and gives a hint to the conception of 1 mol. Among the experienced educators, 'praxis' is to determine 1 mol via mass measurements and the molar masses. 1 mol is only implicitly conceptualised as identical to Avogadro's number of elementary entities.

This concludes the phase of the interview which reveals how mole is measured. Now we turn to the question What is measured by 'the mole'?.

3.4.2 Conceptions of 'the mole'

Results and discussion

In constructing the individual patterns of reasoning for the 30 students, their statements about 'the mole' were connected to the physical quantity *amount of substance* (Lybeck, Strömdahl & Tullberg, 1985a,b,c,d), even if only one of the students explicitly used the phrase 'amount of substance'. This description obscured the fact that 'the mole' could have different meanings to different students. This was most evident via the registered answers to the question: "When I say mole, what do you think of?". The variation was taken as self-evident and implicit in the individual patterns of reasoning, but was not focused on in the original analysis of the students' transcribed interviews. A renewed analysis resulted in four qualitatively different ways of conceptualising 'the mole', where a vast majority considered mole as a number. (Lybeck, Marton, Strömdahl & Tullberg, 1988, p. 96):

A. Mole as something to be used in calculations
B. Mole as a mass.
C. Mole as a number
D. Mole as a number and as related to mass
E. Mole as related to number and mass.

With this categorisation as a background, analyses of the 28 interview protocols of the educators resulted in four qualitatively distinct categories of description. However, eventually five categories of descriptions were identified. Each of the categories determine a conceptual structure (cf. chapter 8, a *conceptual locality*). Since these categories of description are basic for the conceptualisations of 'the mole' they are denoted *fundamentals* (F). With this denotation it is also emphasised that on a collective level the categories are foundational to calculations within stoichiometry. As we have shown they are also decisive for the choice of teaching designs (Tullberg, Strömdahl & Lybeck, 1989, 1994).

The qualitatively distinct categories of description of 1 mol are

F_0	One mole (1 mol(e)) is a defined portion of substance..
F_1	One mole (1 mol(e)) is an elementary entity dependent (individual) mass.
F_2	One mole (1 mol(e)) is equivalent to a number (Avogadro's number).
F_{2a}	The term mole (1 mol) is excluded and replaced by a number N_0 (alt. L_0 or 1 hen) (identical with Avogadro's number), as a conversion factor between the two units of mass 1 g and 1 u).
F_3	The mole (1 mol) is a unit of the physical quantity *amount of substance*.

The category F_{2a}[35] is a complementary category to F_2, both account for the quantity *number*. F_{2a} is not explicitly found in our empirical data, but a possibility elaborated and advocated by Weninger as a solution to the mole controversy both on practical, educational and especially on theoretical and logical grounds (see, chapter 6).

The fundamentals are incommensurably separated ways of dealing with the phenomenon of quantitative measurement and calculation of substances involved in chemical reactions. The fundamentals carry the property of incommensurability, not only in a Kuhnian sense (Kuhn, (1962) 1970) but also enclosing mathematical meaning. Physical quantities are said to be incommensurable if they do not measure the same property. Kuhn (1970) says:

> In the transition from one theory to the next, words change their meanings or conditions of applicability in subtle ways. Though most of the same signs are used before and after a revolution- e.g. force, mass, compound, cell - the ways in which some of them attach to nature has somewhat changed. Successive theories are thus, we say, incommensurable. (Kuhn, 1970, p. 266)

Kuhn compares the incommensurability between two paradigms with the translation of one language to another:

> They often have the inestimable advantage that the signs used in two languages are identical or nearly so, that most of them function the same way in both languages, and that, where function has changed, there are nevertheless informative reasons for retaining the same sign. But those advantages bring with them penalties illustrated in both scientific discourse and history of science. They make it excessively easy to ignore functional changes that would be apparent if they had been accompanied by a change of sign. (Kuhn, 1970, p. 269)

This observation is applicable to the fundamentals with their different meanings of the one and the same sign, 'mol'. Even if the symbols and the words are formally identical in different fundamentals their connotations (senses) are totally different. The words in different fundamentals are homonyms even if they refer to the same scientific domain. Thus it is impossible to mix elements (concepts) from different fundamentals, without running into conceptual ambiguities and logical contradictions.

The fundamentals are constituted as generalised, theoretically cultivated systems of concepts, each one with an individual inherent logic. They are decontexualized structures, where one physical quantity is highlighted at a time, with two exceptions. Those are F_0, where 1 mol is a name of concrete portions and F_{2a} where 'the mole' is excluded and substituted by a conversion factor (Avogadro's number).

Further analysis of the empirical data and theoretical considerations have meant a revision of previous findings concerning the fundamentals described in Strömdahl, Tullberg and Lybeck (1988, 1989, 1994). Among other things this revision has meant a separation of the definitional part of the fundamental and the mathematics applied to the specific fundamental. The revised fundamentals are looked upon as lexical definitions in the second order perspective (cf. section 3.1.3). In a first order perspective they are: one ostensive definition (F_0) and four stipulative definitions (F_1 , F_2 , F_{2a} , F_3).

F_0

This fundamental means an ostensive definition of mole. 1 mol is the name of the physical concrete portion of a substance which bears the property to react chemically with other substances in whole value ratios. 1 mol (a concrete portion) has nothing to do with physical quantities or units at all. The portion 1 mol can be described by the physical quantities mass, volume and density (abstracts). The use of the expression 'number of moles' in this fundamental does not explicitly connote a defined physical quantity. 'Number of moles' denotes a number (multiples) of 'mole'-portions (or the fraction of one portion) of a defined substance involved in a chemical context. Since 1 mol in F_0 is a name of a concrete thing it is manifested as a body of variable size

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[35] The category F_{2a} has been denoted F_4 in previous reports (e.g., Strömdahl, Tullberg & Lybeck, 1994.)

(volume and mass) according to the substance under consideration (defined elementary entity, structure, temperature and pressure) .

The discontinuous aspect of matter is expressed by Avogadro's number, 'The number of atoms in 1 mol is equal to Avogadro's number' or '1 mol contains Avogardo's number of atoms'.

When showing portions of 1 mol of different substances (cf. educator M1), in order to make the teaching of mole 'more concrete, by showing how much it is', viz. its concrete extension in space, it is close to the conception of 'the mole' in the F_0 sense. This should not be mixed up with a demonstration of extension in the sense of the physical quantity volume, which is an abstraction.

The statement '1 mol contains $6.02 \cdot 10^{23}$ particles' is only correctly used within F_0. However, few of the respondents using the expression seem to be aware of this.

F_1

One mole is stipulatively defined as elementary entity dependent masses, based on atomic weights (atomic masses). For instance, if aluminium has the atomic mass 27 u (or relative atomic mass 27) then '1 mol Al = 27 g Al'. In other words one mole is an individual mass unit and the corresponding physical quantity is mass. The mole is here synonymous with the Ostwaldian Mole and the other historic denotations gram-atomic weight, gram-molecule weight or gram- formula weight. The expressions 'molar mass' or 'molar weight' are equivalent to the mass of 1 mol in accordance with historical uses (cf. Wallot, 1953).

The expression 'number of moles' in F_1 is logically referring to multiples of masses with the unit 'mol'. This is further explicated in connection to the mathematics applied (see below) .

F_2

One mole is stipulatively defined as a number, Avogadro's number. The identity 1 mol = $6.022 \cdot 10^{23}$ is valid. This means that the number $6.022 \cdot 10^{23}$ has got double names, 1 mol and Avogadro's number! The phrase 'number of moles' is used as multiples of this counting unit 1 mol.

F_{2a}

In a lot of papers Weninger (e.g., 1959,1980,1981,1982,1983,1985) strongly advocates that, as he says, "der vermeintlichen" (= the supposed) physical quantity *amount of substance* and its unit 1 mol should be deleted from SI and replaced by *number*:

> Der Name 'Stoffmenge' bezeichnet keine physikalisch relevante Grösse, sondern ein illusionäres Konstrukt. (...) An die Stelle der vermeintlichen Grösse "Stoffmenge" sollte die Anzahl treten. (Weninger, 1985, p. 159)

Still there is a need to bridge the gap between the discontinuous and continuous conceptualisations of matter. Weninger focus this need to a conversion factor (N_0) between the two units of mass 1 g and 1 u (1g = $N_0 \cdot$ 1u). The factor, N_0, is called "Normanzahl" and is equivalent to Avogadro's number (Weninger, 1983). Dierks (1981b) has elaborated the consequences for stoichiometry calculations with this definition.

In an attempt to solve the "mol"- controversy Dierks, Weninger and Herron (1985b, pp. 1021-1022) have introduced a new term, 1 hen equivalent to N_0 (Avogadro's number). In fact, the proposal implies a renaming of 1 mol with the same connotation as of the mole expressed by F_2. 1 hen is a name of a number like 1 dozen and 1 score. With the proposal nothing is gained beyond what is already known. It is an adoption of the historical conception F_2. However, it is a totally different question to argue against the prevailing fundamental F_3 in favour of fundamental F_{2a} as a norm in the scientific society, which is the aim of Weninger's argumentation.

F_3

1 mol is the SI-unit of the physical quantity *amount of substance* (n).

The physical quantity *amount of substance* is related to other physical quantities by the rules of quantity calculus.

We have constructed a diagram (figure 3.5), showing relationships between *amount of substance* and adequate physical quantities used in elementary educational settings (Lybeck, Strömdahl & Tullberg, 1985a,b,c).

In F_3, molar mass (M) is a physical quantity as well as a elementary entity dependent proportionality constant connecting mass (m) and amount of substance (n) in the proportionality $m = M \cdot n$. The unit of molar mass is 1 g/mol (according to SI correctly, 1 kg/mol).

$$m\text{ (portion of substance)} = m(1\text{ ee}) \cdot N$$

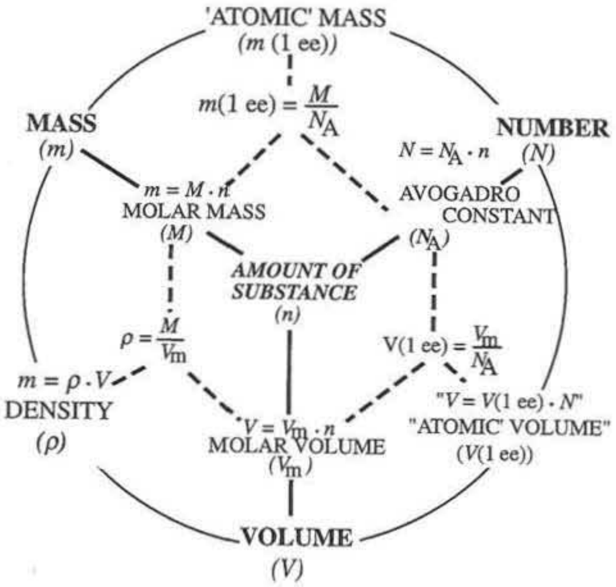

Fig. 3. 5 The relationships between common physical quantities and the base physical quantity *amount of substance*.

Discussion

The fundamentals are qualitatively separated from a mere historical description like the one made by Dierks (1981a), because they are empirically grounded in the conceptions actually and currently held by the respondents found in our data. On the other hand, the fundamentals are validated by historical facts and by the findings of Copley (1961) some 30 years ago:

> 'Mole' is at present used in three different senses: (i) as chemists' unit amount of substance(...), (ii) as Avogadro's number (...) and (iii) as 'gram-molecular weight' (...). The use of *mol* for sense (i) only could do something to clarify this unfortunate confusion. (Copley, 1961, p.777)

Copley's sense (i) seems to coincide with F_3 , (ii) with F_2 and (iii) with F_1.

The established set of fundamentals make up an 'instrument' to 'measure' precision and consistency of statements regarding 'the mole'.

A conception held by an individual in our studies is seldom consistent with one of the fundamentals. On the contrary, elements from different fundamentals are ordinarily mixed (mixconceptions, cf. section 2.2).

The classification of individual educators conceptions of 'the mole' is made by referring to explicit statements to the question "When I say mole what do you think of ?" This puts the individual conception into a fundamental. This is their 'centre of gravity' conception of 'the mole' (Strömdahl *et al.*, 1994, p. 20). But other phases in the interview do not need to be consistent with the fundamental explicitly expressed by the subject. By using the set of fundamentals as an instrument of analysis, when reading the transcribed interviews, reveals internal inconsistencies in individual statements.

The educators' reasoning about the linkage between mass and number is often connected with an ambiguity. On the one hand the linkage is seen as a mass (unit 1 g) of 1 mol (Avogadro's number) of elementary entities under consideration. On the other hand the "mass" is attached to the unit g/mol, which indicates that it is not a mass (m), but a derived physical quantity, molar mass (M).

In F_1, 1 mol equals individual masses e. g. 1 mol Sn = 119g Sn. If one simultaneously uses molar mass, $M(\text{Sn}) = 119$ g/mol, which is valid in F_3, the logical result is $M(\text{Sn}) = 119\text{g}/119\text{g} = 1$ (!).

This result logically excludes molar mass in the sense of F_3 from F_1.

When the equation $m/M = n$ is used within the frames quantity calculus but applied to F_0-F_2, one is 'forced' to adopt the unit g/mol to molar mass even if it is contradictory to the conceptualisation of 'molar mass' in F_0-F_2 as "the mass of 1 mol". The result, n, must have the right unit, 1 mol. Respondent MA advocates that the expression molar mass is tautological and says that the unit g/mol is necessary to manage dimension analysis.

In F_3 the Avogadro constant is a physical quantity, a general proportionality constant ($N_A = 6.023 \cdot 10^{23}$ mol^{-1}). If 1 mol = $6.023 \cdot 10^{23}$, (F_2) is combined with N_A the mathematical result is $N_A = 1 \cdot$ (cf. Lange, 1954, p. 511). This result excludes the Avogadro constant from F_2.

The hypothesis is that inconsistencies found in the reasoning by both students and educators, rest on mixtures of different traditions, and are the main roots of their experienced difficulties with 'the mole'.

Conclusively, every context where 'the mole' is included can be analysed with the set of fundamentals. Foreign elements discerned, compared to an explicitly expressed conception (classified as belonging to a special fundamental) could be put under discussion and be restored and explained in their right context due to their fundamental habitat.

Though the fundamentals are a result of the analysis of the verbatim transcription of 28 interviews with educators, they are applicable to all our interviewees. Based on our empirical data it is confirmed, as was assumed above, that the students' conceptions are reflections of the educators' conceptions, and conceptions communicated through chemistry textbooks. No conceptions have been found in the students' interview data which have not been found in the educators' interview data. In that respect the student is an echo of the educator.

3.4.3 Conceptual shifts of conceptions of 'the mole'

The empirical data about conceptual shifts regarding 'the mole' for the 28 and the 26 educators have been classified in three categories, considering a) resistance against change b) transient change and c) complete change. Complete change is dichotomised in evolutionary and revolutionary change.

Results
The 28 and the 26 educators were individually asked to give an account of their personal development regarding 'the mole'. The aim of this demand was to get proper information to make descriptions of the current individual conceptions against the background of the personal cognitive development of the actual concept. The descriptions are in several cases uncertain because the educator has forgotten or has not consciously registered his/her own conceptual development.

The historical investigations around the mole, especially the study of Swedish chemistry textbooks during the time span 1900-1985, forms a stable ground in identifying specific conceptions of 'the mole' (Lybeck, Strömdahl & Tullberg, 1985d). Originating from these, reconstruction of previous conceptions among our respondents could be made. However, there still remains a residue of uncertainty since other views than the textbooks' could have been communicated by the actual teacher. The probability of such divergence would however be small since during the actual time period (1940-1960) there was almost consensus on 'the mole' as denoting individual masses (Lybeck, Strömdahl & Tullberg, 1985 d).

The empirical data support a description of changes of the conceptions of "the mole" in three categories:

1) resistance against conceptual shifts
2) transient conceptual shifts (cf. Nussbaum (1989) about mixconceptions)
3) complete conceptual shifts, dichotomised in a) evolutionary and b) revolutionary shifts.

Similar categories of conceptual shifts have also been reported in other studies for instance Champange, Gunstone and Klopfer (1985) and Gunstone (1988) . The result is reported in the following two tables.

Table 3. 3
Conceptual shifts among the 28 educators.[36]

	Shift			
Educator	Resistant	Transient	Complete	Don't remember
T	T2,T6,T8 (F_1)	T1,T3,T5,T7 (F_1,F_2)	T9 ($F_1 \rightarrow F_2$)	T4,T9,T11, T12, T13
M		M2,M5 (F_1,F_2)	M4e,M6,M7e M10r ($F_1 \rightarrow F_2$) M12e($F_1 \rightarrow F_0$) M1($F_2 \rightarrow F_3$) M3e($F_1 \rightarrow (F_2) \rightarrow F_3$) M8e($F_1 \rightarrow F_2 \rightarrow F_3$)	M9,M11
U	U3	U2(F_1,F_2)	U1e($F_1 \rightarrow F_3$)	

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[36] The arrow → denotes the conceptual shift from one fundamental to another (e.g. $F_1 \rightarrow F_2$ is a shift from F_1 to F_2). The letters e and r denote evolutionary and revolutionary shifts, respectively.

Table 3. 4

Conceptual shifts among the 26 educators.[37]

	Shift			
Educator	Resistant	Transient	Complete	Don't remember
T		TD, TN (F_1,F_2)	TAe $(\rightarrow F_2)$ TYr $(F_1\rightarrow F_2)$ TMe $(F_1\rightarrow F_2)$ TUe $(F_1\rightarrow F_2)$	TB,TC,TE, TF,TG, TH, TK
M			MSr$(F_1\rightarrow F_2)$ MAr$(\rightarrow F_2)$	
U	UK (F_1) UL (F_2) UX (F_2)		UBe$(F_1\rightarrow F_2)$ UJe$(F_1\rightarrow F_2)$ UMe$(F_1\rightarrow F_2)$ US$(\rightarrow F_2)$ UY$(\rightarrow F_2)$	UH

Resistance against conceptual shifts

No shift has occurred since the subject met 'the mole' in his/her basic education in secondary (Swe. realskola), upper secondary school (Swe. gymnasium) and university education. The conception is characterised by stability even if terms from F_3 have been assimilated. However, those elements are interpreted by the educator within the conserved conception belonging to F_1 or F_2. During the actual time-period, round 1935 - 1965, F_1 was the prevalent scientific standpoint in Sweden, even if alternative conceptions like F_2 were discussed and were sometimes used by some actors in scientific society (cf. Sillén, Lange & Gabrielson, 1948).

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[37] For denotations see footnote to Table 3.3. In addition, in $(\rightarrow F_2)$ the void space before the arrow → denotes a documented state of non-comprehension.

Example

Subject T2 (interviewed in December 1984) exhibited a conception belonging to F_1:

I: If I say "mole" what comes to your mind in the first place?

T2: Well, I'm thinking of how many grams the formula weight or formula mass... What ... the weight, the mass in grams of ... the molar weight... e.g. 27 grams of aluminium."

T2 was asked if he had changed his conception of "the mole" during his career:

T2: No, well,... The difference nowadays is that the basic unit is kilogram instead of gram. But in this context one still uses gram.

T2 referred to one textbook (Sillén, Lange & Gabrielsson, 1948) which had reinforced his conception of 'the mole' in accordance with F_1, a conception which had been stable since.

T2: In that book "the mole" of a substance is defined as so many grams as the formula weight measures. Like that, in two lines!

I: You have been in favour of that definition since then ?

T2:Yes, I have cling to it, yes.

Transient conceptual shifts

The category is characterised by shifts between different fundamentals due to context. Terms are used equivocally. All respondents who belong to this category change between F_1 and F_2, viz. 'the mole' is conceptualised in turns as a mass and a number, respectively. It is worthwhile to notice that this dualism is recommended in the revision of the syllabus of the Swedish upper secondary school in 1965. (Skolöverstyrelsen, 1965, p. 312).

Example

M2 was interviewed both in 1984 and 1987. In 1984 he stated:

M2: Well I've just taught the mole concept and I have taught the pupils, or at least tried to teach them, to think of mole as a word denoting number and having a certain mass.

At the end of the phase in the interview concerning teaching, M2 present what he had said to his students:

M2: If you weigh out 1.01g, 32g, 18g etc., what would you say about the number of atoms and molecules, respectively? Well, most of them understand it, and others perhaps feel it: there ought to be an equal number of atoms and molecules in... and then I say: These masses are called 1 mol of the specified substance and they contain $6.02 \cdot 10^{23}$ atoms and molecules, respectively.

Further confirmation of his transient conception is gained in the second round of interviews in 1987:

I: Concerning sulfur, do you write like this (Note. The interviewer (I) is writing!): $1 \text{ mol} = 32 \text{ g}$?

M2: Yes!

I: Well, is it possible to write like this: $1 \text{ mol} = 6{,}02 \cdot 10^{23}$? Do you think it's correct?

M2: Yes!

I: You are adding pieces! [Note. M2 wrote pieces after $6.02 \cdot 10^{23}$, viz. $6.02 \cdot 10^{23}$ *pieces* (italics added)].

M2: You ought to do that, yes!

I: But you agree upon the equal sign (or approximately equal to...)?

M2: Yes!

Another example is T7:

T7: The practical approach for the pupils is to establish that 1 mol of a substance is equal to the atomic mass expressed in grams. In this case I'm not so terribly strict, but it's a practical way for them to understand mole. Now I ignore the fact that it's equal to Avogadro's number, the number of particles...

I: But you don't think it's essential in this context?

T7: No, not in this context. No, but they can benefit from it in another context, but when we discuss it, we consider it to be like that.

Complete conceptual shifts

In this category only one fundamental is used independent of context actualised in the interview. The respondent stated explicitly or implicitly that the prevailing conception is different from earlier conceptions held.

Two types of shifts are identified:

a) Revolutionary shifts or 'Aha'- shifts

The respondent is highly aware of the shift and is able to account for it, often very vividly, as a revolutionary experience involving deep emotions. Reflections upon the old and the new concepts are expressed.

b) Evolutionary shifts

These shifts proceed gradually and lack dramatically events. On the one hand, they can be conscious adjustments to an altered view of reality where the subject is able to give a report on the shift and is able to discuss earlier conceptions.

On the other hand, the shift can be 'invisible'. The respondent found it difficult to describe the gradual adjustments made, even if s/he realised that there must have been a change. The current conception seemed to be so self-evident that the subject cannot imagine any other way of thinking.

Totally four (4) out of 54 educators reported revolutionary conceptual shifts about 'the mole'.

M10 was interviewed both in 1984 and at the second interview session in 1987.

In the 1984 interview M10 recalled a distinct memory:

M10: I remember one event, one of the greatest experiences in my life. I think it was around 1946, well somewhere between 1946 and 1950 when I had arrived at the university. I have forgotten the details but I remember that suddenly it struck me, I saw it right in front of me in burning letters that 1 mol O_2, or whatever it was, the elementary entity I have forgotten, is a complete analogy with one gross of pencils. I had certainly dealt with mol and molarity for a long time, but I hadn't become aware of it before I arrived at the university... Yeah, it was a great experience.

M10: (...) the first time I saw this definition of the mole was in Lange, Sillén & Gabrielson, the first edition (1948).

I: But this "aha"-experience, was it connected to that book or was it before...?

M10: I only remember that it was a tremendous experience. (...) Well, and it was after I had arrived at the academy, and I had passed the first year at the Chem department and so on.

Later on in the interview:

I: Have you experienced some radical change since then, after this, or do you still believe...?

M10: No. No, I'm still a believer in... Not a dramatic experience like that.(...) No, no. I think, I will remain .... (laugh) as long I'm in duty...

In the 1987 interview M10 confirm that he still clung to the conception of 'the mole' he gained by the revolutionary experience:

I: Has anything happen since, of this kind of aha-character? Since 1950?

M10: No, not that kind...of experience. Since then I have worked with this from a pedagogical point of view, and struggled to serve it in a acceptable way, and predominately as a practical useful tool for the students. And then, it's like a lot of other (concepts), the comprehension emerges when you use things - the deep comprehension. Somebody never gets it...

At a succeeding seminar in connection with the interview session in 1987, the respondent M10 commented and categorised his transcribed interview from 1984 according to the fundamentals.

M10: ... I have written F_2 which seems to be my status...(...) It also describes a conceptual shift ... or conversion I went through in 1948 or 1947, or around those years. Because I'm so old I was brought up with a strong stress in F_1 and I think it was Sillén [the textbook mentioned above] who gave me that push...

M10: I just remember this, well... it was like a flash of lightning. Well, it was just as people talk (laughing) about religious revivals. I can tell you that I was so deeply affected that I couldn't sit down any longer. I was forced to go for a walk.(...) I can't remember what I was working with at that time, in fact, it's still wrapped in obscurity... But I just remember this... as I said, it was like a flash of lightning. I was preparing something...

It is notable that to M10 the textbook Sillén, Lange and Gabrielsson (1948) meant a conceptual shift ($F_1 \rightarrow F_2$), whereas to T2 the book meant a consolidation of a conception in accordance with F_1.

MS has also experienced a revolutionary conceptual shift ($F_1 \rightarrow F_2$). MS was interviewed in November 1988. When he started studying Chemistry at the university he had to pass a preparatory examination. He failed.

MS: ... I was forced to sit down in my room and try to sort it out. And I struggled, and struggled. Suddenly, Oh, Almighty God, it must be like that... the numbers in the periodic table, atomic mass and molar mass, they have got the same numerical value because one has chosen that peculiar $6.023 \cdot 10^{23}$. Then it all sorted out, suddenly there was a change within me. In a new attempt to pass the examination I got everything right. It was 3 weeks after the first attempt. Everything happened during that period. ...(...) I want to give credit to the examination system that kept me down at the first attempt, so I was forced to find out... I worked late into the night. By the way I got such an impetus that I was one of the few that passed the next exam which was in chemical equilibrium.

MS comments on 'the mole':

MS: To me it's a unit of number and nothing else. It took a lot of time before I grasped it and when I grasped that it was only an unit of number things sorted out. But in school I was taught that 1 mol was so many grams as the formula weight stated.

MA got an 'aha'-experience while studying in teacher training She changed her conception through the influence of a lecturer.

MA: Well, I got some kind of 'aha'-experience.

I: Was he [the lecturer] standing there explaining for you or was it an 'aha'-experience within an hour or a minute or something like that, or was it slow process.

MA: I can't remind now... (...) But just that, that he introduced mole as a number, ... and I have a very apparent, in all situations, apparent visual imagination and memory and I saw those particles in front of me. Every sodium ion creates a chloride ion or (...) well, I can really see, symbolically, the chloride molecules, they are coming two and two, and then they can take care of two sodium ions and then my formulas were balanced.

It is evident that the grasping of mole was intimately bound up with the comprehension of chemical formulas and chemical equations, especially red-ox reactions. To sum up MA's experiences, the interviewer said:

I: (...) Well, then... one could say that you changed your conception of mole in that way. That you didn't have any real conception of mole at first and then... [both I and MA are now laughing] you got one.

MA: No, for me, mole was a rather diffuse concept and it was like a, what shall I say,... a whole lump, what shall I say, perhaps it sounds ridiculous. But you had... and sometimes when one talked about half a mole, yes it was like having half an atom or something in that fashion, not that you had $3 \cdot 10^{23}$ or something. (...) To me it was very abstract. (...) ... and to us, when I went to school molar weight and atomic weight didn't have any units, as they now have. Matter in a way... didn't weigh anything, but you said that the atomic weight for oxygen was... pardon, hydrogen atom was 1 (...) You should be very careful to say that one orange weighed 50 g but atomic weight was dimensionless. (...) ... one single atom didn't weigh anything but one mol did. (...) So, one carbon atom it had atomic weight 12, but here it was 1 mol, well then it weighed 12 grams and I found that odd. (...)... perhaps I'm thinking too concretely. If I had a paper and tore it into a smallest piece, which we can call an atom or molecule. Well, if it doesn't have any weight, it can disappear, even if its very small and that I remember, was very difficult for me that the single atom didn't weigh anything but then suddenly...

The link between the atomic weight of an element, without a unit, and 'the mole' of that element with the unit g (gram) was a conceptual trap to MA. It was first when her teacher introduced 1 mol as a number that she comprehended 'the mole'.

TN was forced to change his conception through the demands upon him as a teacher.

TN: Well it was the first N1(natural sciences program, 1st form) when I had to teach the mole concept. I was desperate, because I couldn't manage to present the thing. I struggled and read a lot of books, and eventually I found a model... and I felt, this I understand and then I used that model.(...) It was the thinking of particles.

TY changed his conception of mol due to teaching demands:

> TY: ... calculations here were very diffuse and what I did under my first years as a teacher, when we made calculations, I can't remember... but I have an impression... once, ... and it must have been, it can't have been before -63/64, it became clear that one could persistently use 'mole' as a number... then I believe I myself got something to cling to and then I have tried to cling to it... in my teaching, to... In fact, I belong to that generation, who studied chemistry in upper secondary school without any physics supporting chemistry. It was something, it was substances turning blue, green and red. (...) And then one arrived at the university and suddenly, good heavens, here is a conformity to law...one saw the thing in a new light but at the same time one hadn't got the thing lit up during secondary school so... when the new text-books came, around -64/65 then... I thought myself and I think lots of others, that now, oh dear, now the students get what we didn't.

The common feature of these four conceptual shifts are that the respondents were all involved in deep intellectual activity, struggling with the concept of 'mole' and so suddenly, the key was found when 1 mol was identified (interpreted) as a fixed number. For M 10 the fixed number was grasped analogously to 1 gross of pencils.

TY found around 1965 that one could persistently use 'the mole' as a number, which solved the previous diffuse conception of calculation in chemistry.

The change was initiated by the new textbooks in chemistry appearing due to the new curriculum for the Swedish Upper Secondary School (SÖ, 1965).

MA was triggered by a teacher at a trainee teachers college to look upon 1 mol as a fixed number. The mole as a number fitted her visual imagination of how atoms are rearranged in chemical reactions.

For MS it was the revolutionary discovery that the numerical value of atomic mass and molar mass was connected by the fixed number $6.02 \cdot 10^{23}$, which was equal to 1 mol.

Examples of category b)

M4 has got a clear picture of the shift $F_1 \rightarrow F_2$. At upper secondary school he learnt about the gram-molecule and it was a mass:

> M4: Well, it was introduced the other way around, it was the gram-molecule and it was by definition as much of a substance as the mass of the molecular weight, but in the unit gram.

Nowadays M4's conception is in accordance with F_2 and 'amount' is used in the sense of a fixed number:

> M4: ... I want to define it as it should be defined, as an amount, a quantity of number (...) of the same kind as dozen, gross and score, but a bit bigger.

M4 looks upon F_1 and F_2 as complementary:

> M4: ... if you choose one of them as a definition, than the other follows, it's a question of which end of the rope you are starting with, so to say, the two ends of the rope I was quite aware of, right from the beginning, but that one should start in the second and not in the first end wasn't clear until the syllabus' revision (in 1965).

The conceptual shift for M4 did not contain any dramatic elements. He was aware of the number aspect of 'the mole' in the early part of the 1940's. M4 passed the exam at upper secondary school in 1944 (Swed. 'studentexamen'). But then the number aspect was seen as a consequence of the definition of 'the mole' (gram-molecule) as a mass. The shift to F_2 (around 1965) was a change of origin (startingpoint). Now 'the mole' was defined as a number, and mass was a consequence (the "mass of 1 mol", "molar mass"). M4 looks upon the shift as a alteration of origin of already known facts.

TH cannot remember anything of his personal development in spite of the fact that he says:

> TH: ... 1 mol... it's the number in... it's equal to the number of carbon atoms of the isotope carbon-12 in 12.0 grams of carbon.

TH used the very common textbook Böös, Leden and Lundberg (1953) at the upper secondary school. The definition of mole in that book is a typical articulation of F_1. Evidently a conceptual shift must have happened, even though TH is not able to give a report on it.

U1 has made a conceptual shift from F_1 to F_3. This shift was made in the middle of the 1960's. As a physical chemist he was searching for a physical quantity with the unit 1 mol in order to be able to treat the unit and the requested physical quantity analogously to other units and physical quantities. His searching is in accordance with the contemporary discussion about the need of a physical quantity (*amount of substance*) for 1 mol in order to fit the demands of quantity calculus.

Even if revolutionary shifts are few in the present empirical data, they are very valuable when trying to identify the process and the components (steps) involved in conceptual shifts. They are temporal concentrates of what for other persons happened during a prolonged time period with no dramatically steps. The revolutionary shifts are often remembered because of their sudden emergence, often connected with emotional feelings and by the sharp contrast between the previous conception and the new one.

3.4.4 Conceptions of amount, *amount of substance* and the SI definition of 1 mol.

The following three sections are accounts of the revealed conceptions of amount, *amount of substance* and the SI definition of the mole.

Conceptions of amount

In the studies with the 28 educators, 26 educators and the 18 trainee teachers, we explicitly asked the respondents in what meanings they used the term *amount* (Swed. *'mängd'*). No such question was posed in the study concerning the students' conceptions. Yet their conceptions of amount were revealed during the reasoning around the task. In Lybeck, Strömdahl and Tullberg (1985, p. 50) we stated that the student uses amount in different meanings. Significantly, the meaning of amount is context-bound. The word amount connotes both a general undifferentiated quantification as well as a measure of a physical quantity which in each case must be interpreted from the context. In common parlance the ambiguity of the word means little disturbance, but in scientific language it is decisive. The demand of clarity is especially pronounced for concepts used in mathematical calculations. The students used the word amount about a concrete portion of matter, the physical quantities mass, volume, number, and in one or two cases as a short name for the physical quantity *amount of substance* or as equivalent to 'number of moles' (cf. Lode, 1970).

The use of the ambiguous term amount instead of the actual physical quantity prevented the respondent from narrowing down quantitative problems to the context of quantity calculus.

The expression 'How much?' in statements like 'How much is there in this cylinder?' is an equivalent to 'What is the amount?' and creates similar problems.

The problems are archetypically demonstrated by a student named Ann, when solving the task (Lybeck, Strömdahl & Tullberg, 1985a, p. 50):

Ann: Well, I think that... First about the amount, how much there is in each one.

I: What do you mean by that?

Ann: What they contain. Let's see, amount. There are different amounts in different tubes here. It's different... (inaudiable) always. How many grams they weigh...etc...

For 1 mol, yes, I need to no how much it weighs. Yes, the weight, yes grams then, the amount, the height, then we can say decimetre.

The 18 trainee teachers also use the word *amount* and 'how much?' in the task-solving context with the same connotations as the students. The results of what they preferably meant with the word amount is collected in appendix II, Table 3. The total variation of the conceptions of amount for the three studies are presented in Table 3. 5.

Table 3.5

The distribution of the conceptions of amount among the respondents in three studies.

Conceptions of amount	28 educators*)	26 educators**)	Trainee teachers***)
Mass	7	1	2
Weight	-	-	1
Volume	3	-	3
Number	9	7	12
Amount of substance	2	6	-
Mole	4	2	1
Number of moles	2	1	-
Heap	-	-	1
Portion	1	-	-
Ambiguous	4	3	7
Sort it out		1	-

*) Data is missing for one (1) respondent

**) Data is missing for six (6) respondents

***) Eight (8) of the respondents reported two conceptions and one reported three.

A majority of the trainee teachers had learnt to connect *amount* to 'the mole', and since 'the mole' is generally comprehended as a number, it is consistent that amount is conceptualised as number by a majority of the respondents. Among this majority there are some who refer to amount as equivalent to a set, as used in set-theory.

A tabulation of the conceptions of amount among the educators is also found in Appendix II, Tables 1 and 2.

The ambiguity and different senses of amount are known and commented by the educators and the trainee teachers, but this does not seem to prohibit them using it with different meanings depending on context. However, those who identify amount with mole, number of moles and amount of substance, said that they tried to reserve the word *amount* for "what is measured in moles".

The respondents' reports make up evidence for a nearly complete disagreement about the connotation of the word *amount*. This fact must be noted in comparison to the prevailing scientific convention, where *amount* is given a fixed meaning as an abbreviation of the physical quantity *amount of substance* (cf. Mills *et al*., 1988; 1993).

Conceptions of amount of substance

In the student study only one respondent (Bosse) mentioned the expression *amount of substance*:

I: ...what do you mean by amount?

Bosse: The correct notion is amount of substance. In fact, it's an amount (set), number of molecules, is 1 mol, it's $6 \cdot 10^{23}$ pieces.

I: If you use amount of substance and mole, what is mole then?

Bosse: It's a measure of amount of substance. If one knows that it's a mole, then the amount of substance is 1 mol, it's... because we use amount of substance ... in school, the name is amount, I think.

I: Well, they say so... where have you got the notion amount of substance from?

Bosse: I read a lot of physical tables, a lot of SI-units.

I: So, you are saying that the teacher doesn't use it?

Bosse: He doesn't, in a sense it's up to him, but it doesn't make it easier to use that expression.

I: But you know that it's amount of substance?

Bosse: Yes.

Contrary to this awareness of a student in grade 2 of the upper-secondary natural sciences program, 17 of the 18 trainee teachers, all with academic studies in chemistry, were ignorant of the contemporary scientific meaning of *amount of substance* (cf. Appendix II, Table 3). The ignorance of the trainee teachers is a remarkable fact, and could not be conceived otherwise than that the physical quantity *amount of substance* has not been thematized at the university where they have studied.

However, the Swedish term 'ämnesmängd' (freely, tolerable, in English, 'amount of compound') is known for some of the trainee teachers (TT) and is identified as "number of pieces" and "number of moles":

I: What is *amount of substance*? Have you heard that expression before?

TT8: No!

I: You have never used it?

TT8: No!

I: Not in your education, yet?

TT8: No!

I: Have you met the word 'ämnesmängd'?

TT8: 'Ämnesmängd', well, it's pieces, because it's a number of moles of something.

Thus, 'ämnesmängd' is equivalent to 'number of moles' but it is interpreted as 'pieces' by TT8 since mole is equivalent to a number. This conception is shared by TT18:

I: If I say amount of substance, does it mean something to you? Have you used that expression?

TT18: Not, what I know...

I: Have you met it at upper secondary school, university or in teacher training?

TT18: Well, if I've forgotten it at once.

(....)

I: Is the word 'ämnesmängd' more familiar to you?

TT18: Well, it sounds more familiar.

I: In what way?

TT18: Let me think... (...) If you ask me about this 'ämnesmängd'. Than I answer... that in group I there is 1 mol sulfur.

I: You said before that amount of substance sounds like number. Does 'ämnesmängd' also sound like number?

TT18: Yes, it does, because mole is number.

TT10 has heard about *amount of substance* but has not attained it as an active concept.

TT10: Well, it's an expression, I haven't,... I've heard it, but I don't use it. I feel it's a bit...amount of substance, it doesn't belong to my vocabulary. (...)... I'm a bit hesitant how to use it.

The educators have all heard the expression *amount of substance* but their knowledge of its meaning differ. Mostly they use the short names amount or 'ämnesmängd' to label what is determined in moles (cf. Appendix II, Table 1 and Table 2; cf. Appendix III for confirmatory quotations among the 26 educators).

Eleven (11) out of the 54 educators say that they use the expression *amount of substance*, and out of them there are three (M3, M8 and U1) who use it in a sense that seems to be in agreement with SI. These three are together with UB, who uses "ämnesmängd" as a synonym to *amount of substance*, those who have conceptions of 'the mole' categorised as belonging to F_3.

LB argues in favour of the use of short name amount instead of *amount of substance*.

LB: ... at the introduction I use it...(...) it's laziness that one doesn't use the whole expression.(...) When one's writing... then one avoids writing something unnecessarily long...

(...)(referring to physics teachers) ... some say that something weighs...that much... but the most accurate say ... that the mass is ... that much. (...) ... I think it's analogous to this... one chooses a linguistic usage, which isn't formally correct, but hopes the pupils catch on ...

LB seems to assume a priori that a formally correct scientific use of language is an obstacle to learning. This means that everyday language ("something weighs...that much") is more intelligible to the student than the formally correct one ("the mass is...that much").

The argument that the expression 'amount of substance' (Swed. 'substansmängd') is too long to use, is very common in all the empirical studies. The short name amount (Swed. 'mängd') is preferred. M1 uses the short name 'amount' because:

M1: ... it is very awkward to say amount of substance (Swed. 'substansmängd').

T3 does not use either amount or *amount of substance*:

I: Do you use 'amount of substance'?

T3: ... to be honest, very little. I'm talking of mole, and by that I mean, it's comparable to score and dozen. It's a number, but in chemistry it's more convenient to talk about a dozen atoms of hydrogen for instance, but instead one talks about 1 mol of atoms. (...)

I: You don't need to introduce it in chemistry teaching ?

T3: No, ... on the contrary, a problem is created with amount of substance... so I must say (to the students)... translate it into moles.

I: Are you saying: How many moles is this?

T3: Yes, that's right.

T9 realises the difficulties when she uses the short name amount and her students read 'amount of substance' in the textbook:

T9: ... it happens nearly every year that the students ask, when they have done their homework, after a couple of lessons ... I talk about amount, and then they are a bit puzzled... is it amount of substance or, ... how does it hang together? But, it's me who isn't consistent. It happens.

M5 is uncertain of the meaning of *amount of substance*. He also refers to textbooks, but in a different way than M1:

I: Do you use the expression amount of substance?

M5: At upper secondary school I do, because the textbooks use it, because it's the textbooks that are governing.

I: What do you mean (by amount of substance)?

M5: It's molar mass. (...) Amount of substance and mole,... then you put an equality sign.. it's like a base unit in the SI-system, so it's difficult to grasp it, what it is, in fact. Mole. So, I wouldn't say molar mass. Mole is more correct... (...) ... if I'm not sure of the expression amount of substance... So, I don't really use the expression amount of substance myself, automatically, I only use amount.

M6 is in the same predicament:

M6: If I use the expression, amount of substance, (pause)...Well, then I should...I think, use it in the same way I use the word mass of a substance. I would think in grams... then... then I leave the chemical concept of amount, I think.

UK who has an explicitly combined perspective of mole (F1&F2) discusses the meaning of the words "ämne" and "substans" (Eng. substance). He uses the word "ämnesmängd" to denote what is measured in moles. He is annoyed about the introduction of "substans" in the expression "substansmängd" (Eng."amount of substance") since his preference "ämne" in his view is identical to "substans", a fact that he believes is shared by ordinary people. The fact that *substansmängd (amount of substance)* is the stipulated name of a physical quantity is not touched upon.

UK: ...the introduction of (the word) substance (in the expression amount of substance) it irritated me a bit, I thought it was a needless word. I... I question if one has gained anything, either ... clarity or pedagogical, by introducing this concept. I mean, substance, it means a lot of things,... I don't know perhaps the idea was that "ämne" could mean a lot of things. I mean, substance could mean at least as many different things (as "ämne") and besides I believe, that ordinary people consider "ämne" and substance to be identical.

What is referred to by 'amount of substance' varies. Only one (U1) of the 54 educators and none of the 18 trainee teachers or the 30 students explicitly referred to 'amount of substance' as a unique independent base physical quantity in analogy with mass or length. 'Amount of substance', its short-name amount and the name 'ämnesmängd' all denote something which is in accordance with the individual conception of 'the mole' (cf. Appendix III, for confirmatory statements among the 26 educators).

Thus, the empirical results show that *amount of substance* (alt. amount) is not comprehended by the respondents as an independent physical quantity, but is conceptualised as identical to some other physical quantity, predominantly number.

Conceptions of the SI definition of the mole.

At one of the seminars in 1987 the following discussion was carried out after having talked about historical definitions of mol:

M2 (seminar 1987): (...) And then the IUPAC definition came. But it's terribly complicated to use in school.

M3: Oh, yes, goodness gracious!

M2: Perhaps it's best to say, like one of you said before, that 1 mol is a number of grams of the different substances... (...) and 1 mol contains the same number of particles, that's just the beauty of it...

Beside the fact that M2 is here using both fundamentals F_1 and F_2, these statements summarise our empirical findings about the general attitude to the SI definition of the mole in relation to teaching. The need of the methodological separation made in section 1.3 about the subject-matter domain and the educational domain is here fully demonstrated.

The following quotations are taken from the interview transcripts of the study embracing 26 educators (cf. Appendix III for systematic quotations from all 26 respondents).

UL is not happy with the SI definition of the mole.

UL: An SI-base unit,... I think one ought to define, without mixing up with any other base unit. For instance gram!

I: So, in fact you are a bit discontented with the present definition...

UL: I don't think it's perfect.

I: No. But is it consistent with your own conception?

UL: Well, this is only ... to quibble and philosophise how one defines it. Still, it must be like it's in praxis, shouldn't it? (...) So, if I had the possibility to decide, I would say... that... Avogadro's constant is as many pieces (...) as there are in those 12 grams. And then 1 mol, as many pieces as Avogadro's constant denotes. (...) But if this "mole thing" is going to have any practical implications, then this problem is emerging. This happens when you use mole for the first time. So you must, in fact, in some way convert it into grams, and one must know how much there is, corresponding to... pieces in 12 grams. (...)... one must have a precise determination of Avogadro's constant, and this could be made either in the definition of the mole or when you shall use it for the first time. (...) But if one is to have any use of the mole, one must know the numerical value of Avogadro's constant, anyhow. And it's determined so, ... a simple chemist will never work with such an accuracy so ... his

results aren't valid,... if there is one more decimal on this constant. It's already 6, 7 or 8...

In a discussion with the interviewer about different systems of basic units UH comments the status of 'the mole' in SI:

UH:...I can't say otherwise... than... the mole and like... it's clear,... to get order in the system, but yet, it has another character. They have not the same ... the same status... (...) well, they aren't as necessary, as to have... those... you know before SI, it was the MKSA-system.

UB about the definition:

UB: It's evident that... we... bring up the definition like it is in several books... that it starts from carbon-12, but... but... we stress that we can look upon it as a number. (...) There are those who for instance use the concept 'the Chemist's dozen'. As well as I have got one dozen of apples I can have 1 mol of atoms of sulfur. We believe that.

On commenting older definitions of the mole UB states:

UB: ... in the SI-definition it's evident... that it isn't the mass... it's an amount... it's a number.

UK about the SI definition of 1 mol:

UK: Well, it's not good. Well, not good... it's evident! Perhaps it's good as a scientific definition, possibly. But it lacks nearly all practical significance, because in my opinion one uses this definition, one takes... the formula-weight and puts on the unit gram. And it works in practical life. And everybody is content.

I: So this scientific definition, it... hasn't all that significance? Not even in scientific contexts?

UK: No, but ...I mean, we are measuring seconds with a watch, we don't bother that it's ... some oscillation in a special crystal... I... I do understand that there must be a tremendously sophisticated scientific definition of every... quantity, in the background. But then one creates a handy praxis to use in practical life. And I... I'm not capable to judge if... the definition of the quantity "ämnesmängd" or amount of substance, is good or bad. But I can say, that it's bad in one respect, that it doesn't... use... the units of the SI-system. It's... it should be kilomole instead.

Like the discussion in an excerpt from one of the seminars at the beginning of this section, UK's approach to the definition summarises the view of a great majority educators in this investigation. He presupposes that the definition is too sophisticated (cf. M1, below) to be used in educational settings and is of no relevance in practical problem solving. The "handy praxis" is in focus (cf. US, below). This means that the link of his own conception to the definition is guided by other factors (tradition and praxis) than those inherent in the context of SI and quantity calculus.

UM identifies 1 mol with Avogadro's number and interprets the SI definition of 1 mol as equal to the number of particles in 12 grams carbon, which in fact is Avogadro's number.

> UM: Well, I know the definition... I always keep that in my mind, it's as many entities as there are in 12 grams of the nuclid carbon 12... But... it's simpler to say that 1 mol is 6.0, well..22 or 23, to the power 23 pieces. Well, one could use more digits... well. I think that's the best... It's my conception, in fact it is... a number.

US consider mol as 'the Chemist's dozen'. She showed the interviewer the definition of the mole in the chemistry textbook written by Segal (1985, p. 28):

> ... a new unit called a **mole** (...) which contains a specific very large number of atoms or molecules. This particular number is known as **Avogadro's number**. Avogadro's number N_A is defined as the number of atoms contained in exactly...

Her comment is, without noticing the false statement by Segal that a unit (an abstract) could contain "a specific, very large number of atoms":

> US: So this is the... practical... definition,... well, which the purist doesn't like. But it's practical.

M1 does not dare to teach the SI definition from the beginning when introducing 'the mole' in educational settings:

> M1: ... And then we turn to number. What is mole? And I slow down, and wait some time with the official definition of the mole, because no human being grasps that, at the beginning. But I can't keep it back, it must come. Why it's decided like that ?... and then we look at the SI-system and this and that.
>
> I: Does anyone grasp this definition? (...)
>
> M1: Well, yes, but it's evident they (the students) do so as time goes by, because it must be connected to my planning of the course in chemistry.

M1 substitutes the expression *amount of substance* with the word amount and M1's own interpretation of the definition is clear:

> I: What do you mean by amount, really?
>
> M1: Well, concretely, it's the number of atoms or formula units or particles or molecules. That's my view.

3.4.5 Conceptions of the relationships between physical quantities.

The results of the respondents reasoning about the mathematical relationships between physical quantities are reported against an

introductory analysis of quantity calculus, proportionality and conversion.

Quantity calculus

Guggenheim (1958) called for the use of quantity calculus, as the most profitable way to do calculations. In the American scientific community he addresses the honour of making this clear to Lodge (1888). Lodge had been Guggenheim's teacher.

Copley (1960) confirmed that:

> The first clear expression of the principles of quantity calculus is undoubtedly A. Lodge's very concise presentation of its conventions under the significant title: "The Multiplication and Division of Concrete Quantities". (Copley, 1960, p. 254)

Henderson (1924) had attributed the use of quantity calculus to William Stroud, under the name of the "Stroud system". But Copley (1960, p. 254) declared that there is no written evidence that Stroud ever used the conventions of quantity calculus.

According to Copley (1960, p. 254) it is clear that Everett (1879) used quantity calculus in 1879, even if it was in an inconsistent way. However, the properties of a physical quantity were already expressed by Maxwell (1873):

> Every expression of a Quantity consists of two factors or components. One of these is the name of a certain known quantity of the same kind as the quantity to be expressed, which is taken as a standard of reference. The other component is the number of times the standard is to be taken in order to make up the required quantity. The standard quantity is technically called the Unit, and the number is called the Numerical Value of the quantity. (Maxwell, 1873, p. B)

A stringent and general use of quantity calculus is a much later phenomena. In Germany it begun some 60 years ago (Weninger, 1990).

> Das Rechnen mit Grössen ("Grössenrechnen") setzte erst vor etwa 60 Jahren zaghaft ein. Und das grundlegend wichtige Werk von Julius Wallot, das die endgültige Durchsetzung des Rechnens mit Grössen bewirkte, erschien in erster Auflage erst im Jahre 1953. (Weninger, 1990, p. 206)

In the prevailing IUPAC recommendations, the elements of quantity calculus are expressed in the following way (Mills *et al.*, 1993, p. 3):

> The value of a *physical quantity* is equal to the product of a *numerical value* and a *unit*:
>
> physical quantity = numerical value x unit

> Neither the physical quantity, nor the symbol used to denote it, should imply a particular choice of unit.
>
> Physical quantities, numerical values, and units, may all be manipulated by the ordinary rules of algebra.

In describing the world in physical terms we assign properties to matter. The set of measurable or calculable properties in natural sciences are the physical quantities. They are abstractions, designed to fit the rules of mathematics.

> Physikalische Grössen sind nie „konkrete Dinge", sondern immer „Attribute" von Dingen; Eigenschaften die wir an den Dingen unserer Erfahrung feststellen können. (Wallot, 1953, p. 1)

The values of the base physical quantities are measured in the real number system. The real numbers make up a continuum, which means that the physical quantities represent continua. This means a mathematical abstraction, an *idealisation*, of the phenomenal property. Thus the physical quantities should not be mixed up with life-world experiences.

As physical quantities are presupposed mathematically continuous, this makes them applicable to differentiation.

Time and length are intuitively taken as continua, with the possibility to adopt an arbitrary value in the real number system. But continuum is also applied to macroscopic properties concerning matter. The continuum as an idealisation applied to matter is well illustrated by the physical quantity density.

Take a range of decreasing portions of matter with mass and volume denoted by m_k and v_k, respectively. k denotes indices for portions of matter. $k=\infty$ is the limit when the matter portion is infinitesimal. Then density in a point (P) is defined by the equation:

$$\rho(\mathrm{P}) = \lim_{\substack{k\to\infty \\ v_n\to 0}} m_k / v_k$$

Continuum is presupposed in this kind of derivation. This mathematical operation, which is an idealised physical description should not be mixed up with life-world circumstances. When the portion of matter is reduced to the order of atomic dimensions (10^{-10} m), the definition above collapses. The use of the physical quantity density is restricted to portions of substances with dimensions much bigger than 10^{-10} m.

Hence, density is a physical property applicable only to dimensions of matter where intra-atomic phenomena can be neglected. A restriction must be added to the definition above: the portion of matter with the volume v_k must remain sufficiently large to contain a number of particles not being in conflict with the properties of the single atoms. With this constraint we consider matter as material continuum and use continuum mathematics. It is a question of a restriction laid upon matter when it is viewed as a continuum or as a discontinuum.

In chemistry laboratories and industrial practice, portions of substances are generally larger than the atomic dimensions and the discontinuity of matter can be ignored. However, this is not to say that the grand theory of chemistry as described and explained in the context of atomic theory is ignored. When the corpuscular structure of matter attracts our attention, we change our perspective from a continuum to a discontinuum. The delimitation and range of the perspectives are complementary in our description of a physical phenomenon.

Mathematical relationships between physical quantities, basic as well as derived, make up quantity calculus. It is recommended for use throughout science and technology (Mills *et al.*, 1993, p. 3)[38].

Proportionality.
Proportionality is one of the most important mathematical structures dealt with in physical sciences. Learner difficulties with proportionality have been investigated in several studies. A review of studies concerning proportionality reasoning has been elaborated by Tourniare and Pulos (1985). Their concern is proportionality reasoning in relation to mathematics education. However, as noted by Gamble (1986), the difficulties can also be experienced in relation to the nature of physics and chemistry, viz. how proportionality is used. A study of the understanding of preservice teachers have of direct proportionality across different tasks has been made by Yap Kueh Chin (1992).

Lybeck (1981) has made extensive studies on proportionality reasoning among students by using measuring cylinders, spring balances, and tasks coupled to density. Lybeck's main contribution is the identification of the A- and B- forms, the functional aspects of proportional reasoning. The A-form denotes a reasoning of proportionality as a relation between separate physical

---

[38] A more appropriate name for 'quantity calculus' might be 'algebra of quantities', because it is the principles of algebra rather than calculus that are involved.

quantities (variables) and the B-form, a reasoning within the same physical quantities (variables). This dicotomization has meant a criticism and a reinterpretation of studies on proportionality like those of Karplus *et al.,* (1970, 1972, 1974), Wollman and Karplus (1974) and Suarez (1977) (cf. Lybeck, 1978, 1979 and 1981).

Ward and Herron (1980) have shown that proportional reasoning ability is related to success in chemistry learning and Wheeler and Kass (1977) found that student problem-solving ability was dependent on proportional reasoning ability. These studies, like other studies in the Piagetan tradition, consider proportionality reasoning as belonging to the formal stage. Chiappetta (1976) and DeCarcer, Gabel and Staver (1978) reported that about a half of a group of high school students do not operate on the formal operational level. Thus, the problems of proportional reasoning seem to be extensive in relation to curriculum demands.

In a study aiming to determine whether certain instructional strategies were superior to others in teaching high school chemistry students problemsolving, Gable and Sherwood (1983) found that the factor-label method was the most effective and proportionality was the least effective, when calculating with 'mole'. Contrary, in gas law calculations proportionality was most effective. However, the gas laws were taught later in the school year. Their own explanation was that either the teaching strategies are subject matter-specific or the proportionality method becomes more effective over time. In fact they stated that the gas laws were explicitly given as proportionalities ($y = k \cdot x$). No such statement was made about the teaching of mole. Thus the most plausible explanation to the results seems to be the lack of a teaching sequence of 'the mole' where proportionality is used explicitly.

The students' lack of overall applicable mathematical instruments are supported by results gained in interviews with pupils in 16+ chemistry courses, reported by Lazonby, Morris and Waddington (1982):

> Whereas many pupils could do separate steps in calculations, they have difficulty linking sequential operations, as described by Howe (1975). Often pupils reported to very haphazard ways of solving problems, as the following comments (in answer to the question, 'What do you do when you go wrong in a problem') show: 'I'd start moving the numbers around until I got something that looked right!' 'I start again, because I know I am wrong, and then mix the numbers around'.

Similar answers are found in our student study (Lybeck, Strömdahl & Tullberg, 1985a). The educators' ideas of reasoning around a problem instead of using 'formulae', which is rejected, is typical in our studies with educators. The educators lack confidence in using stringent proportionality which is denoted as 'formulae'-manipulation. The general attitude is that students should be taught to reason anew, and use algorithms ('rule of three') every time they are calculating (cf. Appendix III for confirmatory statements by the 26 educators). Explicit teaching of proportionality in the A-form is not on the agenda.

Davies and Moore (1980) who had adopted SI and quantity calculus concluded:

> We believe that by emphasising the proportionality relationships among the quantities involved in stoichiometric calculations and by providing an outline form in which the logic of a problem solution can be expressed we are able materially to increase problem-solving skills of introductory chemistry students. (Davies & Moore, 1980, p. 306)

Whitmer (1987) has also drawn attention to the importance of managing proportionality, in the form $y = k \cdot x$, in chemistry:

> Students capable of proportional reasoning are armed with a powerful problem-solving tool. (Whitmer, 1987, p. 37)

In order to communicate the empirical findings concerning reasoning about relationships between physical quantities it is necessary to take into account ratio, proportion, rule of three and proportionality. Further, conversion must also be discussed.

Rule of three

From a mathematical point of view a proportion is an equality of two ratios of the form

$$a/b = c/d \quad (1)$$

where $a,b,c,d \in \mathbf{R}_+$ ($\mathbf{R}_+$ denotes the positive real numbers). If three of the variables (e. g. a, b and d) are known the fourth (c) can be calculated

$$a/b \cdot d = c \quad (2)$$

The proportion can be translated to the algorithm 'rule of three', the 'B-form ' of proportionality (cf. Lybeck, 1981):

$b \leftrightarrow a$
$b/b=1 \leftrightarrow a/b$
$d \leftrightarrow (a/b) \cdot d = c$

The double-cusped arrow is often read as 'equivalent to' or 'corresponds to'.

Calculating in the form of 'rule of three' is a reasoning of the logical schema 'if... then':

if b corresponds to a
then 1 corresponds to a/b
if d **then** d corresponds to $(a/b) \cdot d = c$

Hence, the use of 'rule of three' is basically more of a logical schema than formal mathematics. Perhaps this is why several of the respondents among the educators prefer this type of solving stoichiometric problems as a "mathematical simplification", rather than using formal mathematics in the form $y = k \cdot x$.

Simple logic seems to be considered as more accessible, or adapted to the student's learning conditions, than the 'abstract' proportionality sometimes classified as 'formulae'-manipulation and a 'physicalisation' of chemistry.

The use of 'rule of three' is not connected to some special fundamental. It is always applicable in dealing with a proportionality. In fact it is widely used in stoichiometric calculations. However, within F_0, F_1 and F_{2a}, where 'the mole' is not explicitly associated to a physical quantity, 'rule of three' seems to be the usual way to treat proportionality (cf. Appendix III, for confirmatory statements about the use of 'rule of three' among the 26 educators). In fact, in these cases the schema 'rule of three' could rather be conceived as manipulations between units than between physical quantities. For instance within the frames of F_1, the schema of 'the rule of three' expresses a relation (unique for each substance) between the general mass unit 1 g and the individual mass unit 1 mol. Hence, the manipulation due to this schema is a conversion between units (cf. conversion, below).

The functional relationship of proportionality, $y = k \cdot x$.
If the ratio $a/b = k$ (k = constant) then the proportion (1) turns into $k = c/d$, rearranged:

$$c = k \cdot d$$

This is the proportionality in the functional relationship ($y = f(x)$), generally written with variables x and y:

$$y = k \cdot x$$

This is the A-form of proportionality (cf. Lybeck, 1981). When x and y are representing physical quantities, the equation is called an equation of physical quantities (Sw. 'storhetsekvation'). Along with a fixed system of units, e.g. the units of SI, calculations will be straightforward.

Treatment of 'the mole' in the different fundamentals (F_1 - F_3) in the form $y = k \cdot x$ is possible if 1 mol is used as a unit of an explicit physical quantity. Applied to F_3 *(amount of substance)*, some simple proportionalities emerge (see fig. 3.4, section 3.4.2).

Mass (m), number (N) and volume (V) are connected to *amount of substance* (n) by the proportionality constants molar mass (M), Avogadro constant (N_A), and molar volume (V_m) respectively. All constants are *elementary entity dependent*.

The molar quantities are intensive quantities obtained by extensive quantities divided by *amount of substance* (with a few exceptions (not dealt with in this thesis: molar absorption coefficient and molar conductivity meaning divided by *amount of substance* concentration), and since *amount of substance* is dependent on the elementary entities chosen (cf. the SI definition of 1 mol), we have used the phrase *elementary entity specific* in previous studies (Lybeck, Strömdahl & Tullberg, 1985a,b,c,d). However, since the adjective *specific* before the name of an extensive physical quantity denotes the operation *divided by mass*, the word *dependent* is here used instead of *specific*.

Density (ρ), elementary entity mass (m_a(1ee)), and elementary entity volume (V(1ee)), are proportionality constants connecting mass and volume, mass and number, and volume and number respectively. The latter proportionality constants are all elementary entity dependent and can be logically derived from the former proportionality constants by division ($\rho = M / V_m$, $m(1ee) = M / N_A$, $V(1ee) = V_m / N_A$).

A deduction of the equations $m = M \cdot n$, $N = N_A \cdot n$ and the conversion $1 g = N_0 \cdot 1 u$ is to be found in Lybeck, Strömdahl and Tullberg (1985, a,b,c).

The relationship between *amount of substance* and volume is $V = V_m(ee) \cdot n$

V_m(ee) is the molar volume, an elementary entity specific constant (all other conditions held constant) with the common SI-unit unit 1 dm^3/mol. Molar volume is a derived physical quantity and should not be mixed up with the physical quantity volume. Often only the molar volume of gases is considered in chemistry education, because they can be looked upon as approximately equivalent to the ideal gas molar volume (a constant). Molar volumes for solid substances, which are seldom dealt with in elementary education, confused the students in our investigation (Lybeck, Strömdahl & Tullberg, 1985 a,b,c).

A systematic use of quantity calculus and proportionality in the form, $y = k \cdot x$, solves the conceptual problems associated with the relationships between the physical quantities involved.

Conversion

Proportionality should not be mixed up with conversion which is a change of unit of an invariant physical quantity. Conversion between physical quantities is impossible, because of incommensurability. A conversion factor is a pure number (a real number) and not a proportionality constant in the meaning of a *physical quantity* in the functional relationship $y = k \cdot x$.

Example:

$$1 \text{ yard} = 0.9144 \cdot 1 \text{ m}$$

The over all physical quantity is length. The conversion factor between the two units of length 1 yard and 1 metre (m) is 0.9144.

Results and discussion

At one of the seminars in 1987 a spontaneous discussion emerged between three educators about the relationship between the units 1g and 1u. A fourth participant (a lecturer in mathematics education, here denoted M, not individually interviewed) made a contribution at the end of the discussion (I = the seminar leader).

I: (...) The quotient between these two different mass-systems, the unit-systems is the pure number N_0 .

M3: Well, is that dimensionless?

M2: Pardon?

M3: It's odd that N_0 can be dimensionless.

M10: Well, it is... it's introduced as a dimensionless number. It's OK.

M2: But it's two units which can't be reduced!

M3: It disturbs me too.

M2: Well, it disturbs me too.

M10: No, but it's two units of mass, we are allowed to compare them.

M2: Yes, but if we now used to divide cm^3... etc., then we can't combine, divide dm^3 and cm^3, reduce.

M10: What did you say?

M2: When we calculate dimensions, or what it's called, then we divide units with units.

M10: Well, as far as it's possible.

(...)

M2: But, you can't divide, or cancel dm^3 in the numerator and cm^3 in the denominator. We can't divide like that. You know what I mean?

M3: Yes, I do.

M2: You don't encourage that kind...

M3: You are allowed to ... if you convert dm^3 to cm^3, so we get a power of ten. (...) But, this is not a power of ten.

M2: No.

I: But, imagine the conversion between the two units of mass 1 gram and 1 metric ton.

M3: Then you put 10 power to ... somewhere.

M10: Yes, but 1 kg divided by 1g, is one kilo, 1000. It's exactly the same way.

M3: No, it's analogous to that system of powers of ten.

I: So, it must be powers of ten?

M3: Well, one is educated in that (tradition). (...) Well, there is something of this in my account, in the interview. When I introduce the concept of 1 mol, or the concept of 'ämnesmängd' [amount of substance]. There is something... but... it's not explicit in that way... (...) Well, I accept the idea, but it's not elegant.

I: Well, if this number had been 10^{24}, you wouldn't have said anything.

M3: No, No. If there had been a prefix...

M2: No, then you change g to u$\cdot 10^{24}$.

M: Well, then it's only like a rate of exchange

M2: Yes, it's a rate of exchange.

M10: It's a rate of exchange between two units of mass, u and g, isn't it?

The discussion reflects the uncertainty even among experienced educators about units and physical quantities, and the character of relationships between them. M10 is the only one who masters the situation right from the start of the discussion. The quotient $1\text{g}/1\text{u} = N_0$ is a conversion of units (1u and 1g) within the same physical quantity (mass; the units are dimensionally identical) by a conversion factor, a pure number N_0. M3 and M2 consider N_0 to be attached to a unit (probably 1 u/g and implying that N_0 is some kind of proportionality constant). In addition the conception that the conversion factor should be powers of ten, such as 10^3 between 1g and 1 metric ton, is a constraint on seeing the analogue conversion factor of N_0 between 1u and 1g. Finally M3 accepts the idea of a pure conversion factor, by some kind of analogical reasoning, but dislike the numerical value of N_0, from the point of elegance, since it is not an integer power of ten. M3 explicitly says that he is educated in the spirit of that kind of elegance.

This is an illustration of the problems united with general dealing with different unit-scales (here 1 g and 1u) for one and the same physical quantity. However, this stands in sharp contrast to statements about conversions between the multiple units of for example the metre, dm^3 and cm^3 regarding the physical quantity length.

Three molar quantities will be examined in relation to proportionality.

The focus is stressed on *molar mass*. Molar volume and the Avogadro constant (or *molar number*) are largely modelled by the general features of molar mass.

Molar mass

The physical quantity *molar mass* is in focus in the task solving context, and in the phases of the interview where relationships including mass and 'the mole' are mentioned.

A general view among the respondents is that masses of portions of matter are 'translated' by molar mass into 'moles' in order to make stoichiometric calculations. At the end of the calculation, a gained result in 'moles' is 'retranslated' to mass by multiplying 'the number of moles' by the actual molar mass. In the task solving context, 1 mol is often directly 'translated' to masses by knowledge of molar mass (or molar weight, atomic- weight or -mass) as noted above.

Due to the explicit lack of physical quantities within the fundamentals F_0 - F_2 , 'the mole' connotes a device to make stoichiometric calculations. 'The mole' is here a means to make practical solutions to practical quantitative chemical problems. 'The mole' is an exclusive chemistry device. The possibility of integration of 1 mol as a genuine unit of a physical quantity in the wider context of mathematics and physics (quantity calculus) is not clear.

> M2 (seminar 1987): ... I try to stop the students from using these formulas (equations). Unfortunately they are printed in our book, in the margin. I think they should only , eh,...is the molar mass 21 g/mol and we have got 7 mol then it is 7 times 21. I think one should manage it without formulas (equations).(...) So, to convert between gram and mole and mole and gram, they should do it by definitions and not by formula.

When the seminar leader made an analogue to Ohm's law, M10 said:

> M10: But Ohm's law is essentially different... we have different names on the units for all three physical quantities. The exclusive feature in Chemistry is that we haven't found out a special name of g per mol, God forbid it!. So, already this g per mol, if we remember that and don't turn it around to mol per gram (...) It speaks for itself what to do, if we are going in the one or the other direction

M3 is the only one among the respondents who has explicitly adopted molar mass as a physical quantity, but there is a conceptual problem.

> M3: I used to define molar mass as mass per unit of amount. It is for me a new defined physical quantity and I compare this with how the physicists define velocity, as distance, as distance covered per used time.

The seminar leader called M3's attention to the fact that he defined molar mass as mass per unit of amount (Sw. 'mängdenhet') and not just amount (of substance). M3 cannot see the difference and appeals to one of the other seminar leaders.

> M3: ... velocity is, distance per unit time, and density mass per unit volume, isn't it?

This is the B- form of the functional aspect of proportionality. To express the definitions as M3 does, per unit of volume and unit of time, is to use the 'rule of three' to quantify within one variable at a time, it is to stress the property of isomorphy of the proportionality function.

Later on in the seminar the seminar leader asked M3 to explain: Why is the unit g per mol?

> M3: Well, it's easy if you define molar mass as mass per unit of amount (Sw. mängdenhet). What is the unit of for mass, 1 g, and what is the unit of amount, 1 mol, in the amount of 1 mol. The unit is 1g divided by 1 mol, viz. 1 g per mol, viz. 1 g . mol^{-1}. (...) I get it from same operation as I get the definition of velocity [the respondent is very eager].

The most common view among the respondents is that molar mass is the mass of 1 mol (cf. confirmatory statements among the 26 educators in Appendix III,). Since a large majority of the respondents identified 1 mol as equal to the Avogadro's number, molar mass is interpreted as the mass of that number of specified elementary entities. This unit quantity, special for each element or chemical compound, is the 'measure' to use in finding out 'the number of moles' in an actual portion of matter with a specified mass. This is done by dividing the mass of the actual portion of matter with the mass of one mole (the molar mass). Thus the actual number of moles are multiples of the unit 'measure' (amount, quantity) 1 mol.

Even if the division, actually done, is in the form a/b, the conceptual background seems to be the algorithm 'rule of three'. Properly handled the division a/b results is a pure number (mass divided by mass). This is also indicated by the expression 'number of moles' (cf. Ger. 'Molzahl'). But this logical interpretation is contradictory to the empirical data in the interviews, where 'number of moles' is expressed by a numerical value and the unit mol (e.g. "the number of moles is 2 mol"), which semantically must be looked upon as a tautology. However, the mathematical manipulation behind 'number of moles' which makes sense is 'rule of three'. It conceptually overrules the actual outcome of the division (a/b) and the semantic problem of 'number of moles'.

Many educators explicitly declare preference for reasoning in comparison with formal quantity calculus when calculating quantitative problems. Reasoning means the schema of 'rule of three', such as '... if 1 mol sulfur is (equivalent to) 32 grams then the number of moles in 64 grams must be 2 mol....' (note. no authentic quotation). Explicitly constituted:

$$\begin{array}{lcll} 32\text{ g S} & \leftrightarrow & 1\text{ mol S} & (1) \\ 1\text{ g S} & \leftrightarrow & 1/32\text{ mol S} & (2) \\ 64\text{ g S} & \leftrightarrow & 1/32 \cdot 64\text{ mol S} = 2\text{ mol S} & (3) \end{array}$$

When using rule of three, the units are conserved on both sides of the dubble-cusped arrow (one quantity at a time is manipulated). The division in (2) with 32 without any attached unit is the key. This manipulation possibly explains why the unit mol is attached to the numerical value contrary to the semantics of 'number of moles'.

By using the relationship $n = m/M$, within the rules of quantity calculus with an ultimate demand of proper units of the physical quantity, seems confusing when the educator's conception is still within the frames of 'rule of three', and a conception of molar mass as the mass of 1 mol.

> MU: We call this unit portion 1 mol and we state the fact that carbon has the molar mass 12 g /mol. But the pupils ask ' isn't that the same thing twice over to say molar mass has the unit g/mol?'. And I can agree with them there, that it's saying the same thing twice, but it's important for us to say so and so many g/mol, otherwise we'll run into trouble.

The introduction of a new physical quantity, *amount of substance*, meant a break with the phrase 'number of moles' which is noted by Davies and Moore (1980):

> The phrase "number of moles" is used widely because until recently there was no alternative. Lack of word that bears the same relationship to "number of moles" that "mass" bears to "number of grams" has made mole seem somehow unique and more difficult to handle than other units. Fortunately the SI definition of mole and the IUPAC manual have supplied the name *amount of substance* [italics added] and the symbol *n* [italics added]for the quantity that the mole measures. Of course we must remember that the term amount now has a specific scientific definition. (Davies & Moore, 1980, p. 303).

Four years earlier Davies, Moore and Collins (1976) had stated:

> Another major source of confusion is the use of the term "number of moles" rather than "amount of substance". This older term is clearly ambiguous, is being uncertain whether a pure number or a number multiplied by moles is intended. A survey of currently popular general chemistry texts confirms this ambiguity. While some authors write expressions such as no. of moles H_2S = 0.331 others write them in the form no. of moles H_2S = 0.331 moles. A third group, perhaps the majority, employ both conventions. (Davies, Moore & Collins, 1976, p. 681)

Within the context of SI and quantity calculus, the definitional equation for the physical quantity *molar mass* (*M*), $M = m/n$ could be compared to the definition of density (ρ), $\rho = m/V$. But there is an essential difference. Density is most simply determined by repeatedly measured concordant values of mass and volume of probes of the actual substance. A mean of the quotients of mass and volume is then taken as the numerical value of the density. An experimental determination of *molar mass* is not possible by making up a quotient of mass and *amount of substance*, since *amount of substance* is not a measurable physical quantity.

This fact is observed by the respondents. At one of our seminars (1987) this observation is explicitly stated:

> M3: Now, in physics one is able to measure volume and mass. Draw a diagram and find a straight line. One is able to measure *s* and *t* and get a straight line [*s* and *t* represent length and time, possibly M3 is thinking of the proportionality between them]. But we can't measure *n* and *m* and draw a diagram and get a straight line. (...) But they have to accept it by reasoning that it is so.

Molar mass only mimics an analogue physical status in $m = M \cdot n$ as density (ρ) in the relationship $m = \rho \cdot V$. Hence, *molar mass* is only a mathematical analogue to density. *Molar mass* is determined by measurement and calculations outside the immediate frames of the relationship $m = M \cdot n$ [39]. According to CGPM (1973, p. 35) *molar mass*, *M*, is most simply established by the combination of the quotient of relative atomic masses and the definition of 1 mol[40] :

> Une mole d'atome X contient par définition autant d'atomes qu'il y a d'atomes ^{12}C dans 0,012 kilogramme de carbone 12. Parce qu'on ne sait pas mesurer avec précision la masse m (^{12}C) d'un atome de carbone 12, ni la masse m (X) d'un atome X, on utilise le rapport de ces masses $m(X)/ m(^{12}C)$ qui peut être déterminé avec précision (3). La masse correspondant à 1 mole de X est alors $[m(X)/ m(^{12}C)] \times 0,012$ kg, ce que l'on exprime en disant que la masse molaire $M(X)$ de X quotient de la masse par la quantité de matière est:
>
> $M(X) = [m(X)/ m(^{12}C)] \times 0,012$ kg/mol

The following example is given in CGPM (Bureau international de Poids et mesures, 1973, pp. 35-36) to show how to calculate the *amount of substance* for 0.05 kg fluorine (F_2). The molar mass is determined to $M(F_2) = 0,037\ 996\ 8$ kg/mol. Calculation is made via $n = m/M$.

> La quantité de matière corresondant à une masse donnée du gaz F_2, 0,05 kg par exemple, est:
>
> $0,05\ \text{kg}/0,037\ 996\ 8\ \text{kg}\cdot\text{mol}^{-1} = 1,315\ 90$ mol

Note the word 'correspondant' in the sentences "La masse **correspondant** [note. my emphasis] a 1 mole de X est alors $[m(X)/ m(^{12}C] \times 0,012$ kg" and "La quantité de matière **correspondant** [note. my emphasis] à une masse donnée du gaz F_2, 0,05 kg(...) 1,315 90 mol". Nothing is here said of a proportionality in the form $m = M \cdot n$. The reasoning has a resemblance of the 'rule of three'.

Since *amount of substance* cannot be measured, only calculated, it is not possible, by a normal school experiment to calculate a proportionality constant (*M*) between mass and *amount of substance*.

---

[39] No assumptions are needed about the atomic structure of matter to establish the physical quantity *density*. Density is applicable to all kinds of matter, whether being pure substances or mixtures. *Molar mass* can only be applied to pure substances, since it is directly related to the composition of the actual elementary entity.

[40] In the following quotation the footnote (3) says: "On dispose de plusieurs méthodes pour mesurer ce rapport; la méthode la plus direct est l'emploi d'un spectromètre de masse." [There are several methods to measure this quotient; the most accessible is to use a mass-spectrometer.]

Molar mass as an elementary entity constant could only be determined by the measurement of elementary entity masses or ratios of such masses (as shown above), magnified to gram-scale by the definition of the mole. Further, they have one property in common, they are both elementary entity dependent. But even in this similarity there is a difference. Molar mass is intrinsic elementary entity dependent since the physical quantity *amount of substance* is elementary entity dependent by definition. They are elementary entity dependent in a qualitative fashion, since the entities are separated by *kind* of atom or aggregates of atoms. Density is only elementary entity dependent according to the actual substance measured by volume and mass. Neither mass nor volume are by definition intrinsically dependent on elementary entities.

These conceptual circumstances seem to partly explain why educators prefer to calculate 'the mole' by the equation $n = m/M$ and 'rule of three'-reasoning and not by using the formal proportionality $m = M \cdot n$.

Molar volume

Molar volume is traditionally almost exclusively applied to gases in elementary chemistry courses. The general conception is that the gas molar volume is the volume of one mole of a gaseous substance. The reasoning is analogous to the reasoning around molar mass.

The conceptual context constituted by the mole task strongly incites reasoning around volumes since they are immediately visually perceived. By their statements, the respondents seem to ask themselves: What is the phenomenal feature of 1 mol of a substance? What is the volume of 1 mol of a solid substance? Is it a constant value irrespective of substance like the gases? Are the molar volumes different depending on the volumes of the elementary entities making up the macroscopic volume?

These questions caused problems to the respondents, especially to the students and the trainee teachers. Molar volumes of solid and liquid substances are generally not considered in school and undergraduate chemistry education, even if several educators reported that they show their students portions of substances of 1 mol. However, it seems that this is done to show 'how much' 1 mol is in a general sense (space extension) for different substances for comparison, not actually to give numerical measures of volumes.

The Avogadro constant and Avogadro's number

The proportional relationship between number (N) and *amount of substance* (n), $N = N_A \cdot n$ is seldom explicitly expressed by the respondents. Neither is the proportionality constant, the Avogadro constant (N_A), conceptually separated from Avogadro's number, N_0, which is the numerical value of the physical quantity Avogadro constant ($N_0 = \{N_A\}$). Both are conceptualised as the number of elementary entities in 1 mol (cf. Appendix III for confirmatory statements, among the 26 educators, about Avogadro's number and the Avogadro constant)

3.4.6 The results of the empirical investigations summarised

A. The measure with the unit 1 mol is always determined via some other measure, predominantly via the physical quantity mass. Experienced respondents directly translate 1 mol to fixed masses, the 'molar masses' of the actual substances.

B. The total variation of conceptions of 'the mole' is captured by four *fundamentals* (F_i ; i = 0, 1, 2, 2a, 3). Out of 54 educators interviewed, 3 exhibit a conception of 'the mole' more or less coinciding with the SI definition (F_3).

C. Conceptual shifts of conceptions of 'the mole' could be evolutionary (gradual) or revolutionary (sudden). The attainment of a new conception is mainly a result of analogical and metaphorical reasoning. The revolutionary shift seem to be a sudden awareness of the discontinuity between an earlier conception and the new one. gained This type of shift is often experienced via an analogy, e.g. from a conception of '1 mol as an individual mass, e.g. 1 mol S = 32 g S' to 1 mol as a number, 1 mol = 6.0 10^{23} via the analogy '1 mol is like 1 dozen'. The evolutionary change is a process of the same kind, but it is extended over time, where the conceptual discontinuity is not easily recognised by the individual.

D. Conceptions of *amount* and *amount of substance* are equivocal.

E. None (or perhaps one, UH) respondent considered the SI definition of 1 mol as a startingpoint to get information about the scientific meaning of 1 mol and the physical quantity *amount of substance*.

F. The application of quantity calculus and the mathematical structure of proportionality in connection to 'the mole' is not fully developed among the educators interviewed. A plausible explanation is that this is an effect of the non-apprehension of a clear cut physical quantity and 1 mol as a unit of that physical quantity. Hence, the molar quantities (M_i : molar mass M, molar volume V_m and the Avogadro constant (molar number) N_A) are not viewed as physical quantities and constants of proportionality in the general equation $X_i = M_i \cdot n$, where X_i= { mass, volume, number} and n = *amount of substance*.

G. Generally, the empirical investigations show that historical conceptions of 'the mole' and related concepts is manifest among the respondents. These conceptions are handed over to students via teaching. These results fully reveal the importance that the educators' knowledge are in agreement with contemporary science.

CHAPTER 4

THE STRUCTURE AND DYNAMICS OF CONCEPT FORMATION.

In a previous report, a brief historical account has been outlined about the conceptual frames within which the term 'mole' was introduced by Ostwald around 1889. Three areas of development were accentuated, the constitution and refinement of atomic weights, the introduction of the term 'mol' and the use of quantity calculus (Lybeck, Strömdahl & Tullberg, 1985a, pp. 65-76)

The present historical account is not intended as a full historical narrative, exhausting all historical complexity, but is a rational reconstruction under a certain perspective (cf., Lakatos, 1978). It aims at reflecting the fact that 'mole' was introduced as a pragmatic notation of 'combining weights' of matter in a perspective of continuum physics, but was simultaneously implemented in a conceptual environment, where the discontinuity of matter was a well-founded scientific hypothesis (the atomic hypothesis) and was gradually accepted as a physical fact due to experimental concordance with theory. Since its introduction, 'the mole' has been accompanied by this dualism creating manifest conceptual ambiguity. Different solutions to this conceptual problem were possible, but the demand and conclusion on 'the mole' by the legislating organisations of the scientific community as being a genuine unit of a base physical quantity resulted in the prevailing SI definition of 1 mol.

Scientific concept formation is driven by *coherence*. Physical quantities and units are gathered under one "conceptual umbrella". Thus, the unit 1 mol must be a measure of some measurable property, a physical quantity, since 1971 *amount of substance*.

The following steps are considered in the historical account:

* early measurements of masses and volumes of substances converged at chemical reactions.

* found calculated proportional regularities based on these measurements, expressed as 'the law of constant proportions'.

* measurements, predominantly of masses, but also volumes of gases converged at chemical reactions in connection to the Daltonian atomic theory and the introduction of relative atomic weights.

* the introduction of the term 'mole' as a short-term for definite individual masses converged at chemical reactions ('combining weights'; the relative atomic- or molecular- weights expressed in grams).

* the use of the term 'mole' as a 'macro-atom' or a 'macro-molecule', viz. 'mole' as a macroscopic building stone, a concrete portion.

* the use of 'mole', interpreted in a discontinuous view of matter, as identical with the number of atoms in a 'macro-atom' of the sort mentioned in the previous step.

* the radical conceptual reorientation, where 'the mole' is defined as a base SI-unit of a new dimensionally independent physical quantity, *amount of substance*.

Since Ostwald's introduction of 'the mole', as a denotation of fixed individual masses ('combining weights'), its status as a measure (a unit) has been questioned and vividly discussed. The later part of the following historical account reflects the discussion by German physical chemists during several decades. Their theoretical analyses are foundational for comprehending the concept formation of 'the mole' and *amount of substance* (Ger. Stoffmenge).

Homberg seems to have been the first to do quantitative determinations on chemical reactions. In 1699 he neutralised a certain weight of different alkalis with the different weights of one and the same acid. He established that the different weights of the acid were measures of the 'passive force' of the alkalis. He also found that a constant weight of salts was formed when a certain weight of potassium carbonate reacted with various acids (van Spronsen, 1963).

However, systematic quantitative investigations in chemistry started with the Stahlians; Bergman, Wenzel and Richter (Berzelius, 1818, p. 2-5; Walden 1931, p. 55).

Ostwald (1910, p. 11) ascribes Richter as the founder of stoichiometry.

> Die eigentliche Grundlage der Lehre von den Verbindungsgewichten wurde von J.B. Richter seit 1791 gelegt.

Ostwald is referring to Richter's discovery of "the law of equivalent (reciprocal) proportions" 1792 (Richter, 1791; 1792).

Richter, who had coined the name 'stoichiometry,' was convinced that mathematics was applicable to chemical processes. In fact, his dissertation 'De usu Matheseos in Chemia' (1789) was a reply to the philosopher Kant who has denied chemistry as a natural science since in his opinion it was not susceptible to mathematical treatment.

Wenzel had already in 1777 in his dissertation, "Lehre von der Verwandtschaft der Körper", described experiments on neutralisation which

> were with respect to calculations more accurate than the work of contemporary chemists and have in large part been confirmed by the best of subsequent analyses. (Berzelius, 1818, p.3)[41]

Berzelius considered Wenzel to be the discoverer of 'the law of equivalent proportions'. In a lecture 1840, G.H. Hess called attention to the fact that Berzelius has mixed up Wenzel and Richter and incorrectly put the credit upon Wenzel for Richter's results (Hess, J.prakt.Chem. 1841, 24, p. 420 due to Oswald 1910, p. 12 and Partington, 1949, p. 748). These circumstances have been thoroughly discussed, amongst others by Walden (1931, pp. 81-) where Wenzel to some extent obtained redress.

Concerning Lavoisier and the law of equivalent proportions, Berzelius (1818) stated:

> Lavoisier has said nothing of significance concerning this subject. He has only remarked that one compound is produced in terms of definite and unchanging relations whilst another can occur in all kinds of proportions. (Berzelius , 1818, p. 6)[42]

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[41] Translated from the Swedish original by Dr. Dennis Beach.

[42] Translated from the Swedish original by Dr. Dennis Beach.

In "Assai de Statique Chimique" published in Paris 1803, Lavoisier's disciple Berthollet considered the difference between 'dissolutio' (my remark; dissolutio = chemical reactions (compounds)) and 'solutio' (my remark; solutio= dissolving) to be a question of the strength of the bond between the substances. The bond strength is much stronger in the former than the latter.

> The elements, he said, have a maximum and a minimum. These form the outer limits for combinatory possibilities, without which combination cannot take place, but between which compounds are possible in numerable relations, without any define intermediate gradations. When these occur they are dependent on other conditions, of which the most common are cohesion, where with a compound obtain solid state, or expansion, which cases the same gaseous form. When the elements at the point of combination undergo powerful condensation the compound is always formed in unchanging relations, and, because of this gaseous substances are always only combined in definite relations, for example oxygen and hydrogen, nitrogen dioxide and oxygen, an so forth. However, when the compound has the same conditions of density as the elements had previously, combinations can occur anywhere between the maximum and the minimum points. (Berzelius, 1818, p. 7)[43]

Proust tested this hypothesis and rejected it, which resulted in a scientific dispute with Berthollet,[44] which was characterised by Berzelius (1818) as:

> (...) both in its thoroughness, dignity of style and freedom from personality, deservedly a model for the way by which contentious ideas should be forwarded. (Berzelius, 1818, p. 9)[45]

Proust presented a great number of convincing experimental proofs (e.g. metal oxides, coppercarbonate; see also *Rech. sur le Bleu de Prusse Ann Chim 1797, XXIII*, p. 85-101) resulting in a general acceptance in scientific society of 'the law of equivalent (fixed) proportions'. According to Walden (1931) this law was implicitly recognised in quantitative analysis in the eighteenth century, but Proust established it by specific experiments.

The essence of the law of equivalent proportions is summarised by Partington (1949) in the following way:

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[43] Translated from the Swedish original by Dr. Dennis Beach.

[44] For detailed accounts see, Freund (1904) and Kapoor (1965).

[45] Translated from the Swedish original by Dr. Dennis Beach.

> The law of equivalent proportions shows that it is possible to assign to every element an equivalent weight, or equivalent or combining weight, representing the relative proportion in which it combines with other elements. (Partington, 1949, p. 784)

Even if the law is independent of any assumption about the structure of matter, it obtained an elegant theoretical explanation in the atomic hypothesis.

An Irish chemist, Higgins (1789), had in his "A comparative view of the phlogistic and antiphlogistic Theories" put forward a theory that bodies were constructed of particles. No public attention was paid to this theory since Higgins did not give it any empirical support. An experimentally supported version of the atomic theory connected to chemistry was presented by Dalton (1807) as a table of 'absolute weights' of bodies in *Nicholson's Journal*. But it was first when the theory was presented in Thompson's "System of Chemistry" Edinburgh, 1807, 3, p. 425, under the title "A New System of Chemical Philosophy" (also 1808; 1810), that it was recognised by scientific society.

Dalton's hypothesis regarded matter as being corpuscular. Different elements consisted of different atoms characterised by weight (mass) and size. Dalton was influenced by the corpuscular theory of Newton and ancient atomic theory, but the stress on constant weights (mass) of each kind of atoms, making the theory accessible to measurements, separated his theory from previous hypothetical atomic theories. Dalton made the atomic weights into

> ... the keystone of his theory using them as the chief criterion for the distinction of one atomic species from another. (Nash, 1966, p. 235)

The relative weights experimentally established by the law of equivalent proportions were the relative weights assigned to the atoms.

> In all chemical investigations, it has justly been considered an important object to ascertain the relative *weights* of the simples which constitute a compound. But unfortunately the enquiry has terminated here; whereas from the relative weights in the mass, the relative weights of the ultimate particles or atoms of the bodies might have been inferred from which their number and weight in various other compounds would appear, in order to assist and to guide future investigations, and to correct their results. Now it is one great object of this work, to shew the importance and advantage of ascertaining the *relative weights of the ultimate particles, both of simple and compound bodies, the number of simple elementary particles which constitute one compound particle, and the number of less compound particles which enter into the formation of one more compound particle.* (Dalton 1808, pp. 212-213)

Dalton is here arguing for the extrapolation of the measured relative weights ('combining weights') of the constituents in a compound to the relative weights of "...the ultimate particles or atoms of the bodies ... ". By that approach the relative atomic weights became a fact.

Dalton (1808) postulated the general rule that molecules of chemical compounds were constituted of the least number of atoms. The first two rules of combination are

> (...) 1st. When only one combination of two bodies can be obtained, it must be assured to be a *binary* one, unless some other cause appears to the contrary. 2nd. When two combinations are observed, they must be presumed to be a *binary* and a *ternary*.(...). (Dalton, 1808, p. 214)

(See further Dalton, 1808, p. 218-219, Plate 4)

In 1809 Gay-Lussac presented an investigation showing that gases chemically unite by volume in integer multiples ("Sur la combinaison des substances gaseuses, les unes avec les autres", *Memoires d'Arceuil* 1809, 2, p. 207). However, Dalton's settled conception that different atoms had different sizes prevented him from

> ... enjoying the honourable confirmation his ideas had won through Gay-Lussac's discovery ... and seeking instead ... to show that Guy-Lussac was mistaken. (Berzelius, 1818, p. 14)[46]

Dalton (1808) wrote:

> Some observations on nitric acid, and the other compounds of azote and oxygen, have been made by Gay Lussac, in the 2nd vol. of the Memoires d'Arcueil. He contends that one *measure* of oxygenous gas unites to two *measures* of nitrous gas to form nitric acid, and to three measures to form nitrous acid. (...) In fact, his notion of measures is analogous to mine of atoms; and if it could be proved that all elastic fluids have the same number of atoms in the same volume, or numbers that are as 1, 2, 3 &c. the two hypotheses would be the same, except that mine is universal, and his applies only to elastic fluids. Gay Lussac could not but see (page 188, Part 1. of this work) that a similar hypothesis had been entertained by me, and abandoned as untenable; (...). (Dalton, 1808, pp. 555-556 (appendix))

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[46] Translated from the Swedish original by Dr. Dennis Beach.

Dalton's arguments about his assumption and conviction of different atomic sizes are found in a couple of places in his main work (Dalton, 1808, p. 188 and ibid., p. 70-71).

> At the time I formed the theory of mixed gases, I had a confused Idea, as many have, I suppose, at this time, that the particles of elastic fluids are all of the same size; that a given volume of oxygenous gas contains just as many particles as the same volume of hydrogenous; or if not, that we had no data from which the question could be solved. But from a train of reasoning, similar to that exhibited at page 71, I became convinced that different gases have not their particles of the same size: and that the following may be adopted as a maxim, till some reason appears to the contrary:
>
> namely,
>
> *That every species of pure elastic fluid has its particles globular and all of a size; but that no two species agree in the size of their particles*, the pressure and temperature being the same.
>
> (...)
>
> It is evident the number of ultimate particles or molecules in a given weight or volume of one gas is not the same as in another: for, if equal measures of azotic and oxygenous gases were mixed, and could be instantly united chemically, they would form nearly two measures of nitrous gas, having the same weight as the two original measures; but the number of ultimate particles could at most be one half of that before the union. No two eleastic fluids, probably, therefore, have the same number of particles, either in the same volume or the same weight.

After additional criticism of Gay-Lussac's experiment he concludes (Dalton, 1808, p. 559):

> The truth is, I believe, that the gases do not unite in equal or exact measures in any one instance; when they appear to do so, it is owing to the inaccuracy of our experiments.
>
> In no case, perhaps, is there a nearer approach to mathematical exactness, than in that of 1 measure of oxygen to 2 of hydrogen; but here, the most exact experiments I have ever made, gave 1.97 hydrogen to 1 oxygen.

An attempt to explain Gay-Lussac's law of volume was presented by Avogadro (Avogardro, 1811, *Journal de Physique* 1811, 73, p. 58). Avogadro assumed that equal volumes of all gases (elements, compounds, and mixtures of these) at the same pressure and temperature contain equal numbers of molecules (Avogardo's term is 'molécules integrantes' = molecules of chemical compounds

(cf. Partington, 1949, p. 768); molecules in general (cf. Nash, 1966, p. 278)).

Molecule was an important concept in Avogadro's theory because he assumed that even gaseous elements were molecules, consisting of two atoms (the word atom is missing in Avogadro's dissertation; he called them molécules élémentaires).

Avogadro's hypothesis also implied a new theory of gases, which was difficult to accept due to contemporary conceptions of gases.

The hypotheses was seriously considered first in 1858 when Canizzaro used it to explain accumulated experimental data that did not fit the original Daltonian atomic theory.

> By that time chemists were better prepared to accept the kinetic model of a gas because of the revolution underway in thermal physics, the abandonment of the caloric theory and the growing acceptance of the kinetic theory of gases. Thus the atomic theories in Chemistry and in Physics aided each other. (Holton & Roller, 1958, p. 400).

In 1865, originating from the kinetic theory, Loschmidt made an attempt to calculate the size of the molecules.[47] As a consequence of this size determination, the number of molecules in 1 cm^3 gas at 0 °C and 760 mm Hg was calculated. However, this was not done by Loschmidt personally (cf. *Journal of Chemical Education*, vol. 47/11 Nov. 1970).

According to Burger (1983, p. 97), Loschmidt's number was introduced by Boltzman in 1895, as a name for the number of particles in 1 cm^3 'Stickstoff' (Eng. Nitrogen) at 0 °C and normal pressure (cf. above), and the Avogadro constant (constante d'Avogadro) by Perrin 1909 as the name for the number of particles in a gram-molecule.

The different meanings addressed by different scientists to Loschmidt's number and Loschmidt constant, as well as Avogadro's number and Avogadro constant, have been described by Burger (1983, p. 88).

However, no systematic investigation seems to have been made of the different determinations of the number of molecules in one gram-

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[47] Loschmidt, "Zur Grösse der Luftmolekule" [On the size of the air molecule], Sitzungsberichte der mathematischen naturwissenschaftlischen klasse der kaiserlichen Akademie der Wissenschaften zur Wien 1865, 52. II, pp. 395-413, Wien 1866.

molecule or mole and of the historical development of the different names connected to that number.

During the last years of the nineteenth century the discussion of real atomism, contrary to a hypothetical atomism only adjusted for mathematical considerations, was intensified. The development and progress of statistical thermodynamics bound to the names Maxwell, Boltzman and Gibbs added strong support to real atomism. The discussion among scientists about arguments for and against real atomism was a scientific controversy of great dimensions (cf. e.g. Nye, 1976;1984). It was in this conceptual surrounding that Ostwald, at that time a defender of a continuous energetic description of matter, introduced 'the mole'.

The spirit of the times is reflected in a note from 1904 by the Swedish chemist and Nobel laureate Theodor (The) Svedberg (1884-1971):

> Ostwald [...] wanted to put an end to all talk of molecules and atoms as actual units of mass. Instead of molecular weights one should speak of combining weights, etc. I discussed this with my fellow students and many agreed with Ostwald. To me this view seemed far-fetched. (from Lundgren, 1993, p. 328)

Among researchers in the History of Science, there is an accepted distinction between a chemical atomic theory and a physical atomic theory (Thackray, 1970; Lundgren, 1979; Rocke, 1984). The chemical atomic theory is not assigning matter an absolute structure or ontological basis but is a:

> ... conceptual basis for assigning relative weights to elements and assigning molecular formulas to compounds. (Rocke, 1984, p. 10)

Hence, the chemical atomic theory was primarily instrumental, dealing with equivalent weights. Stoichiometric calculations did not need a theory which actually counted with existing atoms. Chemical elements were the simplest substances gained in chemical analysis. No statement was made about the structure of matter. Measurements were made by the continuous physical quantities mass and volume. Not assuming anything about the non-verified structure of matter was a scientific rule of conduct. According to Rocke (1984) nearly all chemists during the 19th century, including Ostwald, held the chemical atomic theory.

Daltonian atomic theory was a merging of the Newtonian physical theory of corpuscles and chemical elements in an empirical chemical tradition expressed by Lavoisier (cf. Lundgren, 1979, p. 81).

The physical atomic theory was ontological, by advocating the clear existence of Newtonian small non-divisible corpuscles.

Originating from Ostwald the term 'mole' was created within the frames of the chemical atomic theory, in a continuum perspective of matter where the existence of atoms was not considered as a physical fact. The empirical measurements of masses were the sound base of a safe scientific approach.

However, the physical atomic theory could be used as an explanation of the stoichiometric results. From the perspective of real atomism, 'combining weights' are a direct consequence of the particularity of matter. The possibility to create a stoichiometry based on calculations of *number* of participating elementary entities in a chemical reaction was evidently present.

The rapid adoption among chemists of 'the mole' and 'Gramm-Molekül' prevented *number* becoming a quantity used in stoichiometric calculations.

> ...obwohl aus den dazu dargelegten Definitionen von NERNST und OSTWALD nicht klar ersichtlich wird, was mit diesen Bezeichnungen eigentlich gemeint ist. (Burger, 1983, p.100).

Ostwald (1899) defined 'the Mol' as equal to the fixed individual masses emerging in chemical reactions .

> Wenn wir die Normal- oder Molekulargewichte der verschiedenen Stoffe bei chemischen Vorgängen in Rechnung bringen, so sind wir meist veranlasst, mit bestimmten Quantitäten zu arbeiten, und beziehen demgemäss diese ursprünglich relativ ermittelten Zahlen auf eine bestimmte Masseneinheit. Da als solche das Gramm dient, so betragen diese Mengen demgemäss soviel Gramm, als das Normalgewicht Einheiten hat. Man nennt diese Mengen, welche die eigentlich messbaren Quantitäten bei chemischen Betrachtungen darstellen, Mole; ein Mol Sauerstoff ist demnach die Menge von 32 g Sauerstoff, und ein Mol Chlorwasserstoff wird durch 36.45 g dargestellt. Auf diese Grössen werden fast alle Eigenschaften der Stoffe bezogen, mit denen wir uns später zu beschäftigen haben werden.

When Ostwald (1911, p. 212) discussed second order reactions in chemical kinetics he stated [48]:

> Damit man die Änderungen beide Stoffmengen durch dieselbe Veränderliche x ausdrücken kann, muss man diese nicht durch gewöhnliches Gewichtmass, sondern durch solche Gewichte messen, welche in Verhältnis der chemischen Äquivalenz in Bezug auf die fragliche Reaktionen stehen. Meist kan man als Einheiten die in Grammen ausgedrückten Molekulargewichte benutzen, die früher schorn mit dem abgekürzten Namen Mol bezeichneten Grössen. So wird in Zukunft stets gerechnet werden: die Menge 0.5 Mol Chlorwasserstoff z. B. ist gleich 18,23 gram.

Here Ostwald is using 'Stoffmenge' (amount of substance) in a general sense, meaning amounts of substances, which could have been ordinary weights ("gewöhnliches Gewichtmass") but in these specific cases are weights, which are multiples of units of molecular weights expressed in grams, denoted 'Mol'. By using the plural form "Einheiten" [units] it is evident that 'Mol' is a denotation of individual units, due to the substance considered.

A general definition was given in Ostwald (1912)[49]:

> Ein Menge irgend eines Stoffs, dessen Massgewicht gleich der Summe der in der Formel vereinigten Verbindungsgewichte ist wollen wir ein Mol des Stoffs nennen. (Ostwald, 1912, p. 199)

The introduction of the term 'mole' seems to have been a pragmatic approach to the quantitative description and calculation of the chemical reaction in a continuous perspective of matter. A re-naming of individual masses into convenient integers to use in description and calculation of chemical reactions.

Compared to the step taken by Dalton (1808), by extrapolating the masses combined (or multiples of these masses) at chemical reactions to the ultimate atoms, regarding matter as corpuscular or discontinuous, Ostwald remained in the continuous view of matter retaining the 'combining weights' by introducing the mole. The individual weights became 'building blocks' in chemical reactions, regarded in a continuous macro level perspective of matter.

---

[48] Ostwald is referring to the equation $dx/d\vartheta = k(A-x)(B-x)$ where A and B are the original amounts and x the change of the amounts during the time ϑ. k is a constant.

[49] [An amount of a substance, whose weight of mass is equal to the sum of the combining weights due to the chemical formula will we denote one Mol]

The feature of the Ostwaldian mole was stated by Stille (1955):

> Ihr Betrag ist so bemessen, daß bei chemischen Reaktionen gerade jeweils 1 mol oder ganzzahlige Vielfache eines mol der einzelnen Partner miteinander reagieren. Somit müssen die für die einzelnen Molekülsorten individuellen chemischen Massen-Größen zueinander in denselben Verhältnissen stehen, die bei chemischen Umsetzungen der betreffenden Molekülsorten beobachtet werden. (Stille, 1955, p. 117)

The continuum approach related to an discontinuous (atomic) view of matter is analysed by Stille (1955):

> ...mol und kmol sind Massen-Größen, deren Wert sich von einer chemisch homogenen Substanz zur andern ändert. Sie werden definiert, um die Gesetzmäßigkeiten des *atomaren Geschehens*, wie es sich in chemischen Reaktionen widerspiegelt, in *formal* einfacher Weise im Rahmen eine für die *kontinuumstheoretische Makrophysik* zweckmäßigen Darstellung behandeln und rechnerisch erfassen zu können, ohne neue, der Atomistik Rechnung tragende Begriffe oder Grundgrößenarten, wie beispielsweise die "Stoffmenge" (...), einzuführen. Anstatt die einzelnen Atome oder Moleküle als individuen zu zählen, geht man von ihrer Eigenschaft aus, Masse zu besitzen, und zwar eine masse, die für die Art des betreffenden Atoms oder Moleküls charakteristisch ist. Eine dem atomistischen Aufbau und Verhalten der Materie entsprechende Abzählung der einzelnen, unter sich gleichen Individuen ersetzt man in der kontinuumsteoretischen Beschreibung der Vorgänge und Zustände chemisch homogener Substanzen durch die Einführung spezieller Massen-Größen, die individuell für jede Substanz so definiert sind, daß sie gleich viele Moleküle enthalten.
>
> Obwohl die Massen-Größen unter sich nicht gleich sind, sondern je nach der chemischen Substanz verschiedene Massen darstellen " die Massen je eines mol Natrium, (atomares) Chlor oder Natriumchlorid stehen im verhältnis 22,991:35,457:58,448 ", spricht man einfach von "einem mol" und nennt es eine "individuelle chemische Massen-Einheit". Hierdurch soll zum Ausdruck gebracht werden, daß das mol keine Einheit im eigentlichen Sinne, sondern eine für jede chemisch homogene Substanz individuelle Massen-Größe darstellt. (Stille, 1955, p. 117)

The pragmatic approach by Ostwald is stressed by Stille, saying that mole is not a unit in the conventional sense but denotes individual mass measures.

Hence, the mole was not introduced because of a lack of a suitable measure (a physical quantity and a unit) of portions of substances conveyed at chemical reactions, but as a short name for individual combining weights. Further, 'the mole' as individual units of mass falls within the frames of continuum physics.

Even if the term 'Mol' in the original Ostwaldian sense was taken as individual masses, it was also taken as a denotation of the concrete portions with these individual masses. This was most evident by using the term 'Gramm-Molekül' or 'g-Molekel' (and even 'g-Mol') introduced by Nernst (cf. Burger, 1983, p. 85). Here 'Molekül' or 'Molekel'[50] connotes a 'macro'-molecule, a building-block measured in grams. This is clear when e.g. Einstein (1904, pp. 358-359) speaks of "wirklichen Moleküle" and " ... Molekül im Sinne des Chemikers" and states 1 g of hydrogen as a unit of measure for the latter.

Lange (1953a) made a definite statement of mole as a 'macro-atom'. According to the smallness of the elementary entities (Lange's term is 'Stoffstück'):

> ... ihr ungewöhnlich kleines Ausmaß, zum Ausdruck kommend in der ungeheuren Größe der Lochmidtschen Zahl N_L. Daher hat es sich als notwendig erwiesen, gewissermaßen ein praktisch brauchbareres, *makroskopisches Ersatzteilchen*, Ersatzatom oder Ersatzmolekül einzuführen: Das *Mol* der *betreffenden Stoffart*. (Lange, 1953a, p. 257)

This approach implies that the individual portions, measured as fixed masses ('combining weights'), denoted 'mole', are taken formally as macroscopic equivalents to the single atoms on the microscopic level.

The dual view of matter as continuous on the macro-level and discontinuous on the micro-level was naturally connected to 'the mol' (gram-molecule).

The value of R^* , the gas constant in the gas-law, $p \cdot V = R^* \cdot T$ is dependent on the mass and kind of the gas used. If masses of different gases are taken equal to the molecular masses of the actual substances, then R^* has got the same value, R, for all gases ($p \cdot V = R \cdot T$).

Planck (1900) showed that the ratio between k (Boltzmann's constant) and the general gas constant R gave the value w, which was

> ...das für alle Substanzen gleiche Verhältnis der Masse eines wirklichen Molecüles zur Masse eines g-Molecüles darstellt.

This value was determined to $w = k/R = 1{,}62 \cdot 10^{-24}$, but Planck (1900) also interpreted the inverse of this ratio

---

[50] 'Mol.' and 'Mol' was both before and after the Ostwaldian definition used as a abbreviation of 'Molekül' or 'Molekel.'

> ...auf ein g-Molecül eines jeden Stoffes gehen $1/w = 6{,}175 \cdot 10^{23}$ wirkliche Molecüle.

Wallot (1953), like Lange (1953a,b), interpreted the Ostwaldian Mol as a portion of substance (konkrete Quantum Stoff). Wallot (1953) states:

> Man merke sich schon hier, daß der Ausdruck -je Mol" trotszdem nicht dasselbe bedeutet wie der Ausdruck -je Masseneinheit". Darum vervendet man besser zusammengesetzte Wörter wie Molwärme oder das Eigenschaftswort molar.(Wallot, 1953, §19, s.26)

Since one mole is regarded as something concrete it is clear that the phrase *molar mass* maintains the connotation of mass, the mass of one mole. But, simultaneously mass has also the unit mol (Wallot, 1953):

> Als einheit des Mengenmaßes Masse wird aber meist nicht das Gramm oder das Kilogramm verwendet, sondern die Masse m_{Mol} eines konkreten Mol selbst oder ein Vielfaches davon. (Wallot, 1953, paragraph 49)

This is expressed by the equation $m_{\mathrm{Mol}} = M \cdot \mathrm{g} = mol$. Here the index Mol denotes a concrete thing and *mol* denotes a unit of mass (M in the equation is 'molecular weight', and is dimensionless (nowadays: attributed the dimension 1).

The molar volume $V_{\mathrm{n\ Mol}} = v_{\mathrm{n}} \cdot m_{\mathrm{Mol}} = v_{\mathrm{n}} \cdot \mathrm{mol} = 22{,}4145\ \mathrm{dm}^3$ and the specific[51] volume $v_{\mathrm{n}} = 22{,}4145\ \mathrm{dm}^3/\mathrm{mol}$ were commented by Wallot (ibid.) :

> Bei der Verwendung der Einheiten mol und kilomol tritt eine praktische - oder vielleicht richtiger psychologische - Schwierigkeit auf,... (...) Die erwähnte Schwierigkeit liegt nun darin, dass leider sehr häufig das spezifische Volum v_{n} , wenn es auf die einheit dm³/mol bezogen wird, -Molvolum" genant wird. Das ist ein sehr unzweckmässiger Sprachgebrauch. Wir sagen -Geschwindigkeit", "Dichte" und lassen die Umschreibungen "Weg je Zeiteinheit", "Masse je Volumeinhet" zu. Aber wir sagen für "Geschwindigkeit" nicht "Stundenweg" und für "Dichte" nicht "Kubikmetermasse". Diese Ausdrucke entsprechen genau dem "Molvolum" in dem von mir beanstandeten Sinn; denn Stunde ist eine spezielle Zeiteinheit, Kubikmeter eine spezielle Volumeinheit, mol eine spezielle Masseneinheit. (...) Es ist also irreführend, zu sagen:
>
> Das Molvolum idealer Gase beträgt im Normzustand 22,4145 dm³/mol.
>
> Es stehen nur zwei richtige Ausdrucksweisen zur Verfugung:

---

[51] Notice the use of 'specific' which means divided by mass, implying that 'the mole' is a measure of mass.

> 1. Das Molvolum idealer Gase beträgt im Normzustand 22,4145 dm^3.
> 2. Das spezifische Volum idealer Gase beträgt im Normzustand 22,4145 dm^3/mol.

Wallot (1953) started in a microscopic, discontinuous perspective of matter. To get macroscopic measures, no prescription was made of the number (N) of elementary entities

> ... sondern das Produkt N mal m_{Molekul}; und zwar hat man es gleich dem seit langem bekannten Produkt aus dem Molekulargewicht *M* (einer reinen Zahl) und der Masseneinheit Gramm gemacht:
>
> $N \cdot m_{\mathrm{Molekul}} = M \cdot g$
>
> Wilhelm OSTWALD nannte das diesem Produkt entsprechende konkrete Quantum Stoff ein -Mol". Es ist also:
>
> $m_{\mathrm{Mol}} = N \cdot m_{\mathrm{Molekul}} = M \cdot g$
>
> Man definiert nun -molare" Grössen ensprechend den molekularen; die Zahl $N = m_{\mathrm{Mol}}/m_{\mathrm{Molekul}}$, die -LOSCHMIDTsche Zahl", ist der Faktor, mit dem die mikroskopischen Grössen in die makroskopischen -transformiert" werden. Nach sorgfältigen Messungen ist:
>
> $N = 6{,}026 \cdot 10^{23}$.
>
> Der erste wichtige molare Begriff ist der -molaren Menge". Darunter verstehen wir die Zahl
>
> $n_{\mathrm{Mol}} = m/m_{\mathrm{Mol}}$ (...)
>
> (Wallot,1953, §19)

m_{Mol} is the mass of one mole and, the "molaren Menge", n_{Mol}, (= m/m_{Mol}) is the number (Zahl) of moles. Loschmidt's number is a numerical factor connecting the microscopic and macroscopic masses.

In fact, Wallot (1953) started his exposition of mol and molar quantities by a discussion of amount (Ger. Menge). According to Wallot (ibid.), DIN[52] 1305 (edited July 1938) defines 'Menge' (amount) and specially 'Stoffenmenge' (amount of substance) as the number of molecules 'Anzahl der Molekule'.

> Wenn gleiche konkrete Einzeldinge ein Größeres Ganzes bilden, verstehen wir unter der Menge der konkreten Einzeldinge einfach ihre Anzahl.

---

[52] DIN, Deutsche Industrinorm.

> (...) In der Wissenshaft und in der Technik, die es mit Stoffen zu tun hat, kan man bei homogenen Stoffen als Einzeldinge die Molküle ansehen, aus denen sie aufgebaut sind. (Wallot, 1953, §18)

The 'amount of molecules' (molekularen Menge) is determined by the ratio of the mass of an actual portion of substance and the mass of one molecule:

> $n_{\mathrm{Molekül}} = m/m_{\mathrm{Molekül}}$
>
> (...) ... die molekulare Menge ist also keineswegs identisch mit der Masse oder dem Normgewicht oder dem Normvolum, diese drei Grössen sind aber der molecularen menge proportional mit bekannten und wohldefinierten "individuellen" Proportionalitätskonstanten. (Wallot, 1953, § 18)

$n_{\mathrm{Molekül}}$ as a quotient between two physical quantities (mass) is a physical quantity itself. The physical quantity 'amount of molecules' (Ger. molecularen Menge) was denoted by Wallot as dimensionless (Ger. dimensionslos). Nowadays we say that such a quantity has the dimension 1.

The proper expression is stressed (cf. Wallot, 1953, § 18):

$n_{\mathrm{Molekül}} = 10^{24}$ and not $n_{\mathrm{Molekül}} = 10^{24}$ Moleküle

'Moleküle' is not a unit in the meaning of quantity calculus. It is a name of an entity, something with physical significance.

Wallot (1953) concludes:

> Die definition der molekularen Menge und die Auffassung, daß die Masse nur ein Mengen maß ist, widerspricht der Darstellung NEWTONs, der quantitas materiae und massa als Synonyme behandelt hat. (...)
>
> ... man könne ja auch die quantitas materiae Newtons, die Stoffmenge, zur Grundgröße machen; jeder wisse, was das ist, und man könne Stoffmengen wie massen unmittelbar mit der Waage vergleichen... (aber) (...) man müßte ebenfalls eine überflüssige Konstante k" einführen und die Masse dann etwas als das Produkt aus dieser Konstante und der Stoffmenge definieren. Nicht Wesentliches wäre gewonnen. (Wallot, 1953, § 18 and 7)

According to Lange (1953a) the need of a base physical quantity 'Stoffmenge' (amount of substance) had been discussed for several years:

> Die Notwendigkeit, für reine Stoffe eine bestimmmte Stoffmenge in ähnlicher Weise wie eine Grundgröße, mit einer eigenen Dimension, einzuführen, ist

> schorn verschiedenen Seiten mehr oder weniger deutlich angeregt worden. Hier sei nur auf einen diesbezüglichen langjährigen Briefwechsel zwischen einegen Autoren, z. T. im Rahmen de AEF und des CITCE[53], verwiesen. Daran haben sich u.a. die Herren Emde, Flegler, Fleischmann, Lange, Lohde, Oberdorfer, Pohl, Wallot beteiligt. Dabei sind zahlreiche übereinstimmende - neben manchen unterschiedlichen - Auffassungen zu Tage getreten. (...). (Lange, 1953a, p. 255, footnote 10)

Wallot (1953) clearly express doubts against the introduction of 'Stoffmenge' [amount of substance] as a new physical quantity. The problems related to phenomenal references of basic physical quantities is an obstacle. Operational definitions are insufficient. Vast problems encounter the researcher trying to explain the meaning of a new basic physical quantity:

> Jede neue Grundgröße muß mit Worten oder durch Beispiele erklärt werden, denn Definitions-gleichungen für Grundgrößen gibt es nicht. Viele meinen, es genüge zu diesem Zweck, für die neue Grundgrösse ein Meß- oder wenigstens Vergleichverfahren anzugeben. Sie sagen z. B.: "Die Stoffmenge ist die Größe die mit der Waage bestimmt wird". Darin läge aber, selbst wenn die Stoffmenge die einzige mit der Waage bestimmbare Größe wäre, kein Erklärung des Begriffs der Stoffmenge. Denn dieser enthält ausser dem Merkmal der Bestimmbarkeit durch die Waage noch andere Merkmale; und erst die Summe aller Merkmale ergibt den Begriff "Stoffmenge".
>
> Je mehr Grundgrößen wir einführen, um so öfter sehen wir uns vor die undankbare Aufgabe gestellt, uns von Begriffen, für die wir keine exakten Definitionen haben, eine lebendige Vorstellung zu bilden. (Wallot, 1953, § 31)

Some ten years earlier Pohl and Stöckman (1944) had expressed doubts about 'Stoffmenge' as a base physical quantity. According to them the introduction of Stoffmenge as a basic physical quantity was made e. g. by attaching the molar volume V = 22,4 Liter another dimension V = 22,4 Liter/MOL (Pohl & Stöckman, 1944, p. 535).

Further,

> Diese Dimensionierung beruht auf einer eigenartigen festsetzung. Die Stoffmenge wird wie eine Grundgröße behandelt. Sie wurden bisher gebräuchlichen fünf Grundgrößen Länge, Zeit, Masse, Temperatur und Ladung als gleichberechtigt an die Seite gestellt.

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[53] CITCE = Internationalen Komitees für electrochemische Termodynamik und Kinetik.

> Der für ihre Einheit benutzte, schon anderweitig vergebene Name wird von uns MOL gedruckt, um Verwechslungen mit den individuellen Masseneinheiten Mol = (M) Gramm zu verhindern. (Pohl & Stöckman, 1944, p. 537)

MOL is a unit of the basic quantity 'Stoffmenge' in the following way:

> 1. Die Stoffemenge (Newton's quantitas materie) wird wie eine Grundgröße behandelt und der Masse als gleichberechtigt an die Seite gestellt. (...)
>
> 2. Als einheitsstoffmenge gilt die Stoffmenge, die ebensoviel Moleküle enthält wie 32 gramm Sauerstoff.
>
> 3. Dieser Einheitsstoffmenge gibt man denselben Namen, den Ostwald für die individuellen Masseneinheiten (M) Gramm eingführt hat, nämlich 1 mol. Wir drucken MOL, um die Verwechslung mit Mol = (M) gramm zu verhindern. (...)
>
> 4. Zur Umrechnung von Grössen, die die Masse *M* als Grundgrösse enthalten, auf solche, die statt *M* die Stoffmenge *Z* als Grundgrösse enthalten, dient das "Molgewicht" genannte Verhältnis
>
> Masse M/Stoffmenge Z = (M) gramm/MOL und daraus folgend
>
> Stoffmenge Z = Masse M/ (M) gramm/ MOL (...).
>
> (Pohl & Stöckman, 1944, p. 535)

Even if 'Stoffmenge' could be used without objections they found it too detailed. Further, they pointed to five disadvantages :

> 1. die behandlung der Stoffmenge Z als Grundgröße;
>
> 2 die Verwendung des bereits vor Jahrzehnten anders definierten Wortes "Mol" für die Einheit dieser Grundgröße
>
> 3. die Notwendigkeit, neben den mit Hilfe der Grundgrösse Masse gebilderten Begriffen spezif. Volumen, spezif. Wärme usw. noch andere mit der Grundgrösse Stoffmenge gebildete Grössen Molvolumen, Molwärme usw beizubehalten und so den Buchstabenbedarf fur die Gleichungen unnötig zu vergrössern;
>
> 4. die verwendung der gleichen Namen Molvolumen, Molwärme usw für die neuen Begriffe, obwohl diese Namen seit Jahrzehnten für die oben aufgezählten, anders Nebenbegriffe festliegen
>
> 5. die Notwendigkeit, neben dem diemensionslosen Moleculargewicht (M) einen "Molgewicht" gennanten Umrechnungsfaktor einzuführen. (Pohl & Stöckman, 1944, p. 536)

Their conclusion was:

> All das läßt sich vermeiden, wenn man konsequent Mole als individuelle Masseneinheiten anwendet.

In a later paper, Pohl (1953) repeated the two meanings of the mole as an individual mass and as a unit for the base quantity Stoffmenge. After a new exposition of the quantities involved, Pohl's conclusion is clear:

> Alle molaren Grössen sind sachlich entbehrlich.

This is for instance demonstrated by Pohl (1953) via the gas law, which can be given three formulations:

$p\,V = M\,R\,T_{abs}$ (M = Masse)
$p\,V = n^*\,R^*\,T_{abs}$ (n^*= Anzahl der Mole)
$p\,V = Z\,R^{**}\,T_{abs}$ (Z = Stoffmenge)

Westphal (1954) gave an explanation why he entered the discussion of 'the mole'. The reason was the introduction of individual units of mass (the Ostwaldian mole). It has no analogue in physics. The demand for uniform integrated standards in science was decisive for his position on 'the mole'.

> Was mir - und auch manchen anderen Physikern - an dem bisherigen Brauch besonders missfällt, ist die Einführung individueller Masseneinheiten, die kein Analogon in der Physik hat, obgleich man solche leicht konstruieren könnte. Dies inbesondere war es, was mich zu den vorstehenden Überlegungen veranlasst hat. (Westphal, 1954, p.407)

Similar arguments against 'the mole' as an individual mass unit was used 25 years later by Weninger (1979a):

> Der begriff der individuellen Masseneinheit ist in sich unlogisch. (...) In den Ausdrucken "3 mol Wasserstoff" und "3 mol Sauerstoff" signalisiert der jeweils gleiche Term "3 mol" - wenn "1 mol" ein Masseneinheit ist -, das die beiden Stoffportionen verschiedene Massen haben, nämlich 6,048 g und 96,00 g. Das ist methodologisch unhaltbar. (Weninger, 1979a, p. 12)

Westphal (1954) commented the conceptual consequences of his exposition on 'Stoffmenge' as a base physical quantity.[54]

> Demnach wird durch die hier von mir eingeführten Definitionen *quantitativ überhaupt nichts geändert.* Es handelt sich um eine reine *Frage der Begriffsbildung,* die für den Nur-Praktiker, den nur die Zahlenwerte interessiern, völlig belanglos ist. (Westphal, 1954, p. 407)

---

[54] In Westphal's reasoning about the quantity "Stoffmenge" its unit, 1 mol, belongs to the same category as dozen, etc. ("Die entsperechende Stoffenmengeneinhet gehört zur gleichen Begriffsgruppe wie Dutzend, Mandel, Schock.").

Westphal saw the change only as a question of concept formation, completely insignificant to the practitioner.[55]

Bantle and Hablützel (1953, p. 63) stated by the demands of quantity calculus that the digit 3 in the expressions 3 Mol chlorine and 3 Mol hydrogen must be a numerical value and Mol a unit of a physical quantity accounting for some joint property:

> Das einzige übereinstimmende quantitative Merkmal dieser Gaskörper ist aber die *Anzahl* der freien Gasteilchen, der Moleküle. Die Einheit 1 mol muss also - ähnlich wie 1 Paar, 1 Dutzend, 1 Gros - ein Zählmass sein, ...

Out of this statement they proposed a definition of 1 mol.

> 1 mol ist eine dimensionslose Zähleneinheit, grösser als die natürliche Zähleinheit 1 Stück. Die Zähleinheit 1 mol ist festgelegt durch die Anzahl der Moleküle in 32 g Sauerstoffgas.

Hence, they had found that number was an indispensable base physical quantity in physical chemistry.

> ... *Anzahl z ist eine in der physikalischen Chemie unentbehrliche Grundgrösse*1), die in jeder der oben angeführten Zähleinheiten ausgedrückt werden kann. (Bantle & Hablützel, 1953. pp. 63-64)

The footnote 1) said:

> Wir halten es nicht für Zweckmässig diese Grundgrösse mit dem vieldeutigen Ausdruck « Stoffmenge » zu belasten. Vgl Note 2 auf Seite 63.

In footnote 2 (Ger. Note 2) Bantel and Hablützel refer to papers written by Pohl and Westphal.

In Westphal (1963) 'Stoffmenge' denoted a mass or a measure of number of (small) particles (Ger. Teilchenmenge). Westphal stressed the number perspective and introduced 'Teilchenmenge' as a base physical quantity (Ger. Grundgrößenart) with the unit 1 mol:

> Diese Anzahl ist aber bei wägbaren Körpern viel zu groß, um wirklich abgezählt zu werden. Deshalb dient zur Bewertung von Körpern nach ihrer Teichenanzahl *eine dieser Anzahl proportionale, meßbare Größe,* die wir als *Teilchenmenge* (Formelzeichen *n*) bezeichen. (...) Je nach der Bewertungsart

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[55] A similar opinion is shared by a majority of the educators in the empirical studies, who do not consider the significance of deep knowledge of the concepts involved in stoichiometry but stress an algorithmic knowledge in order to solve problems and exercises (for confirmatory statements see, appendix III).

> kann eine Teilchenmenge als *Molekülmenge, Atommenge* oder *Inonenmenge* bezeichnet werden. Die Teichenmenge ist als eine Grundgrößenart anzusehen.
>
> Die Einheit der Teilchenmenge heißt *Mol* (Einheitenzeichen mol) und wird durch jeden Körper verwirklicht, der ebenso viele der jeweils gemeinten Teilchen enthält wie Atome in einem Kohlenstoffkörper von der Masse 12 g enthalten sind (...). (Westphal, 1963, p. 46)

Westphal defined not only the ordinary molar quantities ($X_m = X/n$; X, denoting some physical quantity), M_m (molar mass), V_m (molar volume) and C_m (molar heat) but also N_A the 'molar number of particles', in Westphal's terminology 'molare Teilchenanzahl'.

Westphal's suggestion is somewhat doubtful. On the one hand 'Teilchenanzahl' is a base physical quantity, on the other hand it could be substituted by 'Molekülmenge', 'Atommenge' and 'Ionenmenge'. Thus, the term 'Teilchenanzahl' was equivalent to amounts of specified concrete 'things', atoms, molecules, etc. Besides it is wrongly stated that 'Teilchenanzahl' is a measurable physical quantity (Ger. meßbare Größe).The conclusive question is: What is gained by introducing a dimensionally independent physical quantity 'Teilchenmenge' which is proportional to the natural quantity *number*? (Cf. the criticism of Westphal (1963; 1965; 1971) by Weninger (1982 b)).

When Stille (1955) made a review of the different meanings of the mole, besides the Ostwaldian mole, he said :

> In der zweiten, heute vor allem in der Physikalischen Chemie sehr verbreiteten Aufassung sieht man das "Mol" als einen rein zahlenmäßigen Mengenbegriff der Chemie an, und zwar als die *Anzahl* der Atome oder Moleküle, die in einem mol der Atom- oder Molekülsorte enthalten sind. Ihre Anzahl ist eine von der Art der einzelnen Moleküle unabhängige universelle Konstante, die man die *Loschmidtsche* (...) oder Avogadrosche *Zahl L* nennt (...); sie ergibt sich aus den Resultaten von Präzisionsmessungen (...) zu $L = (6{,}0237 \pm 0{,}0015) \cdot 10^{23}$. (...)
>
> Wenn man Mengen chemischer Substanzen, d.h. die in einer betrachteten Menge enthaltene Anzahl N von Molekülen, in dieser Mengeneinheit zählt, pflegt man alllerdings im allgemeinen nicht die in einer "arithmetischen Zählungseinheit" $6{,}0237 \cdot 10^{23}$ gezählten Zahlenwerte der Moleküle und diese "Zählungseinheit" selbst anzugeben. Vielmehr leitet man aus N eine neue Mengengröße so ab, daß sie wieder in der Zählungseinheit Eins der normalen Zahlenreihe gezählt wird. Wir werden die spezielle Mengengröße, die sich auf je L Moleküle bezieht, mit l bezeichnen und die *Molzahl* der betrachteten Substanzmenge nennen. (...) Die Molzahl l wird als chemische Mengengröße gegeben durch die Beziehung
>
> $l = N / L.$
>
> Sie ist eine dimensionslose Größe und wird in der allgemeinen arithmetischen Zählungseinheit Eins gemessen. (Stille, 1955, p. 118)

It is evident that Stille in the quotation above used 'Menge' in at least two senses, as a denotation of a collection of molecules or atoms, and as a denotation of concrete portions.

Stille connects 'mole number' (Molzahl) to the introduction of the basic physical quantity *amount of substance* ('Stoffmenge'), which is a precursor to the definition given by IUPAC and CGPM 1971:

> Wenn man (...) des Mol-Begriffs präziser formulieren will, beispielsweise durch Einführung der (...) Grundgrößenart "Stoffmenge", so können l (...) als zahlenwert der Stoffmenge, gemessen in den zugehörigen Stoffenmengeneinheit angesehen werden. (Stille, 1955, p. 119)

The unit of *amount of substance* ('Stoffmenge') is defined,

> ... als Einheit der Stoffmenge diejenige Stoffmenge festgelegt, die so viele Individuen (Atome oder Moleküle) wie (A_o) g atomarer Sauerstoff Atome enthält.
>
> (...) Bei der Darstellung chemischer Reaktionen und für die einzelnen Elemente oder Moleküle spezifischer Eigenschaften kann in physikalisch sinnvoller Weise die Stoffmenge nur auf chemisch homogene Substanzen angewendet werden. (Stille, 1955, p. 119)

The 'definition' of *amount of substance* accounted for in the IUPAC manual (Mills *et al*., 1993), $n_B = N_B / L$, has got its analogue in the definition of 'number of moles' (Molzahl), $l = N / L$. L in the former case has got the unit mol^{-1} and in the latter case 1 .

Guggenheim (1961) referred to Stille (1955) when he supported the introduction of *amount of substance* as a base physical quantity (see section 5.1).

In the IUPAP proposition from 1958 the unit 1 mol was defined with considerable confusion about a concordant physical quantity, when stating:

> 1 mole (symbol: mol) is the quantity of substance which contains the same number of molecules (or ions, or atoms, or electrons, as the case may be) as there are ...

What does 'quantity of substance' mean? Is it a concrete portion of a substance or is it a physical quantity? Since it *contains* something it must logically be something concrete, thus 'quantity of substance' is a portion and not a physical quantity. The definition does not explicitly refer to a physical quantity corresponding to the defined unit 1 mol.

In the 1967 IUPAC proposition the definition of the mole was changed:

> The mole is the amount of substance of a system which contains as many elementary entities as there are...

This definition of 'the mole' prescribes that it is a unit of a measure of the property *amount of substance (the physical quantity)* of a system. 'System' is the denotation of the concrete portion of matter which contains elementary entities. Moreover, the words molecule, atom, ion, etc. are subsumed under the superordinate denotation *elementary entity*.

Eventually the proposition from 1967 (confirmed 1969) resulted in the 1971 CGPM decision on the prevailing definition. For a detailed discussion of the 1967 IUPAC proposition see chapter 5.

When *amount of substance* was explicitly introduced as a physical quantity in the German discussion in the 1930's, the ambiguity and vagueness of that quantity, whether it should be a continuous or a discontinuous variable, in view of the experimentally verified atomic theory, seems not to be made clear. The old tradition of a chemical atomic theory approach was maintained and gave us the linguistic hybrid 'amount of substance', ambiguously accounting for matter as both a continuum and a discontinuum.

McGlashan (1977) points to the fact that *amount of substance* is adopted for historical reasons. From a physical point of view there is no need of *amount of substance*:

> Although widely used by chemists, the physical quantity called amount of substance and its SI unit called the mole are not necessary in science. It would be perfectly feasible to deal always with molecular quantities, and at least in physics that is often done.
>
> Nevertheless, for historical reasons it is customary in chemistry (and in physics too) to use the redundant physical quantity amount of substance and its SI unit the mole. (McGlashan 1977, p. 276)

This statement is both evidence for historically divided conceptions of matter among chemists and physicists and for the juxtaposition of chemistry and physics views of how to quantify matter mathematically.

The tradition in chemistry of using the pragmatic term 'the mole' is reminiscent of the continuum view of matter (Ostwald's mole as a specific unit of the physical quantity *mass*). The introduction and use of the physical quantity *amount of substance* accounts for a physicalized point of view, meeting the demands of coherence in quantity calculus, with base physical quantities as mathematically continuous variables. Thus, the prevailing definition of 1 mol is a result of joint traditions from both physics and chemistry.

Generally, matter could be described from two different perspectives. By viewing the macroscopic level as associated with a conception of matter as a continuum, the tools of continuum physics and continuum mathematics are applied. The prevailing physical quantity *amount of substance* formally fits into this continuous description of matter.

Describing the phenomenal level of matter as multi-atomic, which is in accordance with Chemistry as a science of multi-atomic descriptions and theories, is to view matter as a discontinuum. In this case the *number* of entities in a portion of matter is a natural quantifier. The choice of perspective is a matter of contextual convenience.

The continuous and particulate description of matter is typically demonstrated in classical and statistical thermodynamics, respectively. The former being independent of the corpuscularity of matter and the latter taking its startingpoint in a corpuscular view of matter.

Summary
Historical developments in the concept of 'the mole' are briefly summarised:

Empirical approach	Experimental measurements of mass (and volume) of substances conveyed at chemical reactions.
Theoretical approach	Measured masses converted to relative atomic- or molecular- weights within the Daltonian theory
Praxis	Relative atomic- or molecular- masses (weights) reconverted to measurable masses (weights) expressed in grams. 1) Those individual masses, 'combining masses', are denoted 1 mol by Ostwald. 2) 1 mol is also used as a label for the concrete

	portion with the weight of 1 mol 3) 1 mol is the number of elementary entities in 1 mol (taken as a concrete portion)
Theoretical convention	1 mol is the SI-unit of the physical quantity *amount of substance*

Originally 'the mol' was introduced as a pragmatic denotation of chemically combining weights (numerically coinciding with the relative atomic weights; or multiples of such weights) and also as a denotation of portions of such weights. Interpreted within the frame of atomic theory the mole was made a general 'unit' by identifying it as a fixed number of elementary entities (Avogadro's number). By the 1971 decision, 1 mol was conventionally defined within the frame of 'base physical quantities' and lost its former connotations as identical to fixed masses, individual concrete portions with fixed masses and a fixed number.

The adjustment, making 1 mol a genuine unit, fitting the features of a base physical quantity, had most far-reaching consequences. Since 1 mol was never a historically 'genuine root-unit' for some dimensionally independent physical quantity, it was necessary to invent a basic physical quantity - *amount of substance* - to adjust 1 mol to the logical needs of quantity calculus. This physical quantity does not emerge as a logical answer to some independent phenomenal property in addition to what is accounted for by mass and number or any other physical quantity. Hence, *amount of substance* is a formal quantity which cannot be measured, only calculated by the mass of the elementary entity of the actual substance (dependent on nature and composition) as well as the number of elementary entities, which could only be calculated from measurements of continuous physical quantities. It lacks the generality associated with other independent physical quantities such as mass and length, which are properties of *things* and not of *substances*.

The physical quantity *amount of substance* is by definition bound to the nature of the elementary entity under consideration (Bureau International, 1973, p. 8):

> (...) 2° Lorsqu'on emploie la mole, les entités élémentaires doivent être spécifiée et peuvent être des atomes, des molécules, (...)

The only easily grasped general phenomenal property that is equal to equal measures of *amount of substance* for two different substances is the *number* of elementary entities, for instance 1 mol gold (elementary entity, Au) and 1 mol acetic acid (elementary entity, CH_3COOH). According to Weninger, (e.g., 1985, p. 156) this fact disqualifies the quantity as physical quantity comparable to the other basic physical quantities in SI. However, as a base physical quantity, *amount of substance* is formally to be regarded as an idealised, mathematically continuous counterpart to the discontinuous variable *number*.

CHAPTER 5

A CONCEPTUAL ANALYSIS OF *AMOUNT OF SUBSTANCE*

5.1 The IUPAC- manual

As a guide for the scientific community IUPAC publish a manual, with recurrent revisions, for the proper use of physical quantities and units. The first edition, with the name 'Manual of Symbols and Terminology for Physicochemical Quantities and Units', was prepared in 1969 with M.L. MacGlashan as editor. As stated in the preface the intention is

> ...to secure clarity and precision, and wider agreement in the use of symbols, by chemists in different countries, among physicists, chemists and engineers, and by editors of scientific journals. (McGlashan, 1970, p. 3)

The 2nd and 3rd editions were delivered in 1973 and 1979. The manual appeared substantially revised and extended in 1988 under a new title, "Quantities, Units and Symbols in Physical Chemistry" and the latest edition is from 1993 with I. Mills *et al.* as editors. The style of the two latest editions is slightly changed from its predecessors

> ...from being a book of rules towards being a manual of advice and assistance for the day-to-day use of practising scientists. (Mills *et al.*, 1988, p. viii)

The IUPAC manual (called 'The green book', due to the colour of the cover), including the definitions made in SI by CGMP, expresses the prevailing scientific standpoint about the physical quantities and units as well as the use of quantity calculus. Thus, the importance of this book as a norm for the individual chemist (scientist and educator) ought to be considerable. This is also stressed in the manual. For instance it is said that the symbols of the seven base units

> ...are internationally agreed and should not be changed in other languages or scripts. (Mills *et al.*, 1993, p. 71)

In the introduction to the section on 'Tables of physical quantities', the manual says:

> ..., it is clearly an aid to scientific communication if we all generally follow a standard notation. The symbols (...) have been chosen to conform with current usage and to minimise conflict as far as possible. (...) Major deviations from the recommended symbols should be particularly carefully defined. (Mills *et al.*, 1993, p. 9)

Out of this claim, as a world wide standard, the manual will now be examined concerning the SI base unit 1 mol and the base physical quantity *amount of substance*.

In the first chapter the prominence of the physical quantity *amount of substance* in chemistry is established:[56]

> By convention physical quantities are organised in a dimensional system built upon seven *base quantities*, each of which is regarded as having its own dimension. (...)
>
> The physical quantity *amount of substance* or *chemical amount* is of special importance to chemists. Amount of substance is proportional to the number of specified elementary entities of that substance, the proportionality factor being the same for all substances; its reciprocal is the *Avogadro constant* (...). The SI unit of amount of substance is the mole (...). The physical quantity 'amount of substance' should no longer be called 'number of moles', just as the physical quantity 'mass' should not be called 'number of kilograms'. The name 'amount of substance' and 'chemical amount' may often be usefully abbreviated to the single word 'amount', particularly in such phrases as 'amount concentration' (...), and 'amount of N_2' (...). (Mills *et al.*, 1993, p. 4)

The statement raises two main questions.

Is the **base** physical quantity *amount of substance* defined by a proportionality, where number is the foundational quantity: "Amount of substance is proportional to the number of specified elementary entities..."?

Does the phrase "amount of substance... of that substance" and the recommended abbreviation 'amount' mean that the phrase *amount of substance* is divisible where 'substance' denotes something concrete and could be substituted by the name of the actual substance like copper, sulfur, iron, etc., or specified by the actual elementary entity? Is it

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[56] The alterrnative name *chemical amount* was introduced at the 36th IUPAC General Assembly in Hamburg in August 1991 (Cvitaš, 1993, p. 100).

possible to manipulate the stipulated name of a base physical quantity without introducing conceptual disturbance and doubts of the univocalness of the name? I start with the second question.

5.2 The name *amount of substance*

In the sentence "amount of substance is proportional to the number of specified elementary entities of that substance", the words 'that substance' logically refer to 'substance' in 'amount of substance'. Since *amount of substance* (taken as a whole) is the name of a physical quantity, an abstraction, and 'substance' in the phrase 'that substance' refers to something concrete (some kind of element or chemical compound or their elementary entities), the reference seems to be illogical.

However, there is evidence in the text that from the authors' point of view the reasoning is logical, since in the name 'amount of substance' the connotation of 'of substance' does refer to concrete substances. A confirmation is found in footnote (1), (Mills *et al.*, 1993, p. 41):

> The words 'of substance' may be replaced by the specification of the entity.

This is explicitly exemplified on, for instance, p. 46 when expressions like "amount of Cl, amount of chlorine atoms" and "amount of (entities) H_2SO_4" are used.

On the one hand it is stated that the name of the physical quantity is *amount of substance* (or *chemical amount*). On the other hand it is stated that the words 'of substance' can be substituted by a specification of the concrete entities. It does not seem to be consistent with the premises of quantity calculus, to mix the name of a physical quantity with names of the entities measured by the physical quantity.

In addition, conceptual certainty is not created by first fixing the word *substance* to *amount* in *amount of substance* and then subtracting it, receiving the single ambiguous word 'amount' again.

The conceptual indeterminacy of *amount of substance* was already present in Guggenheim's (1961) paper on the mole, amount of substance and related quantities. This was, in fact, one of the first texts supporting the introduction of the physical quantity *amount of substance* presented before an American audience of chemists.

Guggenheim pointed out:

> During the past score of years the view has been accepted by a rapidly increasing number of physicists and chemists that there is a third *quantity* [note. my italics] different from mass and weight but proportional to both. This *quantity* [note. my italics] was first named (5) "Stoffmenge" in German and the English translation is "amount of substance". (Guggenheim, 1961, p. 87)[57]

The word *quantity* is here used in the sense of a physical quantity, since it is used about mass and weight. Hence, "amount of substance" is taken as a dimensionally independent quantity (physical quantity). However, in the following part of the paper Guggenheim did not use "amount of substance" as a name of a fixed physical quantity. It was used in expressions such as (ibid., p. 87):

> Admittedly the amount of a pure dry solid substance is usually measured by weighing, but there are numerous other ways of measuring amount of substance.

Here the word amount seems to connote a 'portion', or a general quantity. And the last part of the sentence, "there are numerous other ways of measuring amount of substance", indicate that amount of substance does not have a fixed meaning. Amount of substance is probably used here in the same general sense as the single word amount. The non-fixed (general) meaning of amount and amount of substance is confirmed when Guggenheim stated:

> The amount of a gas (or beer!) is often determined by a measurement of volume. The amount of a substance in solution is often determined by titration... (...). The amount of a radioactive substance may be determined by a Geiger counter. (...) It is clear that amount of substance determinable by any of the mentioned techniques is no more identical with mass and weight than these two quantities are identical with each other. The unit of amount of substance most used and among chemists almost universally used is the mole. (Guggenheim, 1961, p. 87)

In the last sentence, amount of substance is simultaneously connoting two senses. First, in relation to the previous sentences it connotes a portion or a quantity in a general sense. Second, it seems to connote a physical quantity 'amount of substance' by stating "The unit of amount of substance... is the mole". By saying "The unit of amount of substance most used and among chemists almost universally used...", in a context

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[57] The reference denoted '(5)' in the quotation is Stille (1955).

where amount and amount of substance have been given a general sense and connected to the physical quantities mass and volume and measuring devices or methods (Geiger counter, titration), is confusing. Further, in the definition of mole given by Guggenheim, amount of substance is given the sense of a portion (here the fixed portion named 'the mole'), since it contains elementary entities.

> The mole is the amount of substance containing the same number of molecules (or atoms or radicals or ions or electrons as the case may be) as there are atoms in 12 grams of ^{12}C. (Guggenheim, 1961, p. 87)

Compared to the 1959 definition of IUPAP and Guggenheim's suggestion, the 1967 IUPAC (1968) definition was completed by the phrase *of a system*, so the introduction of the definition became "The mole is an amount of substance *of a system* which contains...", viz. it is the system that contains elementary entities and not the unit mole or the physical quantity *amount of substance*.

The full definition of the mole was given in the following way (IUPAC, 1968, p. 11 and p. 27 (italics are used on p. 27))[58]:

> The mole is an amount of substance of a system which contains as many elementary units as there are carbon atoms in 0.012 kg (exactly) of the pure nuclide ^{12}C. The elementary unit *must be specified* and may be an atom, a molecule, an ion, an electron, a photon, etc., or a *specified* group of such entities.

Associated to the work of the Commission on Symbols, Terminology and Units in Prague in August 28 and 29, 1967, the definition of 'the mole' was commented:

> The same definition has been accepted by the SUN Commisssion of IUPAC and by ISO. It is currently being seriously considered by the Commité International de Poids et Mesures (CIPM) for adoption as a seventh basic unit of the Système International. IUPAC is asked to endorse the above definition to inform COPM of this endorsement (an earlier version of the definition was approved by the Bureau of IUPAC (date).) (IUPAC, 1968, p. 11) [59]

Using *an* instead of *the* before amount of substance in the definition of 'the mole' is a linguistic and semantic deviation compared to other definitions of the basic SI units given in the same publication. Compare "The mole is *an* [italics added] amount of substance..." with:

> The metre is the length...
> The kilogramme is the mass...
> The second is the duration...
> (IUPAC, 1968)

This deviation seems to alter (reduce) the meaning of *amount of substance* as a univocal physical quantity into a term comparable to the word 'amount' with its ambiguous meaning (here, possibly a concrete portion). It seems that the physical quantity of the defined unit *the mole* is less explicitly expressed compared to the other physical quantities.

However, in the final 1969 IUPAC definition *an* was replaced by *the*. Some other amendments were also made, for instance the word *unit* in the connection elementary unit was substituted by *entity*. As already mentioned above the definition of 1 mol was approved as a base unit in SI by CGPM in 1971.

McGlashan who was Vice-Chairman in the IUPAC Commission at the Prague meeting in August 1967 used *amount of substance* in a confusing way:

> The physical quantity called amount of substance is denoted by *n* and is regarded as dimensionally independent.
>
> Amount of substance is not the same as mass. The amount of a substance and its mass, unlike its volume... (...) ...the amount of a *particular* substance is proportional to its mass. Any resemblance between amount of substance and mass ends there, however, and in general the amounts of different substances are *not* proportional to their masses. Just as the dimension of mass is simply that of mass, so the dimension of amount of substance is simply that of amount of substance; that is what is implied by the word 'independent in the phrase ' dimensionally independent. (McGlashan, 1977, p. 276)

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[58] The IUPAC (1968) was a "Draft of an extensively revised version of the 1959 Manual of physicochemical symbols and terminology". Comments could be sent to the Chairman of the Commission Professor McGlashan within eight months. The final text would appear after a review of the Commission and an approval of the Physical Chemistry division of the IUPAC.

[59] SUN Commission, Commission on Symbols, Units and Nomenclature of the International Union of Pure and Applied Physics. ISO, International Organization for Standardization

The insertion of an *a* in *amount of substance*, getting *amount of a substance* is a disturbance in the efforts to make an unequivocal interpretation of the text.

In the phrase, "The amount of a substance and its mass, unlike its volume...", "The amount" either refers to amount in a general sense, or to 'amount of substance' in the previous sentence, or are 'amount of substance' and 'amount of a substance' treated as equivalents by McGlashan? But logically the insertion of an 'a' between 'of' and 'substance' changes the meaning of the totality 'amount of substance', as a name of a base physical quantity. It is only the word 'amount' in the quoted phrase that logically has a status as some kind of physical quantity or as a general denotation of a portion of a concrete substance. 'A substance' in 'amount of a substance' is referring to a concrete substance, since it is possible to talk about "its mass" and "its volume". This is even more stressed in the expression "the amount of a *particular* substance is proportional to its mass.", where the word *'particular'* explicitly points to a concrete substance. In this context "Amount" ought to be interpreted as an abbreviation of the phrase *amount of substance*. The sentence "Any resemblance between amount of substance and mass ends there, however, and in general the amounts of different substances are *not* proportional to their masses." is even more confusing, since there is no resemblance at all between different basic physical quantities as stated by McGlashan in the last part of the quotation, by stating that amount of substance is dimensionally independent. The connotation of "amounts of different substances" is a variation on 'amount of a substance' and 'amount of a particular substance'. In all three phrases, 'amount' is probably intended to denote the physical quantity *'amount of substance'* and 'substance' represents some concrete substance. But in the text the conceptual situation is uncertain.

Hence, to sum up there must be two senses of 'substance' in this specific context:

1. $(\text{substance})_1$ in the name of the physical quantity *amount of substance*. $(\text{substance})_1$ is a part of the name *amount of substance*, which must be looked upon as an indivisible entirety.
2. $(\text{substance})_2$ in 'amount of a substance' (and its analogues 'amount of a particular substance' and 'amounts of different substances'). $(\text{substance})_2$ is a superordinate concept for concrete matter manifested in portions of different elements (iron, gold, etc.) or compounds (sodiumchloride, potassiumsulphate, etc.) determined by their elementary entities.

Hence, substance in *amount of substance* could not be substituted with the actual elementary entities as said in the manual. What can be done is to substitute the whole name *amount of substance* with the short name *amount* and if a substance's name is attached to that short name it is in the sense of $(\text{substance})_2$.

The name of the physical quantity is legislated *amount of substance*. If used abbreviated as 'amount', why was not the physical quantity plainly named 'amount' in the decision made by CGPM 1971? And why was *chemical amount* introduced as an alternative to *amount of substance*, if *amount* is passable as a short name?

One of the editors of the IUPAC manual, Cvitaš (1993) has commented the adoption of *chemical amount* as an alternative to *amount of substance* at the 36th IUPAC General Assembly in Hamburg in August 1991.

> The term 'amount of substance' for the old 'number of moles' seems still to bother many chemist and so does the concept introduced in 1969 by Prof. Max McGlashan. 'Amount of substance' is no doubt a mouthful and even more so the 'amount of substance concentration' or 'amount of substance fraction'. To avoid such lengthy names the authors of the Green Book (1988) recommended the use of expressions such as '*amount* of sodium chloride' instead of '*amount of substance* of sodium chloride' for $n(\text{NaCl})$. (...) 'Amount' having a more general meaning was thought to be inadequate for describing the physical quantity n. (...) A further improvement could possibly be achieved by adding the attribute 'chemical' to amount whether there is a risk of confusion with the general meaning of the word. (...) After all, it will still remain a physical quantity. So in the 1992 edition two alternative names 'amount of substance' and chemical amount' will stand next to each other with a footnote on the practice in clinical chemistry and the future will show what chemists will accept. (Cvitaš, 1993, p. 100)

Actually, the reson for introducing *chemical amount* as an alternative to *amount of substance* seems to be a solution to a linguistic problem regarding the length of the phrase *amount of substance*.

It is evident that the use of the abbreviation, or short name *amount*, can create misunderstanding and contradicts the demand of consequence and univocalness.[60] It also seems as this abbreviation alters the meaning of *amount of substance* as an independent physical quantity into the quantity of *number*. The interpretation of amount as a number is reinforced by the IUPAC recommendation that the symbol $n(Cl_2)$ could be read both as amount of Cl_2 and amount of chlorine molecules (Mills *et al.*,1993, p. 46). This creates confusion as to whether

amount (of substance) is a continuous or discontinuous physical quantity. It seems likely that *amount* in expressions such as 'amount of chloride molecules' can be interpreted as a discontinuous quantity, a denotation of a collection of a number of elementary entities or as a synonym to number.

What does amount mean in ordinary language? Synonyms of amount are, according to 'Webster's new dictionary of synonyms' (1984, p. 40) sum, total, quantity, number, aggregate, whole. In an article a kind of lexical definition of amount is made by 'ostension' (by giving 'prototypical examples'):

> **Amount** denotes the result reached by combining all the sums or weights or measures that form a whole < the *amount* of his purchases> <the *amount* of cotton raised in one year> (Webster's new dictionary of synonyms, 1984, p. 797)

Even if this explication is stressing an amount as a generally bulky thing, the synonyms quantity, number and aggregate demonstrate a near relation to something that is intrinsically structured of separate parts.

According to 'The concise Oxford dictionary' (1984) amount equals a general quantity such as in the expression 'any amount', meaning a 'great deal (of)'.

The word amount is evidently associated with considerable ambiguity compared to number, even if the relationship between amount and number could be acceptably expressed.

> **Number** with its strong suggestion of enumerating, is usually applied to countable aggregates of persons or things and is clearly distinct from *amount*, which ordinarily applies to things in bulk or mass; thus, one may pick a large number of apples to make a large *amount* of applesauce. (Webster's, 1984, p. 797)

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[60] No other base physical quantity in SI is abbreviated.

Even in the Swedish language where the name of *amount of substance* is expressed by one word, 'substansmängd', the authorities of Swedish standards state:

> When misunderstanding is unlikely the shortened form "amount" is used. If required clarifications like amount of electrons, amount of photons and so on can be used. (SIS 01 61 74 3.2, SIS handbok, 1982, p. 129)[61]

Thus, what is said about *amount of substance* and the short name amount is also valid for the Swedish words 'substansmängd' and the short name 'mängd'.[62]

In the current IUPAC manual some additional information is given about the physical quantity *amount of substance*:

> The quantity 'amount of substance' or 'chemical amount' ('Stoffmenge' in German) has been used by chemists for a long time without a proper name. It was simply referred to as the 'number of moles'. This practice should be abandoned, because it is wrong to confuse the name of a physical quantity with the name of a unit (in a similar way it would be wrong to use 'number of metres' as a synonym for 'length'). The amount of substance is proportional to the number of specified elementary entities of that substance; the proportionality factor is the same for all substances and is the reciprocal of the Avogadro constant. The elementary entities may be chosen as convenient, not necessarily as physical real individual particles. Since the amount of substance and all physical quantities derived from it depend on this choice it is essential to specify the entities to avoid ambiguities. (Mills *et al.*, 1993, p. 46)

This quotation shows the intention to establish the status of *amount of substance* as a base physical quantity compared to the common expression 'number of moles'. What is earlier said about the abbreviation 'amount' and the illogical mix up between what is abstract and concrete is contradictory to this clear statement which is in agreement with the inherent logic of SI and quantity calculus.

It seems to be a contradiction to establish a proper name of the physical quantity, *amount of substance*, in one part in the manual and permit usage of a short name *amount* in another part even if there is now a

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[61] Translation from Swedish by Dr. Dennis Beach.

[62] In a recent translation of IUPAC's "Abbreviated List of Quantities, Units and Symbols in Physical Chemistry" edited by Svenska kemistsamfundet 1995 (Swedish Chemists Association) four names of the quantity are used: 'ämnesmängd', '(kemisk) mängd' and 'substansmängd'.

possibility to use the alternative name *chemical amount* to prevent misunderstanding.

And now to the first question.

5.3 About the 'definition' of *amount of substance (n)*

Table 2.10 in the IUPAC manual lists physical quantities in general chemistry (Mills *et al.*, 1993, p. 41). *Amount of substance* denoted "Amount (of substance), chemical amount" in the table with the symbol n is one of them, and is **defined** (my emphasis; the headline of table 2.10 says "Definition") by the equation[63]:

$$n_B = N_B / L$$

where N_B is the number of entities of a substance B and L the Avogadro constant.[64] It is noteworthy that the Avogadro constant is not defined in this table. However, in the previous table 2.9 (Statistical Thermodynamics) the definition is (Mills *et al.*, 1993, p. 39): $L = N/n$, with the SI unit mol^{-1}.

It is notable that *amount of substance* is given as a 'definition' in algebraic form, since it is a basic independent physical quantity comparable to mass, length and time, quantities which are not given as algebraic definitions. The distinctive feature of basic independent physical quantities and their units are that they are not defined by mathematical relationships (Pohl, 1953):

> Grundgrössen und ihre Einheiten lassen sich allein mit Sätzen, also nicht mit Gleichungen, definieren.

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[63] The definition is commented in two footnotes (1) and (2) (ibid., p. 41) :

(1) The words 'of substance' may be replaced by the specification of the entity.

Example When the amount of O_2 is equal to 3 moles, $n(O_2) = 3$ mol, then the amount of ½ O_2 is equal to 6 moles, n (½O_2) = 6 mol. Thus n(½O_2) = $2n(O_2)$. (...).

(2) The definition applies to entities B which should always be indicated by a subscript or in parentheses, e.g. n_B or $n(B)$

[64] Cf. the definition of 'Molzahl', $l = N/L$, in Stille (1955, p. 118) (see, chapter 4).

Also Wallot (1953, p. 1) has commented on the specific nature of base physical quantities:

> Aber Grundgrössen lassen sich nicht durch Gleichungen auf andere schon erklärte Grössen zurückführen. Man spricht auch von "unabhängigen" oder "axiomatischen" Grössen.

If 'amount of substance' is a defined physical quantity by the equation $n_B = N_B / L$, then N_B and L must be foundational to n_B. This statement is made in analogy to the definition of, for instance, the well-known definition of *density* from mass and volume $\rho = m/V$ and the two molar quantities *molar mass* and *molar volume* $M_B = m/n_B$ and $V_{m,B} = V/n_B$ where m, V and n_B are foundational to M_B and $V_{m,B}$) (Mills *et al.*, 1993, p. 41).

In the IUPAC manual, number of entities, N, and Avogadro constant, L, are given without definitions (p. 41). But as the unit of L is 1 mol^{-1}, it is a derived physical quantity from number and *amount of substance* with the SI unit 1 mol ($L = N_B / n_B$). In other words, L, in the equation $N_B = L \cdot n_B$ is the proportionality constant relating the two independent physical quantities number and *amount of substance*, viz. the physical quantity L is **defined** by $L = N_B / n_B$, which is also confirmed by the definition in table 2.9 (p. 39). Hence, if $n_B = N_B / L$ is taken as a definition of n_B, this must be a circular definition (cf. McManus, 1983, p. 6).[65]

The equation $N_B = L \cdot n_B$ states that the number of entities is proportional to the *amount of substance*. This means that *amount of substance* is foundational to number. In other words number depends on the *amount of substance*, n_B, which is the independent variable. These circumstances are a consequence of the definition of the SI unit 1 mol of the physical quantity *amount of substance,* which says: "The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12". The SI definition of the mole establishes a fixed number; the number of atoms in 0.012 kilogram carbon 12. Therefore number must be (logically) proportional to *amount of substance*. However, 'natural

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[65] Here is a possibility to make a misinterpretation, taking the equation $n_B = 1/L \cdot N_B$ as a conversion; N_B and n_B representing the same dimension - number- and L a conversion factor, a fixed number (cf. the category of description F_2, section 3.4.2).

thinking' and the SI definition of 'the mole' underpin a conception of number as foundational to *amount of substance*. This seems to be the reason why it is stated in the manual and by McGlashan (1977) that *amount of substance* is proportional to number via the reciprocal of Avogadro constant ($n_B = 1/L \cdot N_B$).

The statement '*amount of substance* is proportional to number' seems to be an attempt to explain what *amount of substance* is. The statement entertains a conception of *amount of substance* as a kind of measure of number, a mathematically discontinuous measure of the discontinuous variable number. Superficially it also mimics an algebraic definition (an equation) of *amount of substance*. But this is false, as said above, since the proportionality constant L (unit 1 mol^{-1}) is a molar quantity depending on the previous existence of *amount of substance*. This explains the circularity of the 'definition' accounted for above.

In analogy to the relationship $n_B = 1/L \cdot N_B$ it could also be stated that *amount of substance* is proportional to mass, $n_B = 1/M_B \cdot m_B$, with the reciprocal of molar mass (M_B) as a proportionality constant. This statement is **not** made in Mills *et al.* (1988, 1993). A plausible explanation of this fact is that it lacks the generality of the relationship $n_B = 1/L \cdot N_B$. The proportionality constant $1/M_B$ is substance dependent (elementary entity dependent) since M_B is the molar mass. The stress on one of the relationships and the absence of the other in the IUPAC manual could be that the relationship of *amount of substance* and number is 'preferred' by the international standardisation committee as an explanation of what *amount of substance* is. It is evident that the conceptual connection of *amount of substance* to number is stronger than to mass. However none of the relationships have any explanatory capacity of the full meaning of *amount of substance*.

In this context a key question is: If *amount of substance* is directly (monotonously) proportional to number by definition, why not use the physical quantity *number* directly with its natural unit 1, and 1 mol as a multiple unit? This option is strongly advocated by Weninger (see chapter 6).

The SI definition of 'the mole' states that the elementary entity must be specified when the mole is used. This implies that *amount of substance* is an elementary entity dependent quantity and thereby a substance dependent quantity. This means that the quantity *amount of substance* is not comparable to other physical quantities in SI. These account for substance independent continuous properties on the macro-level, and are thereby also independent of composition and structure on the micro-level. *Amount of substance*, by being dependent on qualitative atomic properties, transcends the frames of the set of base physical quantities in SI.

Which phenomenal property is expressed by the physical quantity *amount of substance*? The only property conserved (invariant) by the notation 'the *amount of substance* 1 mol' among different substances[66] is the number of specified elementary entities, a property which is logically and empirically independent of the concept of substance. The only phenomenal property in common between e.g. the *amount of substance* 1 mol oxygen (O_2) and the *amount of substance* 1 mol sodiumchloride (NaCl) is the number of elementary entities, O_2 and NaCl respectively.

Generally, the analogy between the equalities $n_1(\mathrm{Cu}) = n_1(\mathrm{P})$ (e.g., 1 mol Cu = 1 mol P) and $m_1(\mathrm{Cu}) = m_1(\mathrm{P})$ (e.g., 1 kg Cu = 1 kg P) must hold according to the inherent logic of the category of base physical quantities. A fixed numerical value of *amount of substance* of two different substances must denote one and the same *amount of substance*.

Amount of substance cannot easily be comprehended without reference to the discontinuous structure of matter, expressed by the statement '*amount of substance* is proportional to number'. However, the use of the phrases 'number of moles' and 'mole numbers' and nowadays *amount of substance (n)*, in classical thermodynamics does not account for any assumption of the structure or corpuscularity of matter. It is evident that what is denoted by n (*amount of substance*) is a mathematically continuous variable since it is differentiable. This is, for instance, explicitly demonstrated in the definition of *chemical potential*, μ_i:

$$\mu_i = \left(\frac{\partial G}{\partial n_i}\right)_{T,P,n_j}$$

where G = Gibbs free energy, n_i, n_j = *amount of substance* of substance i and substance j, respectively, T = temperature, P = pressure.

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[66] Substances (substance belongs to the macrolevel) are separated on the microlevel due to qualitatively and quantitatively separated elementary entities.

Mills *et al.* (1993) does not explicitly say anything about *amount of substance* being a continuous or discontinuous physical quantity.

According to the factual differentiability of *amount of substance* in the equations of classical thermodynamics and due to the inherent logic of physical quantities in SI, it must be conceptualised as a continuous variable. Logically it is unequivocally determined by number through the SI definition of 1 mol. Hence, *amount of substance* must be regarded as a mathematical idealisation whose metric properties are isomorphic with the positive real numbers $\mathbf{R}_+$, a 'continuous analogy' to the discontinuous variable *number*.

Amount of substance is either

* a physical quantity which is mathematically discontinuous and measures number[67]

or

* a physical quantity which is mathematically continuous and measures number

In the former case *amount of substance* is merely a duplicate of the physical quantity *number*, and, since it is enough with one of them, *amount of substance* seems to be redundant (Cf. the different conclusions of Weninger and Rang (cf. Chapter 6)). However, had *amount of substance* been identical to number, there would have been no grounds for introducing it at all as a **base** physical quantity. *Number* would have been the proper physical quantity. Moreover, requirements are present in the IUPAC manual for a treatment of the domain in a discontinuum perspective. The manual includes the quantity of *number of entities* with the symbol N and SI unit 1. The manual explicitly states that 1 is an SI unit (Mills *et al.*, 1993, pp. 39 and 41). The mass of a discrete entity is denoted m_f or m (p.41). The quantity *number density of entities* or *number concentration* with the symbol n[68] or C is defined $C_B = N/V$ and $C_B = N_B/V$ with the SI unit m^{-3} (p. 42).

Hence, the physical quantity *amount of substance* must have some extra quality compared to *number* to be justified. The justification of the physical quantity *amount of substance* seems to be related to its feature

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[67] The phenomenal ground, the physical significance of *amount of substance* as identical to number, is here directly bound to the corpuscularity of matter within the atomic theory.

[68] The same symbol as for the base physical quantity *amount of substance* !

as a continuous variable. *Amount of substance* is a continuous quantity measuring the number of elementary entities in a portion of matter. According to the SI definition of 1 mol *amount of substance* is unequivocally determined by the number and is one of the seven dimensionally independent basic physical quantities. The relevance of the introduction of *amount of substance* is a question of coherence rather than logic. Coherence to the properties, especially **continuity**, of the category members of the base physical quantities in SI. Thus, *amount of substance* is only comprehensible within the theory of physical quantities. *Amount of substance* is a mathematically continuous variable ($\{n\} \in \mathbf{R}_+$) of a property, particularity of a physical system coherent with the other base physical quantities.

There is a conceptual gap between, on the one hand, all explanations as framed by the atomic theory, where chemical phenomena are described as multi-atomic corpuscular events[69] and on the other, *amount of substance* as a continuous measure of the corpuscles. When the number of elementary entities are low the continuous quantity has a precision that lacks empirical meaning.

A separation must be made between the mathematical idealisation of particularity as a continuity (when the number of particles are so large that their quantification can be idealised as continuous) and particularity itself as confirmed by experiments framed by the atomic theory.

There is an intrinsic qualitative difference between a variable isomorphic with the real number system and a variable isomorphic with the natural number system.

In 1873 Cantor proved that there is no bijection of **N** on **R** ($\nexists\ \overset{\curvearrowright}{\mathbf{N}\ \ \mathbf{R}}$)[70] Gödel proved in 1938 that it is impossible within the frames of the axiomatic system of set-theory (Zermelo - Fraenkel axiomatic system) to demonstrate that R does not have the cardinal number $\aleph_1$. Further, it is proved by Cohen (1966) that the continuum hypothesis could not be deduced from the Zermelo - Fraenkel's axiomatic system. Thus it is impossible to confute (Gödel) or prove (Cohen) the continuum

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[69] Probably the continuity is taken for granted (presupposed) in the shaping of *amount of substance* as the number of particles are so huge that they could be looked upon as a continuum.

[70] There does not exist any bijection between the set of natural numbers and the set of real numbers.

hypothesis. It is independent from the given axiomatic system (cf. the parallel axiom in Euclidean geometry).

As long as there are doubts about the mathematical nature of the metric of *amount of substance,* it will continue to carry considerable ambiguity and indeterminacy.

The commentaries on the 1971 definition as expressed in the 1988 and 1993 IUPAC manuals are not clear about the fact that *amount of substance* (or *chemical amount*) is only interpretable within the theory of continuum physics.

5.4 Conclusion

The analysis of the IUPAC manual (Mills *et al.*, 1988; 1993) demonstrates confusion about the stability of the name and status of the base physical quantity *amount of substance*. Using the word *amount* as an abbreviation of *amount of substance* introduces equivocalness due to the general and multifarious meaning of *amount* as mass, volume, number and as a general arbitrary quantifier which was also emerging in adjacent texts preceding the 1971 definition (e.g. Guggenheim 1961) (cf. also the empirical results about conceptions of amount in chapter 3)

By stating that *amount of substance* is **defined** as proportional to number ($n = 1/L \cdot N$) the status of *amount of substance* as a base physical quantity could be questioned.

If *amount of substance* (n) is not identical to number (N) it is a continuous analogy to the discontinuous variable number. Hence, in the proportionality $n \propto N$, $\{n\} \in \mathbf{R}_+$ and $\{N\} \in \mathbf{N}_+$ where $\mathbf{R}_+$ is the real positive numbers and $\mathbf{N}_+$ the positive integers.

The intrinsic conceptual and mathematical sophistication bound to *amount of substance* seem to contribute a lot to the scientific and educational confusion about it.

Weninger's (see chapter 6) demand for a clear distinction between the continuum and discontinuum perspectives of matter, and his criticism of *amount of substance* (Ger. Stoffmenge) as an illogical construction lacking this distinction is explicitly demonstrated by the present analysis of the IUPAC manual.

The fact is that the legislators of the SI definition of 1 mol have made a mathematical idealisation where number is accounted for by a continuous variable, *amount of substance,* through a proportionality relationship.

Mills *et al.* (1993, p.vii) invite communication about the contents of the IUPAC manual:

> We would welcome comments, criticism, and suggestions for further additions to this book.

Hence, I address the representatives of IUPAC to consider the commentary on the physical quantity *amount of substance* (alt. *chemical amount*) and the SI unit 1 mol in the IUPAC manual in view of the present analysis.

CHAPTER 6

WENINGER'S CRITICISM

The insistent work of Weninger criticising the introduction of the physical quantity *amount of substance* and the definition of mole, both before and after the 1971 definition (CGPM), takes its point of departure in the dual conception of matter. A clear conceptual and terminological distinction is advocated and maintained between a continuous and a discontinuous view of matter throughout his entire work (Weninger, 1982a).

The present conceptual situation is unsatisfactory since even the separate words in the phrase *amount of substance* (Ger. Stoffmenge) connotes a dual perspective of matter. Substance (Ger. Stoff, Sw. 'substans' or 'ämne') connote a continuous view and amount (Ger. Menge, Sw. mängd) a discontinuous view.

However, the two perspectives are not contradictory but complementary.

> Diese Begriffe werden heute als komplementär betrachtet: Sie bedingen einander wechselseitig und bilden eben dadurch eine dialektische Einheit. (...) *Ein Diskontinuum ist* nur kein homogenes, sondern *ein inhomogenes oder strukturiertes Kontinuum.* (Weninger,1987, pp. 246-247)

Weninger's investigations are semantic-terminological expositions, to elaborate an unequivocal language in relation to the actual subject domain, aiming at scientific clarity. Weninger (1977) states:

> Es ist heute jedem Chemiker selbstverständlich, daß wir Dinge als Diskontinua betrachten. Im Denken der Allgemeinheit hat sich die "kopernikanische Wende" hinsichtlich der Chemie bisher nicht vollzogen. Üblicherweise sprechen und denken wir mit Wörtern und Begriffen, die aus der Zeit der ausschließlichen Kontinuumsbetrachtung stammen, und erschweren auf diese Weise den Erkentnisfortschritt der Lernenden, inbesondere den entscheidend wichtigen Übergang vom Kontinuums- zum Diskontinuumsdenken. (Weninger, 1977, p. 44)

But the perspectives must be separated and analysed separately in order to uphold conceptual clarity.

The discontinuity of matter is double, because it means,

> (...), nämlich sowohl eine Diskontinuität im *Aufbau* wie auch eine Diskontinuität in den *Eigenschaften*. Die postulierten Atome sind etwas ganz anderes als kleine Teilchen, die man beim Zerteilen eines homogenen Kontinuums erhielte. (Weninger, 1982a, p. 200)

The terms 'Teilchenaggregat' (aggregate of particles) and 'Monadenaggregat' (aggregates of monads) and 'Henadenaggregat' are used as discontinuum counterparts to 'Stoffportion', the latter word introduced by Weninger (1959, p. 135) and reserved as a denotation for a concrete body of matter in the continuum perspective.

'Monad' was introduced by Weninger (1979a, p. 6) as an superordinate concept to atom, molecule, ion, formula unit, stressing the fact that they are not small bodies of matter (Ger. 'kleiner materieller Dinge') as conjured by the notation 'particle'. As an equivalent in English, the well-known expression 'elementary entity' will do.

What is considered as a substance in a continuous perspective can be looked upon as an structured aggregate of elementary entities (Ger. Monadenaggregatstruktur) in a discontinuous perspective.

> Beim Übergang von einem Teilchenaggregat zu den Einzelteilchen erfolgt eine sprunghafte (diskontinuierliche) Eigenschaftsänderung. Einzelne Teilchen haben nicht nur keine Aggregateigenschaften; sie haben zum Beispiel auch keine Temperatur im Sinne der Thermodynamik. Es gibt also auch Zustandseigenschaften, die wohl Teilchenaggregaten ('Stoffprotionen'), nicht aber einzelnen Teilchen zugeprochen werden können.
>
> Zwischen einem Teilchenaggregat und seinen Teilchen (seinen Aggregatelementen) besteht ein tiefgreifender, kategorial-analytischer (ontologischer) Unterschied. (Weninger, 1977, p. 19)

The properties of a substance are depending on the structure of the aggregate of elementary entities, not only on the kind of elementary entity.

> ... die Eigenschaften der Teilchenaggregate nicht nur von der art der Teilchen, sondern wesentlich auch von den Relationen zwichen den Teilchen bestimmt werden. (Weninger, 1977, p. 21).

A chemical reaction is a rearrangement of elementary entities, meaning new relationships between them, resulting in a new structured aggregate. These circumstances concern elements too. For instance the properties of graphite and diamond are quite different though the atoms are of the same kind.

> Kohlenstoffatome sind weder schwarz (Graphit) noch farblos (Diamant). Wir können ihnen überhaupt keine Farbe zuordnen.
>
> (...) Ein einzelnes Atom ist weder ein Stoff noch eine Stoffportion. (Weninger, 1977, p. 19).

In that respect the discontinuity concerns the structure of aggregates of atoms, not only the atoms themselves.

> Im Verein des Aggregats behalten die Atome ihre Individualität bei, während die Stoffe bei der Stoffeinung, ihre "Individualität" vollständig verlieren.
>
> (...) Permanenz kommt nur den Atomen zu, nicht aber den Atomaggregaten. Die Vorstellung von der Kontinuität im räumlichen Aufbau der Stoffe muss dagegen ganz aufgegeben werden. Erst die Vorstellung von der räumlichen Diskontinuität erschliesst uns ein weiterführendes Verständnis für den Aufbau und die Umbildung der Stoffe. (Weninger, 1982a, p. 200)

The properties of a substance are emerging through collective effects between a large number of particles (a system or a structure). As an example Weninger (1977) discusses the emergence of the brown colour of the element bromine:

> Das Phänomen "braun" kommt also erst zustande, wenn eine Vielzahl von Photonen beobachtet wird, unter denen diejenigen fehlen, die zuvor von (vielen) Brommolekulen aufgenommen worden sind. (Weninger, 1977, p. 21)

The stringent separation between the perspectives of continuity and discontinuity of matter has strong educational (didactical) implications.

> Die Lösung vieler Schwierigkeiten des Chemieunterrichts liegt nicht in einem Verwischen der Unterschiede zwichen einer phänomenologischen Stoffchemie und der Diskontinuumschemie. Dieser Unterschied lässt sich nicht verwischen oder überbrücken. Die Lösung liegt vielmehr darin, dass wir erstens den Chemieunterricht mit einer phänomenologischen Stoffchemie - genauer: mit einer Stoffportionschemie - beginnen (...) und dann zur Diskontinuumschemie übergehen, wobei wir den Schülern in aller Deutlichkeit bewusst machen, dass wir während des ersten, viel Zeit in Anspruch nehmenden Teils der Diskontinuumschemie nur die Monaden behandeln, die die Stoffe aufbauen, nicht aber die Stoffe selbst. (Weninger, 1982b, p. 272)

This implies consequencies for use of language in Chemistry (a review is given by Dierks,1986). The use of the chemical symbols, such as H_2O, must be discussed and settled as to whether they are symbols for substances (continuous perspective) and/or single water molecules (discontinuous perspective). The term red-ox-reaction ought to be used only in a continuous 'substance-oriented' approaches. In a discontinuous perspective, one ought to use the concept of electron-transfer. In a similar way acid would only be used as a term for substances, but proton-transfer would be the proper term in a discontinuous perspective.

From an educational point of view, discontinuous theories of solids and liquids are needed. For gases, there is the kinetic gas theory and the gas law. But, since the complexity of quantitative theories for solid and liquid substances form an obstacle in lower education, good qualitative pictures must be generated instead. On the last point Weninger (1982a) says:[71]

> Hier liegt meine Meinung nach eine der wichtigsten Aufgaben der künftigen Lernforschung. (Weninger, 1982a, p. 269)

In Weningers (1979a, p. 13) opinion the problem of 'the mole' in science and education could be easily solved, if a perspective of discontinuity had been fully adopted. *Amount of substance* (Ger. Stoffmenge) was introduced early in the German discussion as shown in the historical account. However, the inclusion of *amount of substance* among the base physical quantities in SI was a mistake, since

> Die Moldefinition suggeriert, das die Stoffmenge eine physikalische Grösse sei wie andere physikalische Grössen auch, und suggeriert damit wiederhin, dass die Stoffmenge doch eine Kontinuumsgröße sei. Welche Grösse soll die Stoffmenge aber sein? (Weninger, 1979a, p. 14)

By logical reasons *amount of substance* cannot be a continuous physical quantity (Kontiuumsgröße), since

> Wäre die Stoffmenge eine Kontinuumsgröße, könnte ein und dieselbe Stoffportion nur einen einzigen Stoffmengenwert haben. Bedenkt man den Aufbau einer Stoffportion aus teilchen verschiedener Art, hat man den Bereich des Kontinuumsdenkens verlassen und hat es dann mit Teilchenmengen verschiederner Art und Anzahl zu tun: Schwefelatommenge der Anzahl 8L; Schwefelmolekülmenge (S_8-Menge) der Anzahl L.

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[71] [In my opinion this is one of the most important tasks in the research on learning]

> Es is nicht möglich, daß dei Angabe einer Kontinuumsgröße den Aufbau einer Stoffportion aus verschiedenartigen Teilchen beschreibt. Ein Kontinuumsgröß, die das könnte, wäre ein Widerspruch in sich. (Weninger, 1985, p. 156)

Westphal's (1965; 1971) train of thought is a main target for Weninger's (e.g., 1979a, 1982b, 1985) criticism. Westphal stated that it is impossible to enumerate the huge number of particles in portions of substances which are possible to weigh. Hence, *amount of substance* (in Westphals terminology 'Teilchenmenge') is adopted as a physical quantity which is proportional to number ($n \propto N$; $n = 1/N_A \cdot N$) and measured within continuum physics. Westphal (1971, p. 27) defined 'Teilchenmenge' as "Teilchenanzahlen N proportional, also ein *Mass* für solche ist."[*my note*. Ger. *Mass* = measure].

But Weninger (1979a) points to the fact that the number of elementary entities is calculated from measurements of masses and volumes directly without using *amount of substance*.

> Die Monadenanzahle (...) werden immer unmittelbar *aus Massen- oder Volumenwerten*, also immer *ohne* einen Umweg über eine "Stoffmenge" bestimmt. Die Stoffmenge wird erst nachträglich aus der Anzahl konstruiert.
>
> (...)
>
> Der Fehler der bisherigen begrifflichen Bemühungen liegt also darin, dass man sich auf der eine Seite im Bereich des Diskontinuumsdenkens der Bedeutung der Anzahlen bewusst geworden ist, auf der anderen Seite aber an dem Namen "Stoffmenge" festhält und nicht einfach von den Anzahlen spricht - gleichgültig ob diese unmittelbar durch Abzählen oder mittelbar über Massen- oder Volumenwerte bestimmt werden. (Weninger, 1979a, p. 14)

This is repeated in Weninger (1982b, p. 30):

> Die aussage, daß wir Stoffmengen messen, geht an den Tatsachen vorbei. Niemand hat bis heute eine Definition und ein Meßverfahren für die Stoffmenge angeben können. Gemessen werden ausschließ Massen (zum Beispiel 40,1g bei einer Calciumportion) oder Volumina (zum Beispiel 54 ml bei einer Wasserportion), aber nicht Stoffmengen.

and in Weninger (1985, p. 153):

> Niemand hat bis heute die Stoffmenge einer Stoffportion *gemessen*. Es gibt weder ein Verfahren der Kontinuumsphysik noch ein anderes, ein Stoffmenge als solche zu messen.

Weninger's definite conclusion is that the elementary entities in an aggregate are measured by the quantity *number*.

> Das Wort "Stoffmenge" is völlig entbehrlich: Die Grösse eine bestimmten Kupferatomaggregats kann auf keine Weise präziser beschrieben werden als durch die Angabe der Anzahl der Kupferatome, aus denen das Aggregat besteht:
> $N(\text{Cu i Cu-aggregat } 1) = 3 \cdot 602 \cdot 10^{21} = 3\,L$.
> (Weninger, 1979, p. 14)

There is a precise relationship between mass and number (Weninger 1982b, p. 30):

> Zwischen beiden vermittelt die Masse eines einzelnen Teilchens.

So *amount of substance* is obsolete (ibid. p 30):

> Wenn Stoffmenge und Anzahl einander immer und überall proportional sind, ist eine der beiden Größen, und zwar - aus den angefühten Gründen - die Stoffmenge, überflüssig und sollte daher aus dem Größensystem eliminiert werden. Daß man mit der Stoffmenge rechnen kann, besagt nicht, daß sie eine sinnvolle Größe ist.

The arguments are once again considered in Weninger (1985) and he repeats his criticism of the impossible situation created by the mixing of continuity and discontinuity perspectives:

> Mit der Stoffmenge bleibt man in Kontinuumsdenken (um das zu können, wurde die Stoffmenge ja eingeführt (...)), während man sich mit der Anzahl im Diskontinuumsdenken bewegt, in dem einige Größen überflussig sind, ohne die man im Kontinuumsdenken nicht auskomt. (Weninger, 1987, p. 259)

As long as the concept *substance* is used and considered as continuous, there is a need for substance dependent physical quantities, like the *amount of substance* dependent mass, molar mass (M). This intense quantity unites by proportionality the two independent physical quantities *mass* and *amount of substance*.

> Geht man zum Diskontinuumsdenken über, hat man nicht mehr mit Stoffen und Stoffportionen zu tun, sondern mit Henadenaggregatstruktur und Henadenaggregaten (...): Dann hat man das Eizelding "Stoffportion" als Sammelding " Henadenaggregat" zu betrachten (wobei die Elemente der Aggregate als untereinander gleich betrachtet werden, gleichgültig ob es sich um atome, Molekule oder Ionensets handelt). Mit den Sammeldingen (als Mengen) tritt die (bei Einzeldingen nich anwendbare) Grösse "Mächtigkeit" oder "Anzahl" auf. (Weninger, 1987, p. 260)

Henadenmenge, Henadenaggregat, Normhenadenmenge and Normhenadenaggregat were introduced by Weninger as names of systems of elementary entities in a discontinuous perspective. According to Weninger the physical quantity is *number* and the important counting unit within chemistry is 1 hen ≈ 6,022045(31)· 10^{23} (Greek, εν, hen = one). According to Dierks, Weninger and Herron the name follows the idea of naming the atomic mass unit, 1u.

> The Latin root "unus" for "unit" says that there is only one unit when measuring the mass of atoms or group of atoms. When counting sets of atoms or groups of atoms chemists use besides the natural unit "1" only one unit else: 6.022045(31)·10^{23} (hen replaces L_0 or L which we used formerly). (Dierks, Weninger & Herron, 1985, p.1022)

The turn from the continuous to the discontinuous view of matter makes a leap from the category 'substance' (Ger. Stoff) to the category 'thing' (Ger. Ding). Weninger points to the important distinction between 'Aggregaten' (aggregates; things) which have a general meaning and 'Stoffmengen' (measure of substances) which are substance dependent:

> Die Stoffmenge wurde nur eingeführt, um einem Klischee gerecht zu werden. Anders ausgedruckt: Sie wurde eingeführt, weil die Klischeevorstellung von der unbedingten Notwendigkeit stoffkennzeichnender Intensitätsgrössen den Blick dafür verställt hat, dass man diese bei *Sammel*dingen nicht braucht. Wer nicht von Stoffportionen spricht, sondern von Henadenaggregaten, spricht auch nicht von Stoffen, sondern von *Dingen*; und für diese benötigt er keine *stoff*kennzeichenden Grössen. Hinter dem Klischee steht die Unklarheit über den Unterschied zwischen dem Denken im Kontinuum und dem im Diskontinuum beziehungsweise zwischen dem Denken in Substanzen und dem in strukturierten Systemen. (Weninger, 1987, pp. 261-262)

By excluding *amount of substance* and only looking upon substances as structured multi-atomic aggregates, *number* of elementary entities becomes the natural quantity, carrying with it simpler mathematical relationships in stoichiometry. In the equation

$$m_1 \text{ (X-aggregate 1)} = m \text{ (1 X-atom)} \cdot N_1 \text{ (X-aggregate 1)}$$

the total mass m_1 of an aggregate is a multiple (the number, N_1) of the mass of the actual elementary entity, m, in that aggregate. It could also be expressed as, the total mass is proportional to the number, N_1, of elementary entities with the mass m. The proportionality constant is the elementary entity mass, m. However, it is in fact a scaling up from one X-atom to X-aggregate 1.

Since *number* is the neutral element in the system of physical quantities, a division of a quantity, Q, by number gives the same dimension as the quantity Q; dim (Q/N) = dim Q. Hence, by using *number* all molar quantities will disappear.

> Das ist erheblich einsichtiger als der in der Chemie übliche Gebrauch von sogennanten molaren Massen: Die Atom- und Molekülmassen werden im Unterricht verwendet und sind damit bekannt, bereiten also keine Schwierigkeiten; und die nur auf eine unzulässige Weise einzuführenden Grössen "Stoffmenge" und "AVOGADRO-Konstante" und die ebenfalls nur auf eine unzulässige Weise einzuführenden stoffmengenbezogenen Massen (und stoffmengenbezogenen Volumina) brauchen gar nicht erst eingeführt zu werden.). (...)
>
> Wir können also die eigentlich interessirenden Anzahlen ohne die Stoffmengen einführen (nicht aber die Stoffmenge ohne die Anzahl). Damit ist es von vornherein nicht erforderlich, die Stoffmenge und alle anderen mit dieser zusammenhängenden Grössen einzuführen. Nur das Festhaltenwollen an Klischeevorstellungen kan erklären, das dieser Sachverhalt von vielen nicht zur Kenntnis genommen wird. (Weninger 1987, pp. 261 and 263)

Weninger's position is illustrated by Fig 6.1 (see next page).

Weninger states, like Wallot, the demand of phenomenal physical significance of a physical quantity. A physical quantity must be empirically founded. However, a physical phenomenon should not be mixed up with a physical quantity, which is a mathematical abstraction.

Base physical quantities, as well as derived physical quantities, are stipulative definitions. They are not reality itself.

> So ist zum Beispiel die Urgrösse "Volumen" nicht die dritte Potenz der Länge, sondern die Eigenshaft der Dinge, ein Raumstuck zu erfüllen (...). (Weniger,1987, p. 274)

Weninger makes a didactical statement in relation to this exposition.

> Der unterricht hat hinsichtlich der phänomenologischen Definitionen meiner Meinung nach bisher viel versäumt. (Weninger, 1987, p. 275)

The leap between the phenomenal reality (Ger. 'phänomenologische Wirklichkeit') and the mathematical construction of reality means an abstraction where a bit of "realness" is lost.[72]

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[72] Inversely, educators' demand of 'concreteness', stressing 'the mole' as "the chemist's dozen", obscures the attainment of the mathematically continuous physical quantity *amount of substance*.

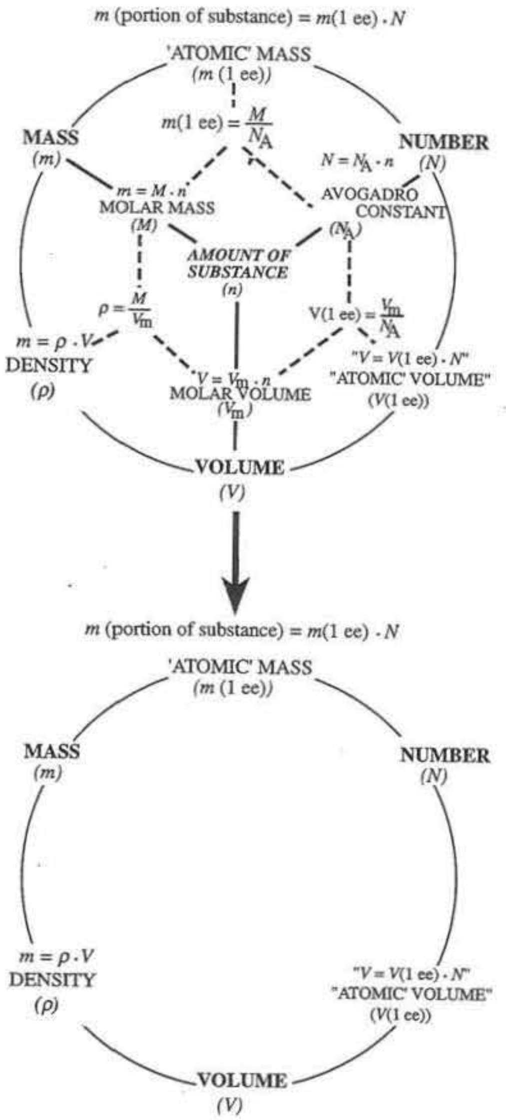

Fig 6.1 The disappearance of the molar quantities when *amount of substance* is deleted.

Weninger's criticism of *amount of substance* has hitherto met little sympathy in the scientific society. The resistance against an acceptance of Weninger's standpoint is risen by upholders of the scientific conventions who support the decisions made by the international organisations GCPM, IUPAC, and ISO. Since, in his opinion the simplicity and logical order introduced in stoichiometry by using number and excluding *amount of substance* is obvious, he indicates possible future research:[73]

> Warum sich so viele gegen einfache Einsicht so hartnäckig sperren, ist ein Phänomen, dessen sich die Wissenschaftssoziologie vermutlich einmal annehmen wird.

The low acceptance or even consideration in the scientific society of Weninger's criticism of the physical quantity *amount of substance* is probably a demonstration of the strength of tradition. It is an example of the fact that rationality, logic and empirical findings do not immediately decide issues in a scientific discourse but create a powerful resistance against novelty, within the reference frames of the accepted tradition (cf. Popper, 1957, 1963; Polanyi, 1958a).

However, some comments on Weninger's proposal will be presented here. In 1977/1978 Merkel (1977a,b; 1978a,b) made a broad exposition of the use of the physical quantities and units in SI. Merkel (1978) stated,

> Betrachtet man die Teilchenantal N als eine Gröl̈e, die keine Zurückführung auf eine andere Größe bedarf, kan man die Stoffmenge über die Teilchenanzahl definieren:
>
> $$n(\mathrm{X}) = 1/\mathrm{N}_{\mathrm{A}} \cdot N\,(\mathrm{X})$$
>
> Die Stoffmenge *n* ist proportional der Teilchenanzahl *N*; der Proportionalitätsfaktor ist $1/N_{\mathrm{A}}$. (...). (Merkel, 1978, p. 189)

and as a commentary to that,

> Eine Diskussion ist im Gange, ob man nicht einfacher die Stoffmenge und die Teilchenanzahl als ein und dieselbe Größe betrachten soll, welche die Einheit Mol und Einheit Tau (Zeichen τ) (oder: Stück) hat - ebenso wie z.B. die Masse die Einheit Gramm und die atomare Masseneinheit u hat [5], [10]. Die Größe sollte "Soffmenge" heißen, um den gerade eingeführten Namen nicht

---

[73] [Why so many are stubborn against simple understanding is a phenomena which the sociology of science probably once will examine.]

> wieder zu ändern, obwohl "Teilchenmenge" von der Sache her der bessere Name wäre [5]. (Merkel, 1978, p.190)

Merkel is here referring to Weninger (1970) [5] and Falk (Vortrag 30.11.77, Karlsruhe) [10]

Weninger (1990) states that the discussion with Rang has come to a good conclusion, since Rang (1987a,b; 1988) as Weninger (1990, p. 198) says: "... is of the same opinion (...) that the amount of substance beside number is not necessary in the system of quantities, and that for instance the AVOGADRO-constant is unnecessary."

However, Rang (1988, p. 5) says that in contrast to Weninger (1985) he has emphasised that *amount of substance* is a conceptually enriched representative of the cardinal number (see, also Rang 1985).

Rang(1988) declares that his interest is

> ...die begriffliche Klärung der physikalischen Größe n und dazu benötige ich eine Terminologie, in der Unterschied zwischen einem materiellen Eigenschaftsträger (Körper), einem davon abstrahierten Träger (Portion), einer Eigenschaft .(Portionsmächtigkeit) und einer physikalischen Größe (Portionsumfang) zum Ausdruck kommt. (Rang, 1988, p. 10)

and his conclusion is

> Der Portionsumfang n ist als Räpresentant der Portionsmächtigkeit bei zahlenmäßig Größenwertangaben informativer als die Kardinalzahl N. (Rang, 1988, p. 13)

If a dimensional system does not contain a dimension like *amount of substance* (in Rang's terminology "Portionsumfang") it would be represented by the cardinal number. But this will be a less rich system since number is the neutral element in the dimensional system of SI (cf. the disappearance of the molar quantities above, Fig 6.1). In that way it could not be a base dimension, since the power of a number is a number. And Rang (1988, p. 13) concludes:

> Geht man durch Schaffung einer Basisdimension Portionsumfang zu einem deutlicheren Dimensionssystem über, so erfolgen die zahlenäßigen Größenwertangaben mit der Einheit Mol. An dieser Einheit ist die Größenart Portionsmächigkeit deutlich erkennbar. (Rang, 1988, p. 13)

In the discussion with van Sprang and ten Voorde (1986), Weninger (1990) shows by stringent analysis that their attack against number is resting on incorrect pre-suppositions and if these are removed their criticism will disintegrate.

The educators interviewed in the empirical studies almost completely agreed in conceptualising 1 mol as a number, 'the chemist's dozen'. Thus, they are no significant upholders of the SI definition but of an older tradition. As shown in the empirical results, only 3 out of 54 interviewed educators have made a conceptual change more or less in agreement with the 1971 definition, even if it superficially can look like nearly all have done so.

Hence, it seems as conditions are present for a re-definition of 1 mol as a symbol for the number $6{,}022\cdot10^{23}$. Weninger (1987) excludes this possibility since:

> Dieser Weg ist aber wohl nicht gangbar, weil man neue Einsichten nicht mit alten Vokabeln verbinden darf, wenn die Kommunikationspartner nicht immer wieder zu den alten Auffassungen verführt werden sollen. (Weninger, 1987, p. 285)

In Weninger (1990) this conviction is repeated:

> Das Nichtunterscheiden der Stoffportion "1 mol (alter Art)" und der Soffenmengeneinheit "1 mol (neuer Art)" zeigt, wie misslich es ist geläufigen Wörtern eine neue Bedeutung zuzuordnen: Das alte Wort ruft immer wieder die alte Bedeutung wach und führt so zu Missverständnissen. Das ist auch der Grund dafür, das ich nicht empfehlen kann, das Wort "Mol" noch einmal umzufunktionieren und diesem die Bedeutung einer Zahl zu geben - obwohl das der einfachste Weg aus allen Schwierigkeiten wäre: Der Gebrauch des alten wortes in einer noch einmal geänderten Bedeutung wurde bei vielen zu noch mehr Missverständnissen führen. (Weninger, 1990, p. 202)

This attitude towards the change of meaning of terms are very much applicable to the introduction of *amount of substance* and the new meaning of 1 mol in 1971. The results of the empirical studies show that next to none of the interviewees have left their old conceptions behind them, instead, the new terms are impaired by the old conceptions. The general supposition of Weninger, about the disadvantageous use of old concept-words for new senses and references, thereby gain support from the empirical results of this investigation.

CHAPTER 7

TOWARDS A THEORY OF CONCEPT ATTAINMENT

The research focus stated in the introductory chapter, 'Why have the educators not attained the 1971 SI-definition of 1 mol and thereby the physical quantity *amount of substance*?' is now re-established in the light of the empirically identified conceptions of 1 mol and adjacent concepts (chapter 3), the rational reconstruction of the concept formation (chapter 4) and the concept analysis of *amount of substance* and 1 mol (chapters 5 and 6). Out of the encounter between empirical and theoretical considerations a theory of the attainment of scientific concepts is proposed. First, some general assumptions about concepts are discussed in the context of current research trends.

7.1 A non-mentalistic approach

Most traditional research in the psychology of education presupposes a definite cognitive structure to be behind the conceptual behaviour of an individual. Knowledge is supposed to be represented and stored in *schemas*. This term was first introduced into modern psychology by Bartlett (1932) in his research on memory and it was adopted in a modified form by Piaget (1952). The somewhat vague concept was also given a renaissance in the 1970's in research on computer based simulations of human cognition. The notion 'schema' has also appeared renamed as 'frame' (cf. e.g., Minsky, 1975;), 'script' and 'plan' (Schank & Abelson, 1975)

Rumelhart (1975) and Bobrow and Norman (1975) retained the term *schema* and used it originally in a similar way to Kant (1787/1963) (cf. Rumelhart & Orthony, 1977; Rumelhart & Norman, 1978).

Within this perspective Rumelhart and Norman (1978) separated three qualitatively different kinds of learning:

* *Accretion* - the encoding of new information in terms of existing schemata.

* *Tuning* or *schema evolution* - the slow modification and refinement of a schema as a function of the application of the schema. They suppose that this kind of process is the central mechanism in the development of expertise. An adaptation between schema and situations to which it is to apply.

* *(Re)structuring* or *schema creation*. This happens through modelling one schema on another. When confronted by a new situation interpretations are made in terms of existing schemata. An iterative process starts to find the most appropriate schema to fit the situation. If no schema exists the "best" contingent schema acts as a model for modelling a new schema. Their hypothesis is that analogical thinking is essential in learning new fields.

Accretion and tuning are in fact an exposition of the Piagetean concepts assimilation (accretion) and accommodation ((re)structuring or schema creation). Hence, a conceptual change is described as a change of schemata. However, from being static structures in the mind and the major content of memory, packets of specialised procedures in which knowledge is embedded, schema have been abandoned in their traditional form within the PDP-model[74] of cognition. The "static view" of the original schema-model is softened.

> In our case, *nothing stored corresponds very closely to* a schema. What is stored is a set of connections strengths which, when activated, have implicitly in them the ability to generate states that correspond to instantiated schemata. (...). There is no point at which it must be decided to create this or that schema. Learning simply proceeds by connection strength adjustment, according to some simple scheme... (...). As the network is reorganised as a function of the structure of its inputs, it may come to respond in a more or less schema-like way". (Rumelhart *et al.*, 1988, p. 21)

The schema theory in the Kantian-Piagetan tradition, the traditional cognitive science approach as well as the connnectionist (PDP) approach take their point of departure in a brain-based or mentalistic

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[74] PDP= Parallel Distributed Processing, the connectionist approach. Concepts are looked upon as emergent states of neural networks and not as fixed entities.

perspective. The 'schema', the 'units' and 'connection strengths' between 'units' in PDP theory, are supposed to be entities existing in the brain. Those entities are modified during the accretion (assimilation), tuning and reconstructing (accommodation) processes, which is manifested in the conceptual behaviour. These approaches are, so to say, both dealing with the 'hard-ware' and the 'soft-ware' in cognition. The schema model theory and the PDP model are on the fringes of the neurological research on cognition (neural-networks). Furthermore it is related to the Kantian idea of innate categories. The schema model can also be related to the conceptualisation of knowledge as entities that could be transmitted from a sender to a receiver (cf. 'the conduit metaphor', Reddy, 1979).

Within the frames of phenomenography, the mentalistic view is discharged. Nothing is stated about the hard-ware. A conception is constituted in the relationship between a man and a phenomenon and a conceptual shift is a change in that relation. That is, no claims are made about representation of concepts in the mind. Concepts are taken as relationships between man and world as they are manifested in overt communication (cf. Marton, 1981). This relational character accounts for the inter- and intrapersonal variability in sense and reference of concepts due to context and situation (cf. section 3.1.3 and section 7.3 below).

7.2 The trichotomycal structure of concepts

A concept is here treated by its *concept-word* (sign or symbol), *sense* and *reference*.

Frege (1892a, p. 29 (English transl.(1952, 3rd ed. reprinted 1992) p. 59)) separated the objective *sense* (Ger. Sinn), and *meaning* (Ger. Bedeutung, henceforth translated *reference*) from associated subjective individual *ideas* (Ger. Vorstellungen). Frege's project was to create a logical model-theoretic semantics to explicate 'Truth', a relation between language and reality, independent of language users (cf. Jackendoff, 1989, p. 74). However, Frege said:

> [...] we cannot come to an understanding with one another apart from language, so in the end we must always rely on other people's understanding words, inflexions, and sentence-construction in essentially the same way as ourselves. (Frege, 1892b, p. 45 (p. 195))

This statement is an argument for conceptualising *the sense* as a publicly negotiated, intersubjectively agreed *idea* in some speaking community (cf. Wittgenstein, 1967). By this assumption there is no absolute difference between *sense* and *idea*, only a difference of degree.

Reference is the phenomena (instances) giving life-world evidence to the actual concept.

The sense and reference of a scientific concept is established via a stipulative definition, historically rooted and intersubjectively agreed upon, embedded in some theory, and is not some kind of objective eternal Platonian sense beyond any kind of argument.[75]

7.3 The prototypicality of concepts

In a theoretical fashion, Wittgenstein (1953, especially paragraphs 67,71 and 79) made a break with a model of natural concepts as unequivocally determined by definitional features, accounting for necessary and sufficient conditions for category memberships. This initial theoretical challenge of the classical theory of categorisation has been followed by empirical studies which have shown that the members of a category are not equal representatives of a category (cf. Rips, Shoben & Smith, 1973; Rosch, 1978; Smith & Medin, 1981; Lakoff, 1987; Gärdenfors, 1992).

Especially Rosch and her colleagues (Rosch, 1973, 1975,1977,1978; Rosch & Mervis, 1975; Rosch, Mervis, Gray, Johnson & Boyes-Bream, 1976) have shown that ordinary human conceptual categorisation among adults as well as children, is not made in set-theoretical terms by fixing sufficient and necessary conditions for category membership, but in terms of *prototypes* and *family resemblance*. Family resemblance is taken as the extent to which attributes of the actual phenomenon or concept overlap the attributes of known members of the conceptual category (see Wittgenstein, 1953, paragraphs 1:66-71[76]; Austin, 1961; for an overview see, Lakoff, 1987). Family resemblance also accounts

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[75] Concepts isolated from a context can give a doubtful impression of human-free knowledge, autonomously existing, such as the elements in Popper's world 3 (cf. Popper, 1972(1963)).

[76] For an analysis of Wittgenstein's notion *family resemblance* see e.g. , Baker and Hacker (1980).

for the fact that the exemplars of a category do not all share the same properties.

Rosch and her collaborates found that among the elements (members) in a category, one or some exemplars always act as a 'model', a prototype, for the others and the category as a whole. For instance, the category 'bird' is conceptualised by an individual of one of the species belonging to that category. According to Rosch's findings robins and sparrows have such a prototypical function. Moreover, concepts can be categorised in taxonomic hierarchies like superordinate categories (e.g. fruit), basic-level categories (e.g. apple) and subordinate categories (e.g. Red Delicious) (cf. Rosch, 1978; for an overview see Lakoff, 1987). Rosch and her associates (Rosch & Mervis,1976; Rosch, 1978) have empirically shown that basic-level categories form the entry into concept categorisation.

However, criticism has been raised against the simple prototype theory. Other theories have been proposed (for reviews see e.g., Smith & Medin, 1981; 1984; Lakoff, 1987; Medin, 1989; Waxman,1991; Barsalou, 1992,1993; Ashby, 1992). Among these there are variations of 'exemplar theories', where one or all exemplars determine category membership. Categorising a new member is a matching procedure of properties of exemplars from that category.

In other theories the prototype is not a distinct exemplar but a set of frequent properties extracted from exemplars. Concepts are categorised by characteristics, probable features or properties (cf. 'probabilistic models of concepts'; see e.g. Smith & Medin, 1981). In that way membership in a conceptual category is graded.

Another prototype-theory of concepts is *the geometric model* of conceptual categorisation (e.g., Gärdenfors, 1990, 1992). A conceptual category is defined as a *conceptual space* fixed by a set of *quality-dimensions* (cf. Quine, 1960, about *quality space*). Concepts are represented by *convex regions*[77] in the conceptual space represented by a Voronoi-division or classification. The central part of the convex region represent the prototype of the concept (or a prototypical area). The central part of the region can also be an imaginary prototype since the centre of the region specifies prototypicality. The geometrical

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[77] If for every pair of points x_1 and x_2 in a region all points between x_1 and x_2 also are in the region it is called a *convex region*.

model permits estimation of the distance between two objects in the regional space and it is therefore possible to measure their degree of *similarity* (or family-resemblance).

Another approach is the General Recognition Theory accounting for a description of categorisation as a division of the perceptual space into regions, each with its own category label. A categorisation is a determination by the individual of the specific region where the stimulus representation falls (cf. Ashby, 1992).

Osherson and Smith (1981) have proposed a hybrid theory. Each concept is supposed to have a core and an identification procedure. The core accounts for classical categorisation with necessary and sufficient conditions, but identification is made via prototypes. For instance, the core of the mathematical concept, odd number, is the stringent mathematical definition in terms of divisibility, but the decision of whether a number is an odd number is made by matching it against prototypes. The categorial set have definitional features, the prototype has modelling properties within the categorial set.

Lakoff and Johnson (1980, p. 125) have characterised the nature of concepts in relation to the prototype theories in the following way:

> (...) individual concepts are not defined in an isolated fashion, but rather in terms of their roles in natural kinds of experiences. Concepts are not defined solely in terms of inherent properties; instead in terms of interactional properties.
>
> (...) Rather than being rigidly defined, concepts arising from our experience are open-ended. Metaphors and hedges are systematic devices for further defining a concept and for changing its range of applicability.

That is, human every-day categorising is not fixed but can be narrowed, expanded or adjusted relative to our purposes and other contextual factors (cf. Lakoff, 1973). Hence, a concept in action (in an individual) is not predominantly determined by Aristotelian classical definitional (necessary and sufficient) conditions, but by the multifarious dynamic relationships to concepts and conceptions gathered around the actual concept as it is revealed in overt communication, for instance, as it is empirically revealed via an interview.

The empirical findings about ways of categorising natural concepts among individuals stand in sharp contrast to the explicit definitional character of concepts and categorisations used in formal logic, mathematics and science. However, based on the empirical results presented in this thesis it is assumed that, for the individual, even scientific concepts are identified and attained via prototypes.

7.4 Metaphor and analogy as vehicles for the non-linearity of teaching and learning

Small changes or disturbances of physical systems near states of equilibrium are often modelled by linear functions. Incremental learning in relation to a previously well-known domain (a kind of equilibrium state), could also be modelled as a linear process (linear function). Such a linear process corresponds to assimilation in Piagetian terminology.

However, pedagogical experience and research speak against a general (global) linear process of learning, roughly expressed as 'the teaching of a certain concept directly results in learning that concept'. Teaching and learning is not a direct transmission of a package or body of knowledge (cf. Reddy, 1979; about the criticism of 'the conduit metaphor' of learning). If general linearity existed, then all learning would only be some direct memory 'recording', but this is now considered contrafactual.

A distinctive feature of a non-linear physical system is that a small change in some parameter can lead to radical consequences or new and surprising effects (cf. "the butterfly-effect" in chaos theory). The multidimensional complexity of learning processes, like 'aha'-experiences connected with suddenness and abrupt (discontinuous) conceptual attainment induced by some seemingly contingent factor, is probably adequately described as some kind of non-linear process.[78]

Often, metaphorical and analogical reasoning lend initial support for such non-linear processes by bridging previous base knowledge to new target knowledge.

Concepts are dynamically related to each other by metaphor and analogy, both according to sense and reference. Analogy and metaphor bring over structural, functional or topological similarities (invariance) between concepts. This is a kind of morphism. The nature of morphism

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[78] Cf. the possibility to model conceptual change within 'catastrophe theory' (about 'catastrophe theory' see e.g. Woodcock & Davis, 1978).

varies in different analogies and metaphors. Since there is no one to one correspondence between different concepts, the morphisms are only partial (e.g. partial homo- or isomorphism). Here, *metaphors* are taken as *partial morphisms* between concepts in different subject domains and *analogies* between concepts in the same domain. Partial morphism via analogy and metaphor is taken as the general principle of sense-transfer, which is taken to occur by anchoring new concepts (knowledge) to prior known concepts (knowledge).

These properties of metaphor and analogy are assumed as partly responsible for the now taken empirical fact of non-linearity of learning.

Reviews of the role of analogy, simile and metaphor in science instruction is found in e.g. Duit (1991) and Duit and Glynn (1992)[79]. Recently a special issue of the Journal of Research in Science Teaching (1993, number 10) was devoted to the role of analogy in science and science teaching.

Metaphor[80]
In thought-experiments, and modelling experiments a target concept is often modelled by another domain than the one it was meant for. Meaning is supposed to be transferred by a metaphor.

Lakoff and Johnson (1980) argue that human thought processes are largely metaphorical, in fact they even consider the human conceptual system as metaphorically structured and defined. This statement raises the general question: Are there any concepts at all that are understood directly, without metaphor? Lakoff and Johnson answer:

> ... what we are claiming about grounding is that we typically conceptualize the non-physical *in terms* of the physical - that is, we conceptualize the less clearly delineated in terms of the more clearly delineated. (Lakoff & Johnson, 1980, p. 59)

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[79] For use of analogy with modelling, explanatory and heuristic functions in scientific research see e. g. Campbell (1957), Hesse (1966), Leatherdale (1974). For a recent discussion of Maxwell's use of analogy in the modelling of the theory of electromagnetic waves and the kinetic theory of gases see Achinstein (1991, 207ff).

[80] Up to 1971 Shibles (1971) has elaborated an extensive bibliography on metaphor.

Metaphors seem to be used for their relative concreteness. Tangible objects and "tangible" qualities, common or familiar functions or actions, referring to visual or tactile properties (space parameters like up, down, inside, outside; delimitation; container; etc.) (cf. Nyman, 1926, about space-analogies in logic).

The interaction between man and world creates experiences which can be understood non-metaphorically (cf. Rosch 1978, about basic level concepts; cf. Pepper, 1942, pp. 92-93, about 'root metaphors'). Out of this experiential understanding new knowledge is attained via metaphorical or analogical reasoning.

Black (1962) like Lakoff and Johnson (1980), also values metaphor as foundational in knowledge formation:

> Perhaps every science must start with metaphor and end with algebra; and perhaps without the metaphor there would never have been any algebra. (Black, 1962, p. 242)

Algebra can be looked upon as a convenient 'language' to describe phenomena in a logical and clear way without a 'many-word' description, where the essence or the carrying capacity of the idea can get lost or be distorted.

Petri (1986) concurs with Black (1962):

> It is my thesis that metaphor is one of the central ways of leaping the epistemological chasm between old knowledge and radically new knowledge. (Petri, 1986, p. 451)

At least two distinctive theories of metaphor are discerned. The classical and most widely spread is the *comparison theory*, where metaphor is viewed as an implicit analogy or simile (Green, 1971). An implicit comparison is made when saying for instance, 'electricity is a fluid'. The implicit message is a shared fundamental similarity - both move in a fluid kind of way.

The comparison theory implies metaphor to prominently be a matter of language use. A metaphor of the form 'A is B' is comparable to the statement A is like B in certain respects. In that way metaphor describes pre-existing similarities.

> The comparative level of metaphor might allow for extensions of already existing knowledge, but it would not provide a new form of understanding. (Petri, 1986, p. 442)

The other theory, the *interaction theory* of metaphor, accounts for an extension of understanding by creating similarity. The theory is developed by Black resting on the works of Richards (1936).

> It would be more illuminating in some of these cases to say that the metaphor creates the similarity than to say that it formulates some similarity antecedently existing. (Black, 1962b, p. 37)

This view is shared by Lakoff and Johnson (1980). The interaction theory is also in concordance with what is denoted 'generative' metaphor (Gentner & Gentner, 1983; Schön 1983, p. 183; also cf. Oppenheimer, 1956).

Metaphor can alternatively be described as *as if* - thinking dealing with models as heuristic fictions like Vaihinger (1920), also discussed by Schön (1983, pp.182-187).

Black has commented the as-if reasoning in relation to the approaches of Maxwell and Kelvin:

> The difference is between thinking of the electrical field *as if* it were filled with a material medium, and thinking of it *as being* such a medium. One approach uses a detached comparison reminiscent of simile and argument from analogy; the other requires an identification typical of metaphor. (Black, 1962, p. 228)

Theoretical modelling is an activity involving metaphor and analogy. In Black's analysis, Kelvin, Rutherford and Bohr, among other scientists, were working in that way. But:

> In using theoretical models, they were not comparing two domains from a position neutral to both. They used language appropriate to the model in thinking about the domain of application: they did not work by analogy, but through and by means of an underlying analogy. Their models were conceived to be more than expository or heuristic devices. [...] theoretical models (whether treated as real or fictious) are not literally constructed: the heart of the method consists in talking in a certain way. [...] It is therefore plausible to say, as some writers do, that the use of theoretical models consists in introducing a new language or dialect, suggested by a familiar theory but extended to a new domain of application. In theoretical modelling the properties of the source field [...] are better known than those of their intended field of application. (Black,1962, pp. 229-232)

However, the question whether the source field is more or less concrete than the target field is unimportant. Black also points to the fact that there is more to modelling scientific theory than simple every-day metaphor:

> We can determine the validity of a given model by checking the extent of its isomorphism with its intended application. Use of theoretical models resembles the use of metaphors in requiring analogical transfer of a vocabulary. Metaphor and model making reveal new relationships; both are attempts to pour new content into old bottles. But a metaphor operates largely with commonplace implications. You need only proverbial knowledge, as it were, to have your metaphor understood; but the maker of a scientific model must have prior control of a well-knit scientific theory if he is to do more than hang an attractive picture on an algebraic formula. Systematic complexity of the source of the model and capacity for analogical development are of the essence. (Black, 1962, p. 238)

Gentner and Gentner (1983) have carried out empirical studies in the target domain of electricity with the water and the moving-crowd models, respectively, as base domains. Their findings support the 'generative metaphor' hypothesis.

> When the two things seen as similar are initially very different from one another, falling into what are usually considered different domains of experience, then *seeing-as* takes a form that I call "generative metaphor".

Ortony (1975) discusses the notion *particularisation* in relation to metaphorical reasoning:

> [...] it is the language comprehender's digital-to-analog converter; it takes him nearer the continuous mode of perceived experience by taking him further away from the discrete mode of linguistic symbols. What metaphor does is to allow large "chunks" to be converted or transferred; metaphor constrains and direct particularisation. (Ortony, 1975, p. 47)

However, the need of metaphor as a necessary epistemological step in knowledge acquisition has been questioned by Green (1986), who has compared the acquisition of a metaphor with how one "gets" a joke. Telling a joke is something other than giving the argument of the joke.

Analogy

The importance of analogy in science has been demonstrated by Campbell (1957) and Hesse (1966). As a tool in generating scientific theories, analogy was explicitly stated and used by Maxwell (see e.g., Achinstein, 1991). The active use of generative analogies in contemporary scientific research has been demonstrated by the 1991 Nobel Laureate in physics, professor Pierre-Gilles de Gennes, who has modelled analogue qualitative and quantitative order phenomena in magnets, superconductors, liquid crystals and polymers.

According to Szabó (1978) the term analogia (Greek, αυαλογια) was from the beginning a mathematical term meaning proportion. Hellenistic linguistics and grammarians borrowed the term from mathematics. Formally, analogy can be looked upon as the linking of two relationships A:B and C:D (A relates to B as C relates to D, formally, A:B::C:D).

Analogy is often unidirectional or asymmetrical, contrary to the mathematical concept proportion, since the known domain (the base domain) is usually the foundation for the target domain.

As noted above, a metaphor could be seen as an implicit analogy. This is the "comparison" view of metaphor identified and criticised by Black (1962).

Pimm (1981, p. 48) has suggested following links between some figures of speech and mathematical notions (concepts). He has adopted the "comparison" view of metaphor.

Simile (the comparison of one thing with another)	↔	relation (equivalence)
Analogy (a resemblance of relations)	↔	morphism (isomorphism)
Metaphor (change based on an analogy)	↔	embedding (transfer via the morphism of analogy; equality)

A morphism preserves structure, but not content (attributes, meaning). According to Gentner and Gentner (1983):

> The analogy, in short, conveys overlap in relations among objects, but no particular overlap in the characteristics of the objects themselves. (Gentner & Gentner, 1983, p. 101)

Generally, an analogy can be characterised as structure-mappings between systems. It

> ...asserts that identical operations and relationships hold among nonidentical things. The relational structure is preserved, but not the objects. (Gentner,1983, p. 102)

Thus structural stability (invariance) is the main feature of analogy.

Formally analogical reasoning can be described in the following way (cf. Gentner & Gentner, 1983; Issing, 1990).

Concepts in the base domain ($b_1, b_2, b_3,...b_n$) are mapped onto the concepts of the target domain ($t_1, t_2, t_3,...t_n$)

$$R(b_i,b_j)\ ) \rightarrow (\ R(t_i,t_j))$$

$R(b_i,b_j)$ is a relation that holds in the base domain and predicts the same relation in the target domain, $R(t_i,t_j)$

Attributes (A) are not preserved between the two domains

$$(\ A\ (b_i)\ ) - / \rightarrow (\ A(t_i)\ )$$

Relations of higher order (R') are described as

$$R'(R_1\ (b_i,b_j),R_2\ (b_k,b_l)) \rightarrow R'(R_1\ (t_i,t_j),\ R_2\ (t_k,t_l))$$

If one of these relations can be imported to the target domain, the others are strongly predicated.

Noteworthy is the conclusion made by Gentner and Gentner (1983) that it is not possible to:

> ... produce correct distinctions in the target domain unless subjects have grasped these differentiations in the base domain. (Gentner & Gentner, 1983, p. 124)

An analogy is only as effective as the base domain is transparent. A fact with far-reaching educational consequences. There is always a possibility that the use of analogy or metaphor in teaching transfers non-intended and irrelevant details leading to erroneous interpretations of the target domain.[81]The hypothesis entertained in the theory of attainment, presented below, is that the use of figurative language, whether it be metaphor or analogy, accounts for the non-linearity of the conceptual attainment process

7.5 Meta-comprehension

Attainment of scientific concepts is assumed to be supported by *meta-comprehension*. This notion denotes both metacognitive awareness/action and meta-knowledge of science.

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[81] Perhaps this is a key source of 'mis'-conceptions, not fully accounted for in the educational 'mis'-conceptions-research?

It seems to be indicated by the empirical findings study that organising principles on the meta-level are superordinate factors ruling the conceptual behaviour of the individual. The term organising principle is here used to denote the description to 'see' a concept, task, problem or domain under a certain perspective. To interpret, structure and perform a concept is ruled by claiming a special position. Thus, a beneficial approach to science (scientific concepts) is to be conscious of the *strategies* and *epistemological commitments* that are rewarding in scientific reasoning, such as *generalizability* and *internal consistency* (cf. Posner & Gertzog, 1982; Posner, Strike, Hewson & Gertzog, 1982; Hewson & Hewson, 1984; Hewson 1985).The apprehension of the dialectical relationship between science content and the nature of science (cf. Wolze & Walgenbach, 1992) includes working processes in science such as idealisation, limiting case studies and imagistic representation (cf. Nersessian, 1992).

Level II in the pedagogical content knowledge research model accounts for meta-comprehension (cf. section 3.1.2).

7.6 Focus on concept attainment

With the assumptions of concepts and concept learning accounted for above in mind, the question arises: What theories are available for modelling concept attainment?

In literature on science education, concept acquisition is generally looked upon as a *conceptual change*, a notion imported from theories of conceptual processes in scientific research within philosophy of science.

As mentioned in section 2.1, the hitherto dominant theory of conceptual change is a theory elaborated by Posner, Strike, Hewson and Gertzog (1982), (Strike & Posner, 1985; cf. also Hashweh, 1986) which assumes that there are analogous patterns between the scientific conceptual shifts, both as described by Kuhn (1962/1970) and as described by Lakatos (1970), and conceptual change in the individual learner. The theory is also inspired by Piagetan theory (cf. Piaget,1962; 1971). Assimilation is compared to the activities within "normal science" or an existing "research program". Accommodation is looked upon as a "scientific revolution" or a change of "research programs".

> That an accommodation is a radical change does not, however, entail that it is abrupt.(...) Accommodation, particularly for the novice, is best thought of as a

> gradual adjustment in one's conception, each new adjustment laying the groundwork for further adjustments but where the end result is a substantial reorganization or change in one's central concept. (Posner *et al.*, 1982, p. 222)

Posner *et al.* (1982) model conceptual change as dependent on four 'variables' within some 'conceptual ecology' (cf. Toulmin, 1972) of the learner. One variable, *dissatisfaction*, concerns the existing conception and the other three, *intelligibility*, *plausibility* and *fruitfulness* the target conception. Posner *et al.* assume that,

i) there must be *dissatisfaction* with existing conceptions[82]. Dissatisfaction is present when something appears that is contradictory to the existing interpreting structure. As such an *anomaly* creates a "crisis" in normal science (Kuhn), analogously a "cognitive conflict" is released in the learner. Posner *et al.*(1982) seems to look upon this as synonymical situations.

ii) A new conception must be *intelligible*, make sense. Analogies, metaphors exemplars and images are lending initial meaning and intelligibility to new concepts (cf. Ortony, 1975; Belth, 1977; Black, 1962).

> Grasping the meaning of an idea is normally a matter of seeing how that idea is interpreted or applied within a certain conceptual context (...) When an accommodation is required, the difficulty is that the context in which a new idea is to be understood is uncertain. (Posner *et al.*, 1985, pp. 225, 227)

iii) A new conception must appear initially *plausible* and have a capacity to solve the problems generated by its predecessors. It must also be consistent with other knowledge. It is assumed that conceptual change occurs against the learners current concepts, the 'conceptual ecology' (Toulmin, 1972). People's ideas or concepts exist as a result of a process of 'natural selection'. The intellectual environment acts as an ecological niche for conceptual development

> Initial plausibility can be thought of as the anticipated degree of fit of a new conception into an existing conceptual ecology. (Posner *et al.*, 1982b, p. 218)

iv) A new conception should suggest the possibility of a *fruitful* research program, be a resource for solving current problems, to

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[82] This idea was also put forward by Hewson (1981). Similar ideas are presented by Piaget (1964), about 'disequilibrium'; Festinger (1957) about 'cognitive dissonance'; Berlyne (1965) about 'conceptual conflict'. The motivational drive, according to Berlyne, was an 'epistemic curiosity' to solve the actual conflict.

interpret experience and open up new areas of inquiry. Fruitfulness can be internal and external (cf. Gunstone, 1988, p. 87)

Learning is seen as a rational activity, a kind of inquiry where judgements are made on the basis of available evidence. Comprehension and acceptance of ideas are made because they are seen as intelligible and rational.Other features important for conceptual change are epistemological commitments such as explanatory ideals and general views about the character of knowledge like elegance, economy, parsimony, not being ad hoc., etc. Further, metaphysical beliefs about science are influential.The conceptual change approach does not model any specific domain.

Among others, criticism has been raised by Wang and Andre (1991, p. 115) to the fact that no direct measures of dissatisfaction have been made to designate whether this is a necessary condition for conceptual change to appear. Perhaps clearer explanations, increased study, more concrete examples, etc. are responsible for conceptual change. Their own research points in that direction, inducing conceptual change in students by using adjusted science texts. Wang and Andre (1991) conceptualise the approach of Posner *et al.* (1982) as a set of technical prescriptions for conceptual change rather than a theory.

Pintrich, Marx and Boyle (1993) have criticised the approach by Posner *et al.*(1982) for excluding motivational and emotional 'variables' from their notion of the process of conceptual change.

Strike and Posner (1992) have revisited their approach, elucidating their original intentions and present standpoint. Even if some modifications are suggested, their basic idea is unaltered.

According to the assumptions of concepts presented in the previous section, concept acquisitions are more of concept extensions than conceptual conflict, crisis and abolishment of the old or everyday conceptions (cf. diSessa, 1993, p. 109, on development and refinement of p-prims). It can also be questioned if the conditions for conceptual change are similar in scientific research and in educational settings (cf. e.g. Pintrich, *et al.*, 1993, 192-193; Lidner 1993; Caravita & Halldén, 1994). For instance, in the educational setting, predetermined goals accounted for in some curriculum, are supposed to be reached within tight time frames in a classroom. The students' knowledge-status and intellectual environment is not comparable to the researchers'. The students are supposed to attain what is already known by the teacher and written in textbooks. There is no evidence of some necessary parallelism between factors ruling concept formation in scientific research and concept attainment in educational settings. Under such conditions, the metaphor of the student as a "researcher" or "scientist" (e.g. Driver, 1983) have been questioned (Caravita & Halldén, 1994).

To make the distinction clear, theories related to 'conceptual change' in science are here denoted *concept(-ional;-ual) formation theories* (e.g. the paradigm theory of Kuhn, 1962) and theories in educational settings *concept(-ional;-ual) attainment theories*. The distinction is focused on the discrepancy between *formation* and *attainment*. *Formation* of scientific concepts is a process of creating non-preexisting perspectives, an enterprise of scientists within scientific communities. *Attainment* is seen as a process of socialisation to become a participant in a pre-existing discourse. In other words a process of enculturation.

Consequently there is no incitement to presume, that the attainment of a scientific concept necessarily presupposes 'cognitive conflict' or 'dissatisfaction' with existing common-sense conceptions ("pre-/mis-, naive or alternative conceptions") of the actual concept domain with the explicit intention to delete them. As is often described in the literature of science education, cognitive conflict is induced in the learner by arranging "learning by doing"- situations. This is an empiristic approach to knowledge acquisition, with questionable results. The students see what they see from the point of their theory-context.

It is not even necessary that the target concept should be plausible in an initial phase of the process of attainment. In educational settings, the assignments given by the teacher are on the one hand intended to make the learner aware of different possible perspectives and delimitations, and on the other hand to accept a special view, often odd and seldom plausible from an everyday perspective. It is a task of apprehending discourses of science which are usually quite distant from pre-existing perspectives. The mission of the teacher is to intervene in the attainment process by elucidating constraints and extensions of senses and references of the scientific concepts parallel to concepts used in everyday discourse.

A scientific concept is only comprehensible within the context of a scientific theory, viz. scientific concepts are always embedded in theories (cf. e.g., Murphy & Medin, 1985; Vosniadou & Ortony, 1989; Tiberghien, 1994). To attain a scientific concept is to contextualize it within the actual scientific theory (cf. Linder, 1993). Correspondingly, common-sense concepts are contextualised and comprehensible within common-sense theories. This context-dependency explains why conceptual conflicts can emerge when one concept-word is bound to both common-sense and scientific senses (cf. e.g. 'work' and 'energy' which have several senses bound to various contexts).

A scientific approach to phenomena is not self-evident nor can it be taken for granted out of unguided perception. Science is persuasive via theory.

7.7 A theory of concept attainment.

It is here taken as an empirical fact that a focused concept is always related to other concepts, embedded and apprehended in some conceptual context determined by the theory in which it is embedded. Concepts are theory laden.

Let c be a set of concepts, $c = \{c_1, c_2, c_3, \dots c_i\}$. Let **C** be a focused concept in the set c.

A general postulate

For every focused concept, **C**, there exists a set of possible *conceptual localities*[83,84], $\Lambda = \{\xi_1, \xi_2, \xi_3, \dots \xi_n\}$ each one, ξ, consisting of a set of concepts $c_{\xi}C = \{c_1, c_2, c_3, \dots c_i\}$ and a set of relationships $s_{\xi}C = \{s_1, s_2, s_3, \dots s_j\}$ connecting the concepts in $c_{\xi}C$, viz. $\xi_C = \{c_{\xi}C, s_{\xi}C\}$. The ξ_C :s are located in common-sense or scientific theories $\tau_1, \tau_2, \tau_3, \dots \tau_k$.

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[83] Sw. 'konceptuell omgivning'. Possible alternatives to locality are *region, domain, territory, field, surrounding, neighborhood, vicinity*.

[84] The conceptual locality encloses what is jointly among terms such as tacit knowledge (Polanyi, 1958, 1966, 1969), mental model (Garnham, 1987; Gentner & Gentner, 1983) mental images (Johnson-Laird, 1985), conceptual map (Novak, 1980; Novak & Gowin, 1981; Matthews, 1984; Heimlich & Pittelman, 1986; Rumelhart & Norman, 1988), schemata (Kant, 1787; Piaget, 1952 ; Rumelhart & Ortony, 1977), scripts and plans (Schank & Abelson, 1975) horizons (Gadamer, 1972, Merleau-Ponty, 1976;), 'gestalt' (Wertheimer, 1945) cognitive ecology (Toulmin, 1972). The awareness of the differences and non-equivalence of these terms, which rest on widely separated approaches, should not prevent us from seeing one common background of all these notions. All these terms in one way or another connote the fact that a single concept does not exist alone but expands surrounding concepts emerging as relationships with a dynamic structure.

Formally[85]:

$$\forall \mathbf{C} : \exists\, c_{i...l} \wedge s_{j...k} \mid \mathbf{C} - s_{j...k} - c_{i...l}$$

Each *conceptual locality* ξ_C is divided in a proximal and a distal region. The proximal region ($\xi_{c,prox}$) embraces the elements in the superordinate category to which the focused concept belongs. Within the superordinate category concepts are related to each other via family resemblance by sharing topological, structural and functional features.

The distal region ($\xi_{c,distal}$) comprises the concepts and their relationships to **C** outside the proximal region but within the actual theory τ.

Concepts are either in focus or in a conceptual locality, due to intentionality (about intentionality cf. Brentano and Husserl; about 'focus' see Polyani; cf. 'theme' in Gurwitsch, 1964). The relationships in the conceptual locality could be casual, logical-lingual and mathematical.

Non-mathematical relationships can be of the type *(A)... is like ...(B), (A)... is a kind of...(B), (A)... is a part of... (B) , (A) ... is an analogue to ... (B).* Thagard (1992) has suggested that: kind-part relationships have been neglected in research on concept-schemes as they are important for understanding the notion of conceptual revolution:

> Kind and part-whole hierarchies serve to structure most of our conceptual system, providing backbones off which other conceptual relations can hang. Although well known to psycholinguists, the importance of these hierarchies has been neglected by philosophers who have tended to speak of "conceptual schemes" entirely in the abstract. (Thagard, 1992, p. 28)

Mathematical relationships can be of an algorithmic type; e.g. *divide mass with molar mass and you get number of moles;* or of a functional type; such as *y is proportional to x;* $y = k \cdot x$.

The introduction of the term conceptual locality is an attempt to model the dynamic nature of concept attainment. When a concept is actualised in a specific context, a conceptual locality is expanded. A conceptual locality emerges in the encounter between the individual and the specific situation/context. The locality shows both stability and instability according to context. What is stable and what is variable can only be empirically determined.

In a study of conceptions of different cases of physical motion amongst first year students' at a university of technology in Sweden, Svensson (1989) found that:

> The analysis of the conceptualization of the cases of physical motion points very clearly to the very restricted contextual character of the conceptions of the cases. The conceptions are dependent on which aspects and parts of the cases are focused on, and in what order. [...]
>
> The students' starting-point for their reasoning about the cases is not in any conceptual framework or abstract concepts and principles. The students do not try to abstract certain general characteristics but try to describe/explain each case with the help of whatever concepts and principles they have access to and seem to fit the meaning given to specific aspects and parts of the cases focused on. Some of the concepts and principles used clearly have an abstract and Newtonian (or rather post-Newtonian) theoretical character for some of the students. However, they seem to be subordinate to a common sense analysis of the case. Thus, the conceptualisation is very restricted concerning relations to a general theoretical framework (if we do not consider general common-sense thinking as such a framework). (Svensson, 1989, p. 543)

This is evidence for a reasonable assumption that each individual exhibits her/his own *conceptual locality* around a focused concept due to the individual conceptual biography, situation and context (cf. Frege's *ideas*). Accordingly, individual conceptual localities are only revealed by empirical investigations which give evidence that there are contingent attributes and relationships due to the situational and contextual frames. Prototypes and family resemblance of previous experienced exemplars of similar situations, not only within a scientific frame, arouse the actual conceptual behaviour.

A *conceptual locality* determined by overt communication with an individual is an open 'system', including biographical and idiosyncratic elements with vague borders. In a detailed determined conceptual locality, unique situations are included (cf. 'event structures', Nelson, 1977). However, in praxis only a part of a possible conceptual locality with biographical nuances is possible to be considered due to the delimitation of the actual investigation and the research aim. In other words, only partial possible conceptual localities with delimited sets of concepts and their relationships can be considered. From such a

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[85] For every concept **C** there exist concepts $c_{i...l}$ and relationships $s_{j...k}$ such that **C** is related via the relationships $s_{j...k}$ to the concepts $c_{i...l}$.

revealed conceptual locality it can be possible to identity the actual theory in which it is located.

At the attainment of a new scientific concept, a conceptual locality emerges when triggered by some features of the new concept. The primary conceptual locality is a dynamic conjecture, bound to prototypes of some conceptual category due to family resemblance (cf. Rosch & Mervis, 1975). The identification of a prototype of a conceptual habitat seems to be a *perception* of similarity. Prototypes are often themselves in some way *percepts.* The use of the expression 'seeing...as' is a metaphor for the pictorial activity behind the 'modelling' process.

Concepts, building up a conceptual locality, are ruled by some organising principle, a theory and can be adjusted by a number of iterative steps, such as reflection, acting and communication. The acquisition of the new concept is generally a process of different temporal length. Sometimes the acquisition is reported by the respondent as 'sudden'. The suddenness is logical when the process is seen as a discontinuous leap of the type 'on - off'. However, it could also be a change on a sliding scale, implying the presence of a 'floating' conceptual habitat of the concept where an experience of suddenness would not be anticipated.

A salient property of an existing conceptual locality is more or less interia (stability, invariance or conservation) when it has reached a saturation state due to a number of iterative steps. The individual conceptual biography, representing a tradition, is a decisive factor. Inertia of knowledge, the tradition determines the knowledge to be learned and to be used (cf. e.g., 'tacit knowledge', Polanyi, 1958, 1966, 1969).

A stipulatively defined concept **C** (cf. Frege's *the sense*) has a fixed conceptual locality with fixed sense and reference, intersubjectively agreed upon in a specific discourse. Scientific concepts are of that kind.

Let ξ_α be the conceptual locality surrounding a scientific concept α framed by a scientific theory, τ.

The theory τ makes up the scientific context of α, where it has a fixed sense and reference by scientific convention. Two types of attainment of α will be discussed:

Type 1.
α is attained via prior scientific knowledge by analogical reasoning via one or more prior known prototypes, $\beta_1,\beta_2,\beta_3,\ldots,\beta_i$ in the target superordinate concept category $\xi_{\alpha,\mathrm{prox}}$. Analogical reasoning is taken as an act of identifying partial (homo-, iso-) morphism between the senses and judgements about references of α and the actual β. This singles out common properties (specific aspects) between α and β, thereby pointing out their habitat in a common superordinate concept category ($\xi_{\alpha,\mathrm{prox}}$) which is comprehensible within theory τ. Some qualitative properties of α and β are always separate, viz. all concepts in a superordinate category do not share all properties. In that sense the concepts only show *family resemblance.* Accordingly, α must be connected with its unique qualitative properties and reference.

Type 2.
If there is no prior knowledge of the target superordinate category, concept attainment can be executed via some detour of metaphor(ical) reasoning, which anchors α in prior known common-sense or scientific knowledge perhaps initially belonging to a domain separated from the target domain (cf. as-if-reasoning; Vaihinger, 1920; Oppenheimer, 1956; Schön 1983; about root metaphors, cf. Lakoff, 1980).

Let γ be a prototype of a superordinate category separated from the target superordinate category. α could be partially attained via γ or multiple prototypes γ_1, γ_2, γ_3,... in that superordinate category. The metaphor gives a 'hint' or a 'chunk' of initial sense to the target concept. Gradually or suddenly a transition into scientific discourse by some analogy. The scientific concept α is *channelled* to the target! (cf. "bridging analogies", Brown & Clement, 1989). The non-linear and dynamic attainment process is probably different and in some sense unique for each individual. As mentioned in section 7.6, reasoning by analogy or metaphor presupposes metacomprehension since there are potential mistakes to be made if the delimitations of them are not recognised. .[86]

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[86] A brief comparison between this theory proposal and the two theories proposed by, on the one hand Chi, Slotta and de Leeuwe (1994) and on the other Tiberghien (1994) (see also, Tiberghien & Megalakaki, 1995) is to be found in Strömdahl (in progress).

CHAPTER 8

THE STRUCTURE AND DYNAMICS OF CONCEPT ATTAINMENT

8.1 The 1971 extension of the base physical quantities

Before 1971 mathematical physics was structured by the base physical quantities *length (l), mass (m), time (t), electric current (I), thermodynamic temperature (T), and luminous intensity (I_v)* making up a set

$\Phi_{\text{SI pre 1971}} = \{m, l, t, T, I, I_v\}$

and a set of concordant units

$U_{\text{SI pre 1971}} = \{1\text{kg}, 1\text{m}, 1\text{s}, 1\text{K}, 1\text{A}, 1\text{cd}\}$

In 1971 the set of base physical quantities was extended by a new quantity *amount of substance (n)*.

$\Phi_{\text{SI post 1971}} = \{m, l, t, T, I, n, I_v\}$

Hence, the set of base units is extended with one new unit, 1 mol

$U_{\text{SI post 1971}} = \{1\text{ kg}, 1\text{ m}, 1\text{ s}, 1\text{ K}, 1\text{ A}, 1\text{ mol}, 1\text{ cd}\}$

As shown in chapter 4, before 1971 there was no general agreement in scientific society on the meaning of 1 mol. Around 1971 the most common standpoint in Swedish textbooks was that 1 mol was a fixed number (F_2). This conception is still dominant according to the empirical results accounted for in section 3.4.2. In view of this fact, the following analysis is delimited to the conditions for the attainment of F_2 and F_3

In the following section the attainment of F_2 is modelled via the proposed theory. In next section a theoretical description of the attainment of F_3 is given via the same theory. This is followed by an analysis of the conditions needed for an attainment of F_3 when F_2 is already attained. This will make it possible to give an answer to the main research question of this thesis: Why have the educators not attained the SI definition of 1 mol from 1971? The concluding section

of this chapter is devoted to a brief analysis of two recent papers on 'the mole' by Staver and Lumpe (1993; 1995). This analysis is as an example of how the results of this thesis can be used.

8.2 The attainment of 1 mol as a number (F_2)

With the acceptance of the atomic theory, 1 mol was concurrently categorised as a fixed number, Avogadro's number. Hence, 1 mol belongs to the superordinate category *units of fixed numbers* Ψ={1 dozen, 1 gross, 1 score, 1 ream,...1 mol}.[87] Together with a set of relationships, S_Ψ = {a kind of, analogue, part of,... proportional to} the set Ψ make up the proximal region of the conceptual locality, $\xi_{\text{1mol,(F2) prox}} = \{\Psi, S_\Psi\}$. All of the elements in Ψ have the same dimension, the physical quantity *number* being the steering factor in the distal region, $\xi_{\text{F2, distal}}$. For instance 1 mol is directly convertible to dozen by a conversion factor (1 mol = $(6.02 \cdot 10^{23}/12)$ dozen).

This attainment procedure is confirmed in the empirical data where the respondents typically reveal that 1 mol was not attained via general properties (necessary and sufficient conditions) but via a prototype in Ψ. Empirical evidence for this is provided by statements of the form: "suddenly I realised that 1 mol *is like* a fixed number" (cf. M10, MS, MA and TY, all accounting for revolutionary shifts into F_2 ; cf. also UB, Apendix III). 1 mol is channelled to and comprehended within the superordinate category Ψ, often by analogy with 1 dozen, which is the predominant prototype of the category. 1 mol is often referred to as 'the chemist's dozen' (a 'big dozen'). This is an analogy of sense. Reference analogies are of the type "1 mol carbon atoms are like 1 dozen tennis-balls".

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[87] Contrary to the other elements in the set, the numerical value of 1 mol is approximate if 1 mol is identified with an experimentally determined value of Avogadro's number.

Schema 8.1

The category character of F_2, 1 mol as belonging to the category units (names) of fixed numbers (dimension: number)

	Concept	Relationship	Prototype
Sense	1 mol		1 dozen
	molar mass (the mass of 1 mol)		'dozen mass' (the mass of 1 dozen)
Reference	1 mol atoms of sulphur	is partially isomorphic with	1 dozen tennis balls
	number of moles		numbers of dozen
	the mass of 1 mol elementary entities		the mass of 1 dozen objects

8.3 The attainment of 1 mol as a base unit of the base physical quantity *amount of substance* (F_3)

If *amount of substance* (n) is focused the proximal region of the conceptual locality is the superordinate category base physical quantities, Φ ($n \in \Phi$), and a set of relationships, S_Φ (an element in that set is e.g. proportionality), $\xi_{\mathrm{n,\ prox}} = \{\Phi, S_\Phi\}$, within the framework of the theory of physical quantities and their units, $\tau_{\mathrm{phys\ quant}}$.

Hence, *amount of substance* is attained via partial isomorphism with one or more prototypes from the set Φ. For example *amount of substance* is partially isomorphic with mass (e.g. their metric structures are isomorphic with the positive real numbers $\mathbf{R}_+$). On the other hand, the qualitative properties of the concepts are totally different, they are incommensurable (dimensionally independent). This is an essential property of base physical quantities. However, via proportionality (an element in S_Φ), they are related to each other by the relationship $m = M \cdot n$.

The adherent SI unit of the physical quantity *amount of substance* is 1 mol. If 1 mol is in focus the proximal region of the conceptual locality is the superordinate category $\mathbf{U}$= {1 kg, 1 m, 1 s, 1 K, 1 A, 1 mol, 1 cd} and the relationships between them, S_U, viz. $\xi_{\mathrm{1mol,(F3)\ prox}} = \{U, S_U\}$. 1 mol is attained through partial isomorphism with the elements in U via some prototype. For instance, 1 mol is partially isomorphic with 1 kg since they are units of base physical quantities.

The individual qualitative senses and references of the quantities and units are gained via the SI definition of the actual unit. In that respect the different quantities and units only share family resemblance within the superordinate categories, Φ and $\mathbf{U}$. They are incommensurable.

Schema 8.2

The character of F_3, 1 mol as the SI-unit of the base physical quantity amount of substance.

Concept	Relationship	Prototype[88]
1 mol	is partially isomorphic with	1 kg
a SI-unit u_i		a SI-unit u_j
amount of substance		*mass*
a physical quantity Q_i		a physical quantity Q_j

The salient features of base physical quantities like e.g. *length, mass and electrical current* are:

* that they connote properties which have apparent physical significance or reference.

* that they are measurable with unique instruments

Two questions arise about *amount of substance* according to these features:

What property is measured by *amount of substance*?
What instrument is used when measuring *amount of substance*?

As shown in chapters 5 and 6 *amount of substance* is a mathematical idealisation (introduction of mathematical continuity) of the measure of

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[88] The prototype (1 kg) is here radomly chosen within the set of base units in SI. Any other unit among the SI base units would have been possible.

number since a general proportionality between them; $n \propto N$ always holds. In some foundational sense n and N are measuring the same underlying property (cf. the text of the 1971 definition of 1 mol).

The fact is that there is no general instrument to measure the base physical quantity *amount of substance,* at least not in an equivalent sense to e.g. an ammeter to measure *electric current*. Both *amount of substance* and number are determined (calculated) via measurement of the macroscopic and atomic masses of pure substances. According to these circumstances the substance dependence of the base physical quantity *amount of substance* is evident.

8.4 Demands for attaining 1 mol as a unit of the base physical quantity *amount of substance*

A transition from F_2 into F_3 means a leap from 'the mole' as a fixed number of elementary entities within discontinuous physics into the structure of base physical quantities within continuum physics. This process could not be described as a question of dissatisfaction with F_2 or cognitive conflict between F_2 and F_3. It is a conceptual extension, a redefinition from $1\ \text{mol} = 6.02 \cdot 10^{23}$ with the category habitat *units of fixed numbers*, to 1 mol as a unit for the base physical quantity *amount of substance*. To make a transition into F_3 is to change the categorial habitat of 1 mol. It is a change of theory and of language use. To reach the new category habitat the existence of the base physical quantity *amount of substance* must be apprehended. 1 mol can only be comprehended as a base unit if there exists some dimension for which it is a unit. For example 1 m is only comprehensible as a base unit of the dimension *length*. The dimensions precede the units. Thus, first *amount of substance* must be attained via some prototype in the set Φ. Second, 1 mol, as a unit for the base physical quantity *amount of substance* is attained via a prototypical member of the target categorial set U.

Schema 8.3.

Comparison of the conceptual habitats for 1 mol as a fixed number and 1 mol as a unit for the base physical quantity amount of substance.

F_2	F_3
1 mol	1 mol
concept category:	**concept category**:
units of numerical quantities (alt. units of fixed numbers, multiple units of number)	base units of SI
prototype:	**prototype**:
one among the members (elements) in the set	one among the members (elements) in the set
Ψ={1 dozen, 1 gross, 1 ream,..., 1 score}	U={1 m, 1 kg, 1s, ...,1 cd)
sense:	**sense**:
1 mol ($6 \cdot 10^{23}$) is an analogue to 1 dozen (12). Both are fixed numbers and of a commensurable dimension (number)	1 mol is an analogue to 1 m as a consequence of both being SI-base units, but of incommensurable dimensions.
Dimension of **1 mol**: *number*	Dimension of **1 mol**: *amount of substance*
Dimension of **1 dozen**: *number*	Dimension of **1 m**: *length*
Reference to natural systems:	**Reference** to natural systems:
a unit ($6 \cdot 10^{23}$) for 'number of elementary entities' measured by the physical quantity *number*	a unit for 'number of elementary entities' measured by the mathematically continuous physical quantity *amount of substance*

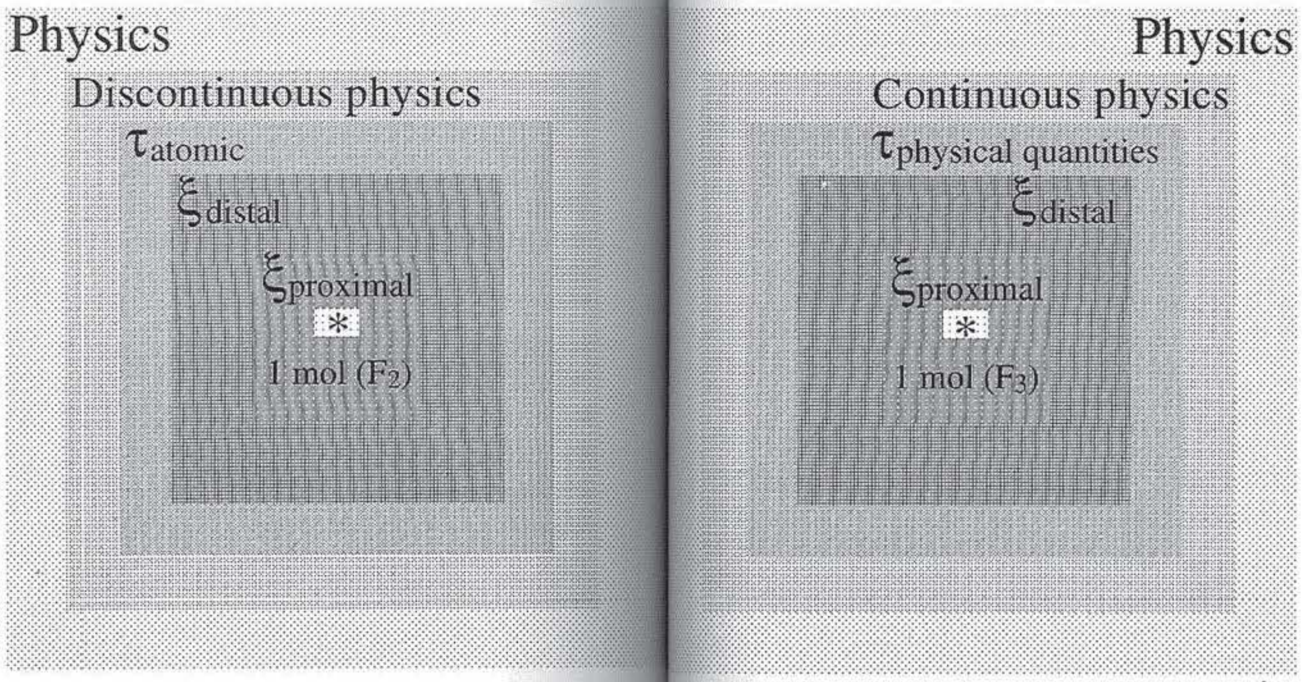

Figure 8.1 The transition $F_2 \rightarrow F_3$.

This figure aims at elucidating the two different categorical habitats of 1mol (F_2) and 1 mol (F_3) and the dynamical shift between them.

Both categorisations are embedded in physics (physical chemistry). 1 mol (F_2) belongs to discontinuous physics and 1 mol (F_3) to continuous physics. 1 mol (F_2) is embedded in the atomic theory (τ_{atomic}). 1 mol (F_3) has its direct habitat in the theory of physical quantities ($\tau_{\text{physical quantities}}$). The conceptual locality of 1 mol (F_2), $\xi_{1\text{mol}(F2)}$, is structured by the distal region, ξ_{distal}, with *number* in focus and the proximal region, ξ_{proximal}, comprising the categorial set $\Psi = \{1 \text{ dozen}, 1 \text{ gross}, 1 \text{ ream}, \ldots 1 \text{ mol}\}$ and the relationships between the elements in that set , S_Ψ.

On the other hand the conceptual locality of 1 mol (F_3), $\xi_{1\text{mol}(F3)}$, is structured by the distal region ξ_{distal} with the set base physical quantities, $\Phi = \{m, l, t, T, I, n, I_v\}$, and their relationships, S_Φ, in focus and the proximal region, ξ_{proximal}, comprising the categorial set of base units $U = \{1 \text{ kg}, 1 \text{ m}, 1 \text{ s}, 1 \text{ K}, 1 \text{ A}, 1 \text{ mol}, 1 \text{ cd}\}$ and the relationships between the elements in that set, S_U.

If F_3 is going to be attained when F_2 is already attained implies that the interpretative frame must be extended to enclose continuous physics, the theory of physical quantities, the apprehension of the base physical quantity *amount of substance* and 1 mol as a base unit for that quantity. To change between the two categorisations is a sort of shift of 'gestalt'.

A comparison of the categorisations in schema 8.3 are briefly outlined. The transition is a non-linear, qualitative conceptual step. But this does not mean that the previous structure must be deleted. The concepts can live side by side but there must be an awareness of their different contexualizations. This means that it is possible to communicate parallel conceptions of the concept 1 mol, as confirmed by our empirical results (e.g., M3, M10, U1).

The categorical habitats of 1 mol in F_2 and F_3 are also illustrated by the figure 8.1. The shadowed areas denote concepts and their relationships according to their categorical habitat.

8.5 Why is the SI definition of 1 mol from 1971 not attained among the respondents ?

The respondents' frame of interpretation

The 1971 SI definition of 1 mol was founded on a convention (a didactic decision) to provide coherence, not a conceptual solution to an accumulation of anomalies about the observation of matter. Nothing has made the traditional apprehension of 1 mol as a fixed number (Avogadro's number) of elementary entities within the frames of the atomic theory, τ_{atomic}, invalid or obsolete. The atomic theory is still in charge. Hence, there are good reasons for the respondents to cling to F_2, since 'natural thinking' is in accordance with *number* as a measure of the size of the particularity of matter. The strong connection between the corpuscular explanation of the chemical reaction and the measure of particularity by the physical quantity *number* is decisive for conceptualising 1 mol as a unit of number. The number of atoms is a salient, relevant property accounting for chemical reactions as rearrangements of numbers of elementary entities. It is 'concrete', 'tangible' and 'functional' and is a sensible explanation of the stoichiometric laws viz., the invariant proportions of masses and volumes of substances involved in chemical reactions.

1 mol as a fixed number elementary entities is also in accordance with the strong pedagogical ideology of *concretion.* According to the empirical data, teaching and learning 'the mole' stresses analogies made 'tangible' via material models. 'The mole', the huge number ($6.02 \cdot 10^{23}$) of elementary entities (atoms, molecules, ions, etc.), is often pointed out as an analogue to fixed numbers like 1 dozen, often 'materialised' and made perceptual by real models such as 1 dozen marbles, beads, tennis-balls, screws, buttons, oranges, etc. . In accordance with this analogy, 'the mole' is referred to as 'the Chemist's dozen' in order to relate to the students' 'life-world' experiences. This is an indirect ostension via reference-analogies since the target 1 mol of elementary entities is hidden from our senses (this became evident for e.g. educator M1 during the interview). The analogy fulfils the demand of the pedagogical ideology of teaching 'the real things', however indirectly.

A vast majority of the educators in the empirical studies have obtained their elementary education in chemistry before 1971. The results of the interview studies provide empirical evidence for sustained conceptions about 'the mole' from his/her own education. If there is some change, it is towards F_2, since 'the mole' is generally approached within the framework of atomic theory (cf. Appendix III).

The respondents' encounter with the SI definition of 1 mol

According to the respondents interpreting framework as described above, their interpretation of the SI definition of 1 mol is evidently mainly made within F_2 and framed by atomic theory, τ_{atomic} .

With this interpreting frame it is intelligible that some of the educators explicitly regard the 1971 definition of 1 mol as a too complex, too wordy and an unnecessary circumlocution of the fact that 1 mol equals Avogadro's number. With this 'taken for granted', the definition is too difficult to use in practice and is therefore dispatched. The interpreting frame is firm, which is illustrated by the interview with M4. After some discussion about interpreting problems and interpretative frameworks and definitions, the interviewer let him read the SI definition of 1 mol in a text-book in chemistry. His conclusion came immediately without any hesitation "It is a number".

Moreover, according to the statements of the educators, scientific definitions per se are looked upon as rigid, too complex and of no practical use (for confirmatory statements see Appendix III). The opinion among several educators seems to be that scientific definitions must always be simplified to be comprehended by the students both in upper secondary school and at the university (and evidently also by themselves).

The educators agree that the scientific definitions must have a detailed and unequivocal semantic structure and wording. However, there seems to be a tendency for them not to really bother about the scientific definition and to ignore the demands to penetrate this complex structure. Idiosyncratic simplifications are dominant. Such simplifications distort and mystify, evidently leading their users missing the intended meaning of the definition. The educational demand of simplification comes into conflict with the scientific demand to reach an understanding on intrinsically scientific grounds. The 'practical' need of 'the mole' in stoichiometry is typically stressed by the educators. - Further, they have no incentive to make a unprejudiced interpretation of the 1971 definition of 1 mol, distinct from the traditional 'taken for granted' conception because this conception works. The apparent closeness between $1 \text{ mol} = 6.02 \cdot 10^{23}$ and '1 mol is proportional to $6.02 \cdot 10^{23}$' is a sophisticated distinction to make against an internalised conceptual tradition of 'the mole' as 'the chemist's dozen'.

The original scientific definition of 1 mol is only intended for the 'purists', not for the 'practical chemist' (cf. e.g., UL, UM and US in Appendix III). The definition is not even examined on its own terms at the university level. Who should use the scientific definition? According to our empirical results: Nobody!

The fact is, that the intended meaning of the definition of 1971 is not even noticed by the respondents because of their persistent interpretative frames.

Two exceptions

There are two exceptions among the educators in our empirical studies. M3, who dutifully accepts the SI definition in analogy with the other SI definitions of base units, and U1 who had actively searched for a physical quantity of the unit 1 mol, and was quite satisfied when the SI definition appeared in 1971. The organising principle of base units and base physical quantities was decisive for U1's standpoint. The conceptual shift for U1 into F_3 was ruled by the organising principle that the unit 1 mol must be connected to a physical quantity in alignment with other units in SI. However, neither of these two chemists, explicitly talk about *amount of substance* as a numerically continuous physical quantity.

A non-awareness of the theory of physical quantities

In the empirical data there is nothing to indicate that the respondents consider the continuous/discontinuous perspectives of the actual concept domain. Thus, the nature of physical quantities as continuous variables is not brought up in the interviews.

There is no explicit interpretation and conception of *amount of substance* as a base physical quantity comparable to *length, time, temperature,...* etc. Thereby 1 mol is not interpreted as a unit similar to the units 1 m , 1 s, 1 K,... etc., even if there are statements about 1 mol as a SI-unit in some general sense.

In these circumstances an attainment of 1 mol as an SI unit for a continuous variable, *amount of substance*, is far-fetched and is not even a reflected possibility. As mentioned above, the scientific definition is not thematized and analysed in a manner which would allow the sophisticated nature of *amount of substance* to become apparent. From the perspective that all chemical phenomena are interpreted as corpuscular events within the atomic theory, this absence of reasoning about 1 mol as a unit for a continuous variable *amount of substance* is comprehensible.

Reasoning about quantity calculus among the respondents is limited. Instead the respondents are talking about how to use the correct units in calculation, how to cancel some of them, ending up with the final correct unit (factor-label method). For instance, M12 and M2 have not solved the inconsistency of molar mass as the mass of 1 mol and molar mass as a physical quantity, but cover it up by accepting 'molar mass' as satisfying the demands of unit analysis.

A dominant pedagogical idea is that the most simple ('concrete') logic and mathematics as possible should be used. As mentioned above, calculation in stoichiometry is generally made in the logical schema 'if... then' manifested in the 'rule of three'. This means that there is more logical reasoning and compartmentalisation than using the general mathematical relationship proportionality. The possibility of *mathematical integration with other areas of chemistry, biology and physics* is not noticed. The algorithm 'rule of three' is accepted without reflection, the manipulation is instrumental. The criteria of success is simply determined by getting correct answers to stoichiometric exercises. Praxis and procedural goals are stressed. By using the 'rule of three', the functional aspect of proportionality is only implicit, meaning absence of the advantages of quantity calculus as a unifying, integrated mathematical structure in scientific calculations including stoichiometry. The usage of the proportionality relationship in the algebraic form of $y = k \cdot x$, is seldom noticed in this context.

The specific general use of the 'rule of three' in stoichiometry compared to other areas of the natural sciences ought to be subjected to an investigation of its own.

The existing tradition communicated by the educators about 'the mole' framed by the atomic theory reveal an absence of tools for handling the sophisticated definition of 1 mol in SI. As mentioned above attainment of the SI definition of 1 mol has to be made in a theoretical context separated from discontinuum physics, namely the theory of physical quantities, $\tau_{\text{phys quant}}$, which belongs to continuum physics.

Since the necessary prerequisites not seems to be present, there is no possibility for the educators to attain F_3.

Conflicts between scientific and educational demands
The empirical data indicates that the respondents are more guided by educational demands than by the demands expressed by scientific conventions. As mentioned above, the contemporary scientific definition of 1 mol is not conceptually thematized in depth nor made explicitly available in the educational setting.

Instead, driven by the educational ideology of concretion, the educator tries to find a 'concrete' practical strategy to teach the mole with the immediate intention to solve 'real' stoichiometric problems and exercises (cf. the quotations in Appendix III).

The conceptual step into F_3 is an abstraction opposing the pedagogical ideology of concretion. Thus, there is a double hindrance toward the conceptual shift $F_2 \rightarrow F_3$, not only regarding the scientific status of *amount of substance* as being a continuous physical quantity, but also the educational ideology of concretion. Since a conception in accordance with F_2 work in practice (giving right answers to exercises) there is no incentive to conceptualise 1 mol as something other than identical to a fixed number (Avogadro's number).

As mentioned above, the attainment of *amount of substance* and 1 mol within the contemporary scientific categorisation is not an act of creating a 'cognitive conflict' and deleting the traditional categorisation, rather it is an act of a meta-comprehensive adoption of a new approach. The different categorisations can be attained separately and live side by side. However, there must be some meta-comprehension of the fact that they are differently contexualised when used in different discourses.

The non-attainment as related to the mol-controversy
The intuitive criticism of educators' against the physical quantity *amount of substance* is in alignment with the elaborated criticism delivered by Weninger (cf. above). This is perhaps an additional argument for the bodies of IUPAC to make some comments, in a future revision of the IUPAC manual, to elucidate the nature of the physical quantity *amount of substance*.

8.6 A case study - two recent articles on the conceptualisation of 'the mole'

In the final section of this chapter, a brief analysis of two research papers will be made to test the potential of the instruments elaborated in this thesis. The criteria for the selection of which texts to consider has been that these papers are amongst the most recent research papers on ´the mole´ known to me. Searching in the latest volumes of the international journals in science education in March 1996, two papers by Staver and Lumpe (1993) and Staver and Lumpe (1995) were found. The first study is a content analysis of the presentation of "the Mole Concept" in 29 American chemistry textbooks[89] for high school and introductory college levels and the second comprises two investigations on student's understanding of "the Mole Concept" and its use in problem solving. The present analysis is limited to identification of the interpretative frame for 'the mole' as it emerges in the papers.

Staver and Lumpe explicitly adhere to the SI definition. However, there are some indicators in the text that they to some extent are deviating from the SI definition.

1) The authors use the expression "the Mole Concept" throughout the texts. This is contrary to the recommendations in the IUPAC manual (Mills *et al.*, 1993). By denoting the mole as a concept, indistinctness emerges. This is illustrated by comparing one of their sentences with a sentence where *amount of substance* is substituted by *length* and *mole* by *metre*.

> Amount of substance is not only a physical quantity, it represents one of seven standard units of measurement defined by the international system (SI). Named the *mole*, the SI unit of measurement for amount of substance is one of the most fundamental concepts in science. (Staver & Lumpe, 1993, p. 322)

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[89] No text had a copyright earlier than 1986. (Staver & Lumpe, 1993, p. 324)

'Length is not only a physical quantity, it represents one of seven standard units of measurement defined by the international system (SI). Named the *metre*, the SI unit of measurement for length is one of the most fundamental concepts in science.'

2) Their version of the SI definition used as a base in their investigations is taken from a textbook by Kotz and Purcell (1987). This states that the mole is "... the amount of substance that contains as many entities...". Their source of information lacks the very important words 'of a system' inserted after "amount of substance". It is the system that contains the elementary entities and not the *amount of substance*.

3) In one section Staver and Lumpe (1995, p. 182) discuss strategies for instruction: "... an emphasis that Avogadro´s constant does not define the mole, but rather is the mole's experimentally determined value. The instructor points out, as does the textbook, that Avogadro's constant, $6.022 \cdot 10^{23}$, is... "

It should be noted that what is here called Avogadro's constant lacks a unit. The correct unit of the Avogadro constant is, according to SI, 1 mol^{-1}. Possibly the authors mean Avogadro's number when they write "Avogadro's constant". But what is most remarkable is that it is stated in the text that $1 \text{ mol} \approx 6.022 \cdot 10^{23}$ ("...the mole's experimentally determined value.").

Moreover, in the conclusion of their paper it is stated:

> At this point we need to emphasize that students who state that a mole contains Avogadro's number of particles or that a mole of substance is its atomic or molecular mass expressed in grams do have the facts correct. (Staver & Lumpe, 1995, p. 189)

Even if they continue the text by saying that the SI definition does not define the mole in either fashion, their interpretative frame for 'the mole' is impaired by earlier traditions in chemistry as formulated in the fundamentals F_1 and F_2 by saying that the students "...do have the facts correct". Their students conceptions, according to the quotation above, are typically coincident with F_1 and F_2.

Staver's and Lumpe's investigations have several merits, but as mentioned in section 1.3, many studies on 'the mole' with the best of intentions to sort out conceptual problems, do not separate the educational and scientific demands. This is problematic. In that perspective Straver's and Lumpe's serious intention to analyse textbooks and students' understandings suffer from a deficiency, since the scientific ground and interpretative frame is uncertain.

CHAPTER 9

EDUCATIONAL IMPLICATIONS

In the introduction a methodological distinction was made between the scientific and the educational domains. After having already analysed of the scientific domain, the educational domain is now focused.

Decisions about teaching and learning stoichiometry in schools are represented in curricula and syllabi. In Sweden stoichiometry is first and only taught to students at upper secondary school on the natural sciences programme, and the technological programme beginning at the age of 16. In some countries the subject matter is prescribed in curricula to younger pupils and to pupils who do not have science as their main line of interest.

On the curriculum level, some questions could be posed (cf. level III in the pedagogical content knowledge research model, see section 3.1.2). Why should stoichiometric calculations be made at all in compulsory and upper secondary schools? What are the educational goals of stoichiometry teaching? Is it necessary to treat the subject matter in a stringent scientific way for those pupils/students who are not choosing science as their main study? Is it meaningful to make stoichiometric calculations for those pupils/students at all?

Independent of the answers to these questions, it seems plausible that if stoichiometry should be taught, the concepts involved should be treated in accordance with correct contemporary conventional science. In serious teaching, deviations from this main rule ought always to be fully accounted for. At least the educator him/herself ought to be fully aware of such deviations.

If the prevailing physical quantity *amount of substance* should be used, it should be used correctly (cf. McGlashan, 1977, p. 276).

If the educational assignment is intended to encourage the students to become participants in contemporary scientific discourse concerning *amount of substance* and 1 mol, this must be attained within the theory of physical quantities and units, $\tau_{\text{phys.quant}}$.

Rather than abolishing earlier conceptions, the issue is to extend the concept repertoire of the learner to include the conventional scientific standpoint.

When educators teach 'the mole' they start with some preliminaries (cf. e.g., Tullberg, Strömdahl, & Lybeck, 1994) making a preparation of a prospective conceptual locality for the implementation of the focal concept, 'the mole'. The target concepts of 'the mole' are then introduced. The student is immediately or very soon confronted by a number of stoichiometric exercises, exemplars or prototypical cases. The educational strategy and tactic is to reach 'praxis' (viz. stoichiometric calculations) as soon as possible. The knowledge of how to use 'the mole' gets priority over knowledge of the conceptual features or the theory context of 'the mole'. Thus, the student is often left with algorithmic knowledge but with no conceptual knowledge of how to handle stoichiometric problems (not exercises). They are given a 'praxis' to handle the stoichiometric problems only.

The findings of the empirical studies show that students have similar conceptions as educators (generally F_2), an expression of the fact that the students have been made participants in a tradition handed over bythe educators.

In contemporary science, quantitative treatment of physical systems imply an application of physical quantities and relationships among these. In introductory chemistry, some of the quantities are base physical quantities, such as *mass* (m), *amount of substance* (n), and *number* (N), others are derived, such as *volume* (V), *molar volume* (V_m), *density* (ρ) and *molar mass* (M). Simple stoichiometric calculations involve an algebraic combination of some of these quantities under reference to some physical system under investigation. Or otherwise expressed, simple stoichiometry can be looked upon as an algebraic structure on the set $Q=\{m, V, n, N\}$.

Within the frames of physical quantities, SI and quantity calculus, the Avogadro constant, molar mass and other molar quantities are comprehensible as derived physical quantities within the coherent theory of physical quantities. In other approaches the different concepts must be explained one by one when they emerge (cf. Avogadro's number and the Avogadro constant and 1 mol sulfur = 32 g sulfur in connection with the common algorithm $n = m/M$).

The use of well-defined concepts, like the physical quantities, seems to be a sound ground for teaching stoichiometry. Furthermore, for pedagogical-didactical reasons there ought to be a strong demand of integrative structures between different science disciplines and mathematics: e.g., proportionality in the form $y = k \cdot x$. An algorithmic treatment of exercises and problem-solving by using 'rule of three' could mean a compartmentalisation of calculations in chemistry compared to calculations in physics. Such a compartmentalisation prevents the advantages of natural integration between physics and chemistry.

As the present educational situation appears in our empirical investigations, conceptual uncertainty exists about 'the mole' and *amount of substance* and is distorting an integrated learning process. Besides, as is shown above there are foundational intrinsic scientific problems connected to the physical quantity *amount of substance*.

As presented in the preface in the IUPAC manual unequivocalness of concepts is needed for an improvement of communication among members of the scientific community (Mills, *et al.*, 1993, p. vii) . This statement ought to be a hallmark also for science teaching and learning in our schools and in undergraduate education.

If *amount of substance* is used as a base physical quantity and 1 mol as a base SI unit, these should be introduced along with the other base physical quantities and units together with proper mathematics (quantity calculus), within the frames of physics.

According to the results of this investigation, two approaches to stoichiometry are possible. These involve calculations, on the one hand made within a continuous, and on the other a discontinuous approach to the quantification of matter. The present situation, as it is reflected through the empirical findings, is characterised by conceptual uncertainty and a mixture between the two. A separation between these approaches as advocated by e.g. Weninger seems to be a foundational step to take, in order to create a clear conceptual ground for learning and teaching.

However, because of the scientific conceptual problems concerning the reference of the physical quantity *amount of substance,* it also seems advisable that introductory stoichiometry teaching could be done within the frames of atomic theory. In an approach to chemistry where the description of matter and chemical reactions is erected on reasoning about rearrangements of numbers of elementary entities, viz. the discontinuity view of matter, making stoichiometric calculations by the quantity *number* becomes very plausible.

The foundational prerequisites for such an approach includes the masses of atoms, measured by mass-spectroscopy as relative atomic masses, and expressed as atomic masses with the unit 1 u ($1u = 1/12\ m(1^{12}C)$), 'ordinary' measured masses (unit 1 kg or 1 g) of substances (looked upon as aggregates of atoms; matter as multiatomic) and the conversion $1\ g = N_0 \cdot 1\ u$. N_0 is the conversion factor between the two units of mass (1 g and 1 u) and could be interpreted as the number of elementary entities, each with the mass 1 u, in a system of these elementary entities with the total mass 1 g.

Even if it is possible to be a skilful practitioner of stoichiometric exercises using *amount of substance* and the SI unit 1 mol, this does not mean that the sophistication of the physical quantity is penetrated. The referential problem about *amount of substance* could still remain undiscovered and unresolved, where with all the stoichiometric calculation would still merely be algorithmic and lacking comprehension. The conceptual difficulty of distinguishing between 1 mol as identical to Avogardo's number and 1 mol as proportional to that number must not be underestimated. Especially when the property one wants to measure is the *number,* in alignment with the common explanation of the chemical reaction as rearrangements of numbers of elementary entities.

An approach using the physical quantity *amount of substance* is a sophisticated step, which could be delayed to a later part in the curriculum. Every calculated number of elementary entities (of a system) in the discontinuous approach could be measured by the physical quantity *amount of substance* by using the equation

$$n = \mathrm{N}/\,\mathrm{N}_0 \cdot \mathrm{mol}^{-1}$$

where n denotes *amount of substance*, N is the calculated number of elementary entities and $N_0 = 1g/1u$. The need to penetrate the conceptual nature of the physical quantity *amount of substance* has been questioned by practitioners as non-relevant in praxis. But the situation is the other way around. By interrogating prevailing scientific sense and reference, an awareness of educational simplifications that are logical, intellectual, scientifically tenable and defensible, and do not do violence to the concept is made possible. What is a simplification worth if the scientific meaning of the concept is not known? From the position of the learner, correct teaching is a legal and moral right.

I now deliver four commented solutions to an elementary stoichiometric problem. Each is founded in a different perspective, including one solution with the correct use of the physical quantity *amount of substance* and its SI-unit 1 mol.

Problem

In a chemical reaction 8.90 g iron (elementary entity Fe) reacted completely with excess oxygen (elementary entity O_2). Calculate the mass of the product di-irontrioxide (elementary entity Fe_2O_3).

Solution 0 (a traditional algorithmic approach)

Chemical equation: $4\ Fe + 3\ O_2$ --------> $2\ Fe_2O_3$

4 mol Fe < ------------> 2 mol Fe_2O_3

1 mol Fe <-------------> 2/4 mol Fe_2O_3

Now 8.90 g Fe is 'converted' into moles (number of moles) by dividing with the 'molar mass' ('the mass of 1 mol') of iron, the numerical value of which is taken from a table (generally the periodic table of the elements) and attached to the unit g/mol in order to get the right unit at the end of the calculation. Then the proportion between Fe and Fe_2O_3 *(1: 2/4) from the chemical equation is applied.*

8.90/55.85 mol Fe <--------> 2/4· 8.90/55.85 mol Fe_2O_3 (1)

The "number of moles" on the right hand side of the arrow is 'translated' (or 'converted') back to mass by multiplying with the actual molar mass (frequently labelled as 'the mass of 1 mol') The molar mass must have the unit g/mol otherwise 'mol' would not cancel when multiplied by (1).

$2/4 \cdot (8.90/55.85) \cdot 159.70\ g\ Fe_2O_3 \approx 13.5\ g\ Fe_2O_3$

Molar mass (M) is used as a 'conversion factor' in the algorithmic treatment of the 'formula' $n = m/M$.

Solution 1 (a continuous approach with the physical quantity *amount of substance* and its SI-unit 1 mol in accordance with quantity calculus)

Given: $m(Fe) = 8.90$ g
$m(O_2)$ excess (there is enough oxygen for all iron to react);
iron is the limiting reagent

Asked for: $m(Fe_2O_3)$

Reaction equation: $4\ Fe$ o $3\ O_2$ --------> $2\ Fe_2O_3$

Since oxygen is in excess, only iron and di-irontrioxide need to be considered in the calculations.

From the reaction equation the stoichiometric coefficient says that:

$n\ (Fe)/\ n\ (Fe_2O_3\ ) = 4/2$

This is a sophisticated (crucial) step since the coefficients in the reaction equation should be 'translated' to numerical values of the continuous physical quantity amount of substance ('4 moles of iron 'corresponds' to 2 moles of di-irontrioxid'). Since the coefficient is traditionally interpreted as an integer, the 'translation' to mole often implies a conception of mole as identical with a number (Avogadro's number). This is not true according to SI. The correct relationship is a proportionality between number and amount of substance ($N = L \cdot n$).

Rearranged: $n\ (Fe_2O_3\ ) = 1/2 \cdot n\ (Fe)$

Since $m = M \cdot n$ then

$m\ (Fe_2O_3\ )/\ M\ (Fe_2O_3) = 1/2 \cdot m(Fe)/M(Fe)$

Rearranged: $m\ (Fe_2O_3\ ) = 1/2 \cdot (m(Fe) \cdot M\ (Fe_2O_3))/M(Fe)$ (i)

Since $M\ (Fe_2O_3)$ and $M(Fe)$ are constants, available in tables and $m(Fe)$ is known, $m\ (Fe_2O_3\ )$ is easily calculated.

$M\ (Fe_2O_3) = 159.70$ g/mol
and $M(Fe) = 55.85$ g/mol
inserted in equation (i)

$$m\,(Fe_2O_3) = 1/2 \cdot (8.90\text{ g} \cdot 159.70\text{g/mol})/\ 55.85\text{ g/mol}$$
$$m\,(Fe_2O_3) \approx 13{,}5\text{ g}$$

Solution 2 (a discontinuous approach)

Given: $m(Fe) = 8.90$ g
$m(O_2)$ excess (there is enough oxygen for all iron to react)
Asked for: $m(Fe_2O_3)$
Chemical equation: 4 Fe o 3 O_2 --------> 2 Fe_2O_3

Since oxygen is in excess, only iron and di-iron-trioxide need to be considered in the calculations.

From the reaction equation the stoichiometric coefficient says that:

$N_1(Fe)/\ N_2(Fe_2O_3) = 4/2$

According to the chemical equation, 4 atoms of iron 'corresponds' to 2 elementary entities of di-irontrioxide. This means that the ratio of number of atoms of iron and number of elementary entities of di-irontrioxide is 4/2.

Rearranged: $N_2(Fe_2O_3) = 1/2 \cdot N_1(Fe)$
Since $N = m(N\,X)/\ m\,(1\,X)$
then
$$m(N_2\,Fe_2O_3)/\ m\,(1\,Fe_2O_3) = 1/2 \cdot m(\,N_1Fe)/m(1\,Fe)$$
Rearranged $m(N_2\,Fe_2O_3) = (1/2\,m(\,N_1Fe)\cdot m\,(1\,Fe_2O_3))/m(1\,Fe)$

Since $m(1\,Fe_2O_3) = 159.70$ u
and $m(1\,Fe\,) = 55.85$ u
then $m(N_2Fe_2O_3) = 1/2 \cdot (8.9\text{ g} \cdot 159{,}70\text{ u})\ /\ 55.85\text{ u}$
$m(N_2Fe_2O_3) \approx 13.5$ g

Solution 3

A graphical exposition, showing the proportionality between the actual quantities.

Given: $m(Fe) = 8.9$ g
$m(O_2)$ excess (there is enough oxygen for all iron to react)
Asked for: $m(Fe_2O_3)$
Reaction equation: 4 Fe o 3 O_2 --------> 2 Fe_2O_3

Since oxygen is in excess, only iron and di-irontrioxide need to be considered in the calculations.

From the reaction equation the stoichiometric coefficient says that:

$$N_1(Fe)/\ N_2(Fe_2O_3) = 4/2$$
Rearranged: $$N_2(Fe_2O_3) = 1/2 \cdot N_1(Fe)$$

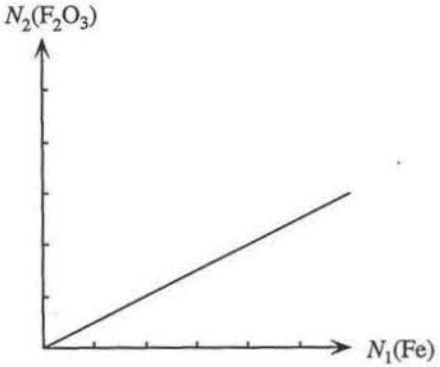

Figure 9.1 Graph showing the proportionality between numbers of the elementary entities participating in the actual chemical reaction. Since $N = N_A \cdot n$, a graph showing the proportionality between the amount of substance for the different substances will be similar.

From $N_2(Fe_2O_3) = 1/2 \cdot N_1(Fe)$
Since $N = m(N\,X)/\ m\,(1\,X)$
then
$$m(N_2\,Fe_2O_3)/\ m\,(1\,Fe_2O_3) = 1/2\,m(\,N_1\,Fe)/m(1\,Fe)$$

Rearranged $m(N_2\,\mathrm{Fe_2O_3}) = (1/2 \cdot m\,(1\,\mathrm{Fe_2O_3}\,) \cdot m(\,N_1\,\mathrm{Fe})/m(1\,\mathrm{Fe})$

Since $m(1\,\mathrm{Fe_2O_{3)}}) = 159.70\,\mathrm{u}$

and $m(1\,\mathrm{Fe}\,) = 55.85\,\mathrm{u}$

then $m(N_2\,\mathrm{Fe_2O_3}) = (1/2 \cdot 159.70\,\mathrm{u}\,/\,55.85\mathrm{u}) \cdot m(N_1\,\mathrm{Fe})$

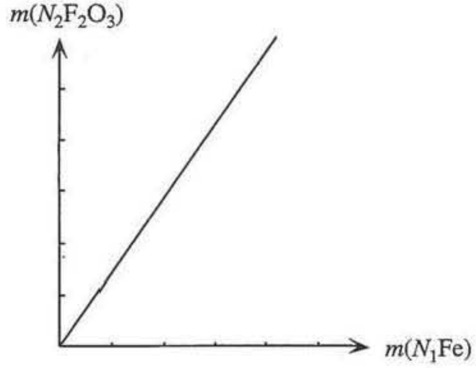

Figure 9.2 Graph showing the proportionality between the masses of the participating substances in the chemical reaction. If 8.9 g iron reacts with excess oxygen the result ≈13.5 g could be determined from the graph.

An essential educational question is whether one should use a lot more time to develop a more fully and complex introduction of a new concept and its locality, rather than immediately or very soon running into the phase of application with only simplified, rudimentary and fragmentary knowledge of the concept in focus. Moreover, the awareness of an *acquisition phase* and an *application phase* of concept attainment seems not to be developed among the educators in the empirical investigations. This is an area which need further research.

It should be noted that no part of this investigation argues for any definite normative standpoint regarding problem-solving methods or strategies in stoichiometry, but rather provide a base for considerations on what activities could be run in class-rooms and lecture-theatres.

CHAPTER 10

GENERAL DISCUSSION

Scientific concepts, such as the physical quantities, are not inherent in Nature but are abstractions derived by reflection based on experiential perception (cf. Carr, Baker, Bell, Biddulph, Jones, Kirkwood, Pearson & Symington, 1993). They are reductions of the infinitely multivariate life-world perceptions to a few manageable idealised variables (measurable properties) within theory boundaries.

As shown in the historical account *amount of substance* was shaped and introduced to fulfil the role of being the physical quantity of a historically existing unit, 'the mole' within the coherent theoretical context of physical quantities. But fitting a formal mathematical structure as quantity calculus is not enough. The ultimate question is: What property of matter is measured by the physical quantity *amount of substance*?, or equivalent: What property is measured in moles?

The 1971 SI definition (CGPM, 1971) and the IUPAC-manual (Mills, *et al.*, 1993) as a conventional scientific norm tells us that *amount of substance* is proportional to number. The fact that it is also proportional to mass, with the reciprocal molar mass as a proportionality constant, is not mentioned by the IUPAC-manual. The annotated proportionality to number seems to be a message to the scientific community that *amount of substance* is implicitly a measure of number of elementary entities (which is also indicated in the SI definition of 1 mol). These circumstances raise doubts about the status of *amount of substance* as an independent physical quantity. However, *amount of substance* can be looked upon as a continuous macroscopic counterpart to *number* as belonging to the categorial set *physical quantities* embedded in the theory of physical quantities included in the theory of continuum physics. The metric of the macroscopic quantity *amount of substance* (n) is mathematically isomorphic with the positive real numbers ($n \in \mathbf{R}_+$) and the metric of the microscopic quantity number (N) is isomorphic with the positive integers ($N \in \mathbf{Z}_+$). *Amount of substance* and *number* are directly proportional to each other. However, no explicit phenomenal reference (physical significance) is attributed to *amount of substance* which transcends number.

The context is decisive for the meaning of a single concept. Thus, the educational difficulty in attaining *amount of substance* lies in the fact that concepts connected to chemical phenomena are generally interpreted and explained within the frames of discontinuum physics where 1 mol as a number of atoms is salient and essential for stoichiometric calculations.

The qualitative conceptual step, which is needed to attain the 1971 definition is huge. This is made explicit by the proposed theory of concept attainment. The fact is that the explanation of chemical processes in classrooms and lecture-theatres naturally leans heavily on the atomic (particulate) nature of matter. The explanation of quantitative chemical conversions is also bound to the individual masses of the elementary entities and their number. Correct calculations with 1 mol as a number work in practice, hence there is no incentive to make an interpretation of the SI definition where 1 mol is not a number. No special notice is taken to the existence of the physical quantity *amount of substance* and how it should be interpreted. However, even if general conceptions of 'the mole' and 'amount' (amount of substance) is number, the educators seem not to dare to move too far from the common scientific terminology, so the concepts are retained, perhaps to guarantee solidarity to some scientific "causity".

The historical meanings of 'the mole' more or less consciously upheld by the educators seems to be part of present chemistry education. The difficulties created by these circumstances are aggregated in stoichiometry. The mix-up between the coherent system of physical quantities and "the mole", not treated as a unit of a physical quantity, brings conflict into the problem-solving situation.

The present investigation shows the tension between the discourses associated with the stipulative definition of physical quantities in scientific discourse and the conceptions and uses of the quantities in practical teaching, founded in historical discourses, even at university level.

Even McGlashan (1977, p. 278), who was the leading theoretician when the IUPAC text was designed, reflects the ambiguous situation by

considering *amount of substance* as redundant, since it is possible to make stoichiometric calculations with molecular properties.

Generally speaking, a tradition is talking in the individual (cf. Bakhtin 1981; 1986 about 'ventriloquism'). The pupil, student, teacher, professor always participate in one or more linguistic-semantic traditions, discourses. Statements made by an individual are in some sense always discourse laden. Statements in science are no exception. The present empirical research approach uses individual statements as indicators to reveal these discourse traditions in speech-acts. It is a kind of empirical semantics. The number of individuals in such an investigation can be rather low. On the other hand it is obvious that it is decisive for the validity of the results that the individuals should be strategically chosen to get the maximum variation of discourses (traditions).

The empirical investigations show that the institutionalised educational system creates a specific discourse via the educator as a conceptual actor. The teacher's conception of 'the mole' is decisive for his/her teaching (cf. the interaction on level II in figure 3.2, section 3.1.2). By accepting the teacher's statements the students become new participants in the discourse that the teacher is a member of. This put a great responsibility onto the educator.

Packer (1988) has stressed that the 'root cause of students problems' in stoichiometry is due to the lack of comprehension of the principles of measurement, the nature of a property and a unit and the relations between them. Is this a function of the lack of proper teaching? Well, Packer has also found that out of 44 teachers only 4 use the term amount, 12 the symbol n and only 5 proper units.

If making students into participants of a contemporary scientific discourse is an educational issue, then the teacher her/himself must be a full-fledged participant of that discourse. Thus teachers demands qualitatively good and quantitatively well-judged education. A proper knowledge of the coherent structure of physical quantities, quantity calculus, the theory and praxis of measurement and meta-comprehension are some cornerstones raised in this investigation.

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Appendix I

The questionnaire

Educators

0. The test-configuration is presented.
1. What is the content of the cylinders?
2. The mole question: Which of the groups I, II and III contains 1 mol of the substances a) tin b) aluminium and c) sulphur ?
3. When I say (the word) mole, what comes to your mind?
4. What do you mean by amount (Sw. mängd)? Do you use the expression 'amount of substance' ?
5. Is there anything in your mind now (concerning this matter) that you haven't thought of before?
6. This 'mole question' has been given to students (N-programme) in Upper Secondary School. Do you think that the question is relevant?
7. How do you think students solve such a question?
8. How do you think trainee teachers solve this problem?
9. How do you teach 'the mole' to your students.
a) at Upper Secondary School
b) at teacher training schools
c) at secondary school
10. Why do you want to teach like this?
11. Have there been any change in your teaching of 'the mole' through the years?
12. Why?
13. What is your opinion of the discussion of teaching methods and didactics today?
14. Where is it going on?
15. Do you want to add anything?
Thank you!

Additional questions to trainee teachers

1. Which are your main subjects? Why did you choose them?
2. When and how were your interests for mathematics and science awoken?
3. Are there any specialities in maths and science that you are especially interested in?
4. Is there any person who has encouraged and inspired you in your choice (relative or teacher)?
5. Are you interested in social science and human studies?
6. Why do you want to be a teacher?
7. What was this problem all about?
8 What is your opinion about teacher education in Chemistry?
Was it good? Is there anything you want to change? What is lacking?

Appendix II

Conceptions among the respondents in the empirical studies concerning the solution of "the mole task" (pattern, perspective and choice of group) conceptions of mole (fundamental), amount and amount of substance.

Table 1 28 educators

Respondent	Pattern	Perspective	Group	Fundamental	Amount	Amount of substance
T1	(\	C,D	I	F1	mass	does not use it
T2	(\	C	I (III)	F1	mass	mass
T3	(\	C	III	F1, F2	–	does not use it
T4	(\	C	III	F2	number, volume	use it, = mole
T5	\	C	I	F1, F2	mass	use it, = mole
T6	(\	C	I, II, (III)	F1, (F2)	mole	does not use it
T7	(\	C	I (III)	F1, F2	ambiguous	too theoretical to use
T8	(\	C	I	F1, (F2)	number, (mass)	use it, = mole
T9	(\	C	III	F2	number	does not use it, =.mole
T10	(\	C	III	F2	mass, number	does not use it, =.mole
T11	(\	C	III	F2	number	use it, number of moles
T12	(\	C	I	F2	portion, volume	amount in moles
T13	(\	C	I (III)	F2	mole, number, mass	does not use it, = mole
M1	(\	C	I	F2, (F3)	number	sort it out
M2	(\	C	I	F1, F2	number of mole	does not use it
M3	(\	C	I	F3	–	in accordance with SI
M4	(\	C	I	F2	mole	amount, mole
M5	(\	C	I	F1, F2	mass	does not use it, = mole
M6	(V)	C, D	III	F2	mole	does not use it, =.mass
M7	(\	C	II	F2	number of mole	amount, =.mole
M8	(\	C	I (III)	F3	short for AoS	in accordance with SI
M9	(\	C	I	F2	number	amount, = mole
M10	(\	C	I	F2	ambiguous	amount, =.mole
M11	(V)	C, D	I	F2	number	volume, number, mass
M12	(\	C	I	F0	short for AoS	amount, = mole
U1	(\	C	I	F3	data is missing?	in accordance with SI
U2	(\	C	I, (II)	F2	ambiguous	use it, = mole
U3	\	C	I	F1	volume	never used

Table 2 26 educators

Respondent	Pattern	Perspective	Group	Fundamental	Amount	Amount of substance
TA	(\	C	I	F2	number	amount, = number
TB	(\	C	I	F2	short for AoS	amount, = mole
TC	(\	C	I (III)	F2, F1	mole	amount, not used
TD	(^	C, D	I (III)	F2,F1	short for AoS	amount, mass
TE	(\	C	I II (III)	F2	short for AoS	too troublesome, mole
TF	\I/	C, D	I (III)	F2	mole	amount, not used
TG	^/)	D	I	F2	sort out	sort out
TH	\	C	I	F2, (F1)	data is missing	data is missing
TI				tape recording failed		
TK	(\	C	I	F2	number	number of mole
TL[1]				F2	short for AoS	amount, mole
TM	(\^	C, D	(III)	F2	ambiguous	use it, = mole
TN	\ ^I/	C, D	II	F2	number	number
TU	\^I	C, D	I	F1, F2	number, mass	does not use it
TY	^/	C, D	I	F2	number	try to use it
MA	\I	C	I	F2	number	does not use it
MS	\	C	I	F2	ambiguous	use it, unit 1 mole
UB	(\I	C	I	F3	short for AoS	use "ämnesmängd"[2]
UH	(\^	C, D	I	F2	ambiguous	use "ämnesmängd"
UJ	(\	C	I (III)	F2	short for AoS	use "ämnesmängd"
UK	(\I	C	II	F1, F2	data is missing	use "ämnesmängd"
UL	(\I	C	I	F2	data is missing	use "ämnesmängd"
UM	(\^/	C, D	III	F2	data is missing	use "ämnesmängd"
US	\I	C	I	F2	number	does not use it
UX	(\I	C	I (III)	F2	data is missing	lacks significance
UY	\I)	C	I	F2	number of mole	does not use it

1) This teacher participated in a seminar on 'the mole' before he was interviewed.

2) A tolerable translation of the Swedish term 'ämnesmängd' is 'amount of compound'

Table 3 18 trainee teachers

Respondent	Pattern	Perspective	Group	Fundamental	Amount	Amount of substance
TT1	(\	C	I (III)	F1, F2	volume, number	not used, V
TT2	(^)	C, D	I (III)	F2	number, heap	not used
TT3	(^	C, D	III	F2	number	number of moles
TT4	^/	D	III	F2	number	weight
TT5	(^/)	C, D	I	F2	number	not used
TT6	\^/)	C, D	I	F2, F1	volume, number	mass, not used
TT7	(\^	C, D	II	F1	ambiguous	not used
TT8	(\^	C, D	III	F2	weight, number, V	not used
TT9	(\\|	C	III	(F1)	ambiguous	not used *
TT10	(\^/)	C, D	II (III)	F1, (F2)	ambiguous	not used
TT11	(\	C	III	F0, F1	ambiguous, mass	not used
TT12	(\^	C, D	III	F2	mole, ambiguous	not used
TT13	(\	C	III	F1, F2	ambiguous	not used, mass
TT14	(\	C	I (III)	F2	number	not used
TT15	(\	C	II	F1, F2	mass, number	do not remember
TT16	\	C	I	F2	number	not used
TT17	(\^/	C, D	I (III)	F2	number, ambiguous	not used, mass
TT18	\^/	C, D	I	F2	number	not used

Table 4 29 students[1]

Respondent	Pattern	Perspective	Group	Fundamental	Amount	Amount of substance
Ada	\^/)	(C), D	II	F2, F1		
Alf	V	C, D	II	F2		
Anders	(V)	C, D	I	F2		
Ann	(\	C	III	F1		
Arne	(\	C	I	F1		
Axel	(V	C	II	F2		
Barbro	(\^/)	C, D	III	F1, F2		
Bengt	V)	D	III	F2		
Berit	V)	(C), D	I	F2		
Bert	/	D	III	F2		
Bertil	(\	C	I	F2		
Björn	(V)	C, D	II	F2		
Bodil	(\	C	I	F1		
Bosse	(V)	C, D	I	F2	number	use it
Britt	(\	C	II	F2		
Bror	(\^/	C, D	I	F2,F1		
Bruno	(\	C	I	F2,F1		
Börje	(\	C	I	F2,F1		
Egon	\	C	I	F2,F1		
Elin	(\	C	III	F1		
Elsa	|/)	D	Excl.II	F2		
Emil	(\\|/	C, D	I	F2		
Emma	V)	D	III	F2,F1		
Enok	(\\|/	C	III	F2		
Erik	(\	C	I	F1, F2		
Ernst	(\\|/)	C, D	I	F2		
Eskil	(\\|)	C, (D)	I	F1,F2		
Eva	(\\|	C	III	F2)		
Evert	V)	C, D	II	F2		

1)No systematic data is available about 'amount' and 'amount of substance'. Bosse is the only one who spontaneously use 'amount of substance'

Appendix III

Some data and quotations with brief commentaries from the empirical study of the 26 educators

TA

The task[90]: molar mass, density, volume. Group I.

The mole[91]: "I think of a number. (...) Yes, one which isn't a score nor a gross ... but one which is enormous big ... namely,... what is it now ?,... $6 \cdot 10^{23}$.

Amount: "... My intuition says that it is a number too ..."

Amount of substance: "... It doesn't mean anything to me ... (...) synonymous with amount ...". TA never uses "amount of compound" [92]. He speaks of "molar value".

Relationships: TA doesn't use any formal relationships between the physical quantities "... I ... I don't know them by heart ... I can ... never learn what is N and n ... I try to teach it in a rational way, so to say ..." "...and I am very fond of calculation by the 'rule of three' ..."
Molar mass: "... it is the mass in grams of one mole..."

Personal development: "... I can't remember that I understood the mole as a number during my own education at the upper secondary school... I think I understood it like a term for concentrations ..."
About the number aspect: "... it must have been at the university ... I was released ... and I thought stoichiometry was rather simple ... like general bookkeeping ..."

TB

The task: molar mass, density, volume. Group I.

The mole: "Yes, ... I think of a specified number of particles ... it is 6 ... it is $6 \cdot 10^{23}$, $6.02 \cdot 10^{23}$ (...) ... and the other part is ... it is related to what mass ... one mole has. (...) ... which has got the same numerical value as the formula mass ... I used to give a double definition of it ... on the one hand as a number ... or that one mole it's so many grams as the numerical value of the formula mass.
TB uses amount as a synonym for amount of substance. "(...) ... specially when you must write it down you hesitate writing something which is unnecessarily long ..." "... you choose a linguistic form which perhaps isn't fully correct but you hope that the students understand what you are talking about..."

Molar mass: "... the mass of one mole of a specified substance ... and the unit is gram per mole..."

Relationships: TB uses the relation $m = M \cdot n$ as an algorithm.

Personal development: TB doesn't remember anything about how he understood "the mole" during upper secondary school or later at the university.

Textbook at upper secondary school: Böös, & Leden (1953).

TC

The task: molar mass, density, volume. Group I.

The mole: "... primarily I associate it with a number ... on the other hand with the definition of the mole? ... as many grams as ... the molar mass ... or the atomic mass (...) ... I stress the particle aspect ... one mole stands for $6.02023 \cdot 10^{23}$ particles (...) ... to use such a big number to describe this, you must have another unit for number ... (...) and than we define one mole as that number..." (...) "... you can also define or characterise the mole concept ... as the mass which weighs as much as the atomic mass in ... in ... grams.

Amount: "... is something with the unit one mole ... amount, it is a quantity ... with both a numerical value and a unit which is one mole."

Amount of substance: The notion amount of substance is only used at the introduction of the domain but then only 'amount'.

Relationships: "... mass equals ... eh ... amount times molar mass ... I write it down ... the formula and ... then ... I let them (the students) use that formula with units, quite consequently."
Personal development:
TC can't remember any changes in his conception of mole. "... I have never thought of mole ... more than ... I think the concept ... I realise the importance of the concept but purely pedagogically it hasn't been specially difficult ...."

Textbook at upper secondary school: Böös, Leden, & Lundberg.

TD

The task: atomic mass, density, volume. First choice group III, and eventually group I.

The mole: "Yes, I am thinking of the number of particles and amount of substance ... expressed in grams. (...) ... one mole can be as many grams (...) as the numerical value.

Amount: "... in the old times amount was ... it was the weight of something.."

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[90] Under the headline 'The task' the main physical quantities used in the task solving process and choice of group are noted.

[91] When the respondents say "six times ten to the power twenty-three" or some variant of this as a numerical value of the Avogadro constant or Avogadro's number, it is here denoted by the scientific notation.

[92] The Swedish term 'ämnesmängd' is translated into 'amount of compound'.

Amount of substance: But now TD uses amount synonymously with amount of substance.

Relationships: "I never write a formula like $n = m/M$ and things like that. I never do that ... (...) ... we look upon the units instead ... what it's going to be.

Personal development: TD has experienced a successive development but he can't give an account of it.

TE

The task: molar mass, density, volume. First, spontaneously group III, then group II or I.

The mole: "I think of a... well, a number of particles. Yes, this 6.0 power to 23.

Amount: "... chemically (...) ... a number."

Amount of substance: TE uses only 'amount' because "It's too complicated ... (...) the expression is too long."

Relationships: $m = n \cdot M$. After some time this equation is used automatically. TE discusses the mass of one atom: 1 mol Cu-atoms $6.0 \cdot 10^{23}$ atoms, 1 mol Cu-atoms have a mass of 63,5 g , 1 Cu-atom has a mass of $63.5 \text{ g} / 6.0 \cdot 10^{23}$.

Molar mass: "... it's the weight of one mole ... grams per mole."

Personal development: TE doesn't remember any details.
Textbook at upper secondary school: Böös, & Lundberg.

TF

The task: molar mass, number, volume. First, group III (by intuition) then Group I.
"Well, in fact, it's a question of sorting out one's own thoughts. What it's... I ... what I am going to think of and how I am going to think.

The mole: "... a number and I think of Avodagro's number, this $6 \cdot 10$ power to twenty (one word inaudible), it ..." (...) "... instead of saying that we have ... six times ten power to twenty-three atoms, we can say that we have got 1 mol of atoms, it's much simpler to say that, than carrying on with that big ... (...) ... but I wouldn't put a sign of equality in between ... But it's true, it's, instead of saying that (number) you say one mole. Be equivalent to, I would say, not equal to.

Amount: "I am thinking of the mole (...) ... I am careless with ... the concepts (...) ... I am using the mole as an amount (...). I say: number of moles ... and I mean amount. I think I have left saying amount, when I mean mass. I hope that heartily, but it ... well ..."

Amount of substance: "... when I introduce it I speak of amount of substance, but then I think this substance ... perhaps disappears, and you are saying a bit carelessly ... amount, but ... at regular intervals, amount of substance appears."
(I: Why amount?) "Well, in fact it's only,... it's ... shorter."

Molar mass: "... the mass of what one mole weighs ..." "... when you have introduced this Avogadro's number and the mole ... then it's evident that one mole is the same as (one word inaudible) mol ... yes, as the atomic mass, but in grams. (...) ... gram per mole."

Relationships: TF uses the equation $m = n \cdot M$ and, that equation rearranged like $n = m/M$. "... five or six years ago, a pupil introduced a concept, which I adopted , he called it "curl-M" ... it's the molar mass."
The order between n and M in the equation $m = n \cdot M$ is explained by TF's statement: "I used to say that it is the same situation, when you buy ... three hundred grams of cheese, when you know what ... the price of one kilogram is."

Personal development: TF cannot remember any changes in her conception of the mole during her career, even if she is aware of that there must have been changes. E.g. amount of substance has been introduced in recent years. TF says that she has learnt much of the mole by teaching the mole.

Textbook at upper secondary school: Böös, Leden & Lundberg.

TG

The task: number, atomic mass. Group I

The mole: "I think of a number. And ...I... Well, I don't think of anything more. (...)...if I don't stick to number, well, then I will be skating over thin ice."

Amount: "...if it's in the textbook (...) then I pass it,...I avoid amount and amount of substance, and things like that...(...)...in a test I wouldn't use the word amount."

Amount of substance: "...I write number of moles.(...)...to me it's alien to say amount of an acid... (...)...I haven't been educated myself with that expression. This is a word (amount) I have met in upper secondary textbooks. (...)...I don't remember such words from my own education ..."

Molar mass: Denotes molar mass with M, e.g. M_{NaCl}. The unit of molar mass is grams.

Relationships: "$c = n/V$ (...) ...is a natural way to remember concentration as mole divided by volume...by the units. (...)...I see it more clearly if I don't use formulas...when one solve the task (...) yes, you are reasoning about it (...) easier for most of the students to manage...but for others the formulas are so beautiful, so they don't want to have it in another way." TG uses $n = m/M$ but not always explicitly. "...not in tests. But it should be there with digits (...)... so I know where they (the students) have taken it from."

Personal development: TG does not remember anything about the mole from his own education. But, "...I remember when I met it in the textbooks...saw this expression amount of substance... to me amount was connected to set theory, because I was a teacher in mathematics.(...) so amount in chemistry (...) I had never thought about that. (...) ...the mole concept (...)...well, it hasn't been (...)... a problem I have pondered about. It's first as a teacher (...) when you use it... it's very central during upper secondary school...you must use it all the time because the reaction formula is dependent on the number of particles, well, and...in order to connect it to mass you must convert to mole.

TH

The task: molar mass. Group I

The mole: "... when I introduce the mole concept then I speak about number ..." (...) It's a huge number and ... it's not surprising that two pairs of stockings weigh different to two pairs of bicycles... (...) ... one mole ... it's the number in ... it's equal to the number of carbon atoms of the isotope carbon -12, carbon -12 in 12,0 g carbon." "...When introducing the mole concept, then I consider it as a number ... the number which is embedded in Avogadro's constant ... after that I link it (the pupils link it) to those relations, molar mass and mass."

Molar mass: "... it is the mass of one mole ... the unit is grams per mole.

Relationships: Pupils are requested to formulate the equation $M = n \cdot M$ by themselves (m = mass, M = molar mass, n = mol). The unit g/mol is analogous to kronor/kg. TH stresses the order of the factors n and M in the equation $m = n \cdot M$. "... n is analogous to kilogram and M to prices per kilogram."

Amount of substance: TH doesn't use the expression amount of substance. "... amount is ambiguous ... that word ... you say big amounts and small amounts, no ..." "Earlier I said number of moles but now I only say moles.

Personal development: TH doesn't remember anything of his personal development concerning the mole.

Textbook: Böös & Leden (1953).

TI

Tape -recording failed

TK

The task: molar mass, density. Group I

The mole: "I think of number (...) this is the concrete picture of ... how you can work with the mole practically."

Molar mass: "It's the mass of one mole ... of one ... of a specified number of these particles ... (in) grams ... implicit per mole."

Amount: "... it is very likely equivalent to number..." "I don't use (the word) amount in chemistry, no."

Amount of substance: "It is an equivalent to the mole ... (...) calculate the amount of substance and calculate the number of moles. (...) Amount of substance is the number of particles."

Avogadro's number: "... it is a suitable number ... (...) it's such a big number, that we get a direct translation from ... atomic weight ... (to) the unit grams.

Relationships: "... the mole triangle" for the less able pupils. 'Rule of three' is used in teaching.

Personal development: TK doesn't remember anything of his personal development concerning the mole. TK's commentary on his definition of 1 mol: "I have always had that ..."

TL

Data for this respondent is excluded , since he participated in a seminar about 'the mole' before he was interviewed.

TY

The task: atomic mass, number, 'amount of substance'. Group I

The mole: "Well, I think of the long definition ... and short it's ... if you take 12,0 grams of carbon ... it will contain one mole of atoms of carbon. Particles, atoms of carbon. Then it can mean a lot of things, if you are going to translate it to ... Avogadro's number and things like that." "(...) ... if ... students in tests ... write that one mole, eh ... well, they can write one mole water, they can write one mole molecules of water, they can write one mole of H_20 is equal to 18 grams, I don't think it's a formal mistake."

Avogadro's number: "Eh ... well, it's ... is ... Avogadr... I would state ... probably it's not strictly mathematical but ... Avo ... Avogadro's number is ... the number of ... particles ... in one mole." (I: Is it possible to put a sign of equality between one mole and Avogadro's number?) "Well, not directly. Well, intuitively there's something which doesn't tally. But, I, I, I can't say what it is, because ... Avogadro's number is a number, in my opinion. One, one mole, it's it's a ... I don't want to have one mole, as one mole. I want to have one mole of atoms or one mole of molecules. One mole, whatever it is."
TY agrees that one mole molecules equals (=) $6.02 \cdot 10^{23}$ molecules and "... one mole of water molecules is equivalent to 18 grams of water."
About the difference between Avogadro's number and the Avogadro constant "... it doesn't matter, but it's not precise (...) Avogadro's number and the Avogadro constant happen to be the same..."

Amount: "I try to let it mean number."

Amount of substance: "... if want do it simple, then I'll go for number ...(...). I don't know if it's inspired from mathematics, amount (set) and number or ... well, I think it's like that. (...) I try to use the expression amount of substance."
(I:... properly speaking, the words number, amount, amount of substance are synonymous?) "Well, it's a question of proper procedure and that I don't care to take ... (...) Num..num..number and amount of substance are synonymous. Amount is more diffuse.
(I: Would you use the expression 'number of moles'?) "Yes, it's said to be a tautology, but I would. (...) I mean, the mole is a number, a number, it's a tautology, but a handy tautology."

Molar mass: "... e.g. the molar mass of water is ... the mass in grams of one mole water molecules. The mass is expressed in grams. The conclusion is that the unit is grams per mole, if you are going to calculate with ... equations. If you calculate through logic or something, then you cope with gram, old "rule of three" and things like that."

Relationships: "... less able students manage to calculate with a formula, even if they don't understand. n equals m divided by M. Well, (laughing) n equals m divided by M."
About the relation between number and amount of substance he says: "Then you get the number measured in pieces. It's equal to the 'amount of substance' with the unit mole times N_A, but now it's only the numerical values ... then I have got mole there and N_A, well, pieces per mole, or something like that ... (...) If you are going to use this as an equation in quantity calculus, then you must have mole there and pieces per mole." (I: And you name that Avogadro's number?) "Yes."
In TY's opinion the pupils' problems are connected to their poor knowledge in mathematics: "They don't see the relationships. Perhaps they have got too little mathematical training, or simply because they haven't got the ability. (...) They get a number of moles and they know the molar mass and then they are going to calculate the mass. Well, are you going to multiply, or divide, what should be divided by what?" "Perhaps the teaching of mathematics in primary and secondary schools has been too little problem oriented, and they have only done calculations without comprehension."
About beakers containing one mole of each substance as a demonstration of 1 mol: "I want them to comprehend that it's the number ... then, perhaps it makes it easier for them to calculate." (I: Is it possible to show the number?) "No, ... well, I know you can, but, but, but I can't, well it's something you have to 'buy'. (...) Well, a specified number of a ... of different substances doesn't need to have equal masses or equal volumes ... and what I want to stress is ... that in chemical reactions the substances doesn't react in volume to volume, or grams to grams, but particle to particle.

Personal development: At upper secondary school (student 1954) and at university he first used the expression gram-molecule and gram-equivalent and later on mole.
"I don't know if they meant anything to me, I used them just to pass the exams." "... my calculations during my first years as a teacher were very diffuse ... it wasn't until around 1963/64, that I made clear to myself that one could use the mole as a number ... then I got something to cling to and after that I have tried to cling to that in my teaching. I belong to the generation who lack knowledge of physics adapted to the study of chemistry."
It seems to have been something like a revolutionary experience to TY: "I think it almost turned out to be like that. I got something to cling to and suddenly the reactions turned out to be more logical ..."
Textbooks at university: Sillén, Lange & Gabrielsson.

TM

The task: atomic weight, density, molar weight, volume. First choice: group III, then exclude group III, no final choice.

The mole: "I think of ... of a number. Well, amount, amount of subst ... element ... well, that's the name nowadays." TM agrees upon the equality $1 \text{ mol} = 6.02 \cdot 10^{23}$.

Amount: TM considers amount as an ambiguous concept. "... a weight, or ... or a number or a volume ..."

Amount of substance: "When I speak of amount of substance, then I mean the amount of particles of a substance. (...) One mole or fractions of one mole ..." No difficulties are connected to the expression "amount of substance".

Avogadro's number: $6.02 \cdot 10^{23}$ pieces.

Avogadro's constant: has no significance.

Molar mass: "... it's the weight of one mole of particles. (...) grams per mole."

Relationships: "... I want them (the students) to use 'the rule of three', which isn't so easy ... (...) you know the weight of some and then you calculate the weight of one ... (...) and if you know that, then you can calculate the weight of an arbitrary number." TM dislikes equations.

Personal development: Student 1961. Before entering university TM's conception of mole was dim. At university the mole was looked upon as a mass. In the middle of the 70's there was a change. The mole was identified as a specified number. After 5-6 years as a teacher TM found that "... it will be easier for them (the pupils) if it is unequivocal, instead of being several things at the same time."
Textbook at upper secondary school: Böös, Leden, & Lundberg.

TN

The task: molar mass, volume, atomic mass, number. "The weights should be nearly equal in the cylinders containing sulphur and aluminium and much heavier in the cylinder containing tin." Group II.

The mole: "Number ... a specified number. Yes, it is 6 times 10 power to 23, approximately." TN agrees that $1 \text{ mol} = 6.02 \cdot 10^{23}$ and $1 \text{ mol S} = 32 \text{ g S}$

Amount: A number, nowadays.

Amount of substance: Amount of substance is synonymous with amount.

Molar mass: "... it's the weight of one mole. (...) ... grams per mole ..."

Avogadro's number. Avodagro's constant: "... to me, when I speak about it, it's only a number, pieces."

Relationships: About $n = m \cdot M$ "Yes, it is difficult. It is only possible, what I know now, to derive [the equation] by considering the units..."

Personal development: Student 1965. "The mole, it's ... yes, it's something between a unit and a conception. I was a bit confused when I began with the mole and started to ponder it, but nowadays I rather think ... I understand it as ... well, no ..., it's still very like a mixture."
Textbook at upper secondary school: Böös, Leden, & Lundberg.

TU

The task: atomic weight, volume. Group I.

The mole: "... an amount of ... particles, $6 \cdot 10^{23}$. I have double thoughts here, so to speak. On the one hand the particle aspect and on the other hand the mass ... aspect . (...) The number aspect isn't practical (so) ... I must put the latter aspect (mass) as number one, even if (...) the first definition is the primary one - in the textbook I used."

When TU is asked if he agrees that 1 mol = $6.02 \cdot 10^{23}$ or 1 mol sulphur = 32 g sulphur, he answers: "We are very rigorous about having the same dimension on both sides of the sign of equality, you can't oppose that demand as a scientist . (...) but I have allowed pupils to write one mole sodium = 23 grams sodium. Well, I don't think it is an unimportant question. To be honest, I don't think it's an important distinction ... (...) because I think it's a question of method. How to introduce this concept and how to use it without being absolutely ... correct linguistically."
In physics and mathematics you can't resign the demands of the sign of equality, but in chemistry "... it is not decisive" to make exceptions.

Amount: The word amount has double meaning to TU. When he teaches the mole he stresses both the number and the mass aspect. "... first I think of particles, then of masses.

Amount of substance: "In fact, I don't like the word. I think ... I think it is ... I think it is mumbo jumbo, so I am afraid the pupils can't appreciate it. I don't know if it's necessary to use. It, it's good when you explain the whole thing in a precise manner, but I can't say that I use the word in the classroom. (...) I (use) number of moles.

Personal development: TU considered the mole as individual masses up to the middle of the 1960's. But in 1965 a curriculum revision was made at upper secondary school involving new editions of textbooks. The mole was then defined as a number. This was a new conception of the mole, which TU accepted.

MA

The task: molar weight, volume. Group I

The mole: "... I am thinking of a number ... and ... connected to a special number of particles in Chemistry ... To me it's $6 \cdot 10^{23}$ pieces and it can be grains of sand in Sahara and stars in the sky ... it is comparable to score, dozen and gross."

Amount of substance: MA never uses amount of substance.

Amount: "Amount is an arbitrary number."

Molar weight: "... it is the weight of one mole of those particles ... The unit of molar weight is gram.

Personal development: MA doesn't remember anything of her conception of the mole before she started teacher training (after chemistry studies at university!) "I first realised what it was when I comprehended it as a number ... I got some kind of 'aha' experience. I have a good visual memory ... and I saw the particles right in front of me."

MS

The task: molar mass. Group I

The mole: "... to me one mole is a unit of number, exclusively. But since you have chosen that very peculiar number then molar mass equals atomic mass."

Amount: It's confusing. On the whole, I think amount is a confusing concept. It can be volumes and weights ... yes, whatever you want.

Amount of substance: Amount of substance has been consistently used by MS, for the last ten years. "Yes, it appeared in the middle of the 70's or in the end of the 70's (...) ... amount of substance, and I myself thought it was a hard (expression) ... amount of substance, and I looked at the pupils. But no, it's not so hard 'the pupils said ... amount of substance ...' They reacted more positively to it than I did, well, OK, let's use it."

Relationships: MS hates the relation $m = n \cdot M$ because: "Well, it is a mess of letters to learn by heart, without any comprehension. But what we must do is simply to compare ... when you have 30 kronor and you want to buy apples at a cost of 9 kronor per kilogram ... This equation ($m = n \cdot M$) ... forget it as soon as possible because you will comprehend less if you know it." Molar mass is the mass of $6.02 \cdot 10^{23}$ particles.

Personal development: Student 1966. "To me it's exclusively a unit of number. It's nothing else and it took me a lot of time before I grasped that and when I grasped it, that it was a unit of number then things seemed to sort out. But in school I learnt that 1 mol it's as many grams as the formula weight." The shift took place round 1967 when MS entered university.
"... I was forced to sit down and work with it. And suddenly, oh God, it must be like that, the numbers in the periodic table, atomic mass and molar mass. The numbers are the same

because of that peculiar $6.023 \cdot 10^{23}$. It all sorted out, suddenly ... It appeared when I tried to solve problems late in the evenings. It was a sneaking process and suddenly I grasped the whole thing and I managed to solve the problems. ... It happened during two or three weeks ...Since then there have been no change."

Textbook at upper secondary school: Böös, Leden, & Lundberg.

UB

The task: molar mass, density, volume. Group I

The mole: "1 mol - in my opinion it has the dimension of amount. It is the unit. Once upon a time it was, in fact, the quantity. If you can talk about 'number of moles' as some kind of quantity. It was a dreadful language ... (...) there wasn't any difference between quantities and units. It's something which emerged later on ... the formal minus definition is ... 'amount of compound' is the same number of particles as there are atoms of carbon-12 in 12 g carbon-12. And that amount is Avogadro's constant then, $6.022 \cdot 10^{23}$ pieces per mol or mol^{-1}. Piece is no dimension." UB declares that amount is synonymous to 'amount of substance'.

Amount, Amount of substance: " 'amount of compound'... in science I mean ... you should use short and handy words. In Swedish 'amount' ... is better than 'amount of compound' ... 'amount of substance' or 'amount of matter' or whatever you use, names which are too long, awkward and ugly."

Molar mass: "I define it as the mass of 1 mol of a specified substance."

Relationships: About the relations between the physical quantities amount of substance and number: "To me, they are almost identical. (...) and this (N_A) is a conversion factor [sic!]. So, amount of substance and number is much more closely related, than amount of substance and mass, than amount of substance and volume."
To UB the relation $N = N_A \cdot n$ is "... much more direct. Yes it is that old mole as a 'big' dozen. I am stuck to that. (...) My view is more concrete ... avoiding saying that it's so and so many pieces. To say that it is so and so many dozen.
I: Is it a conversion factor...?
UB: Between N and n? Yes, in a way. It's something similar to this old dozen and gross and score.
UB conceptualises M an n as two equal physical quantities. In view of that he doesn't see any difference between writing $m = M \cdot n$ or $m = n \cdot M$ even if "... I would never write $y = x \cdot k$. It would be disgusting ." To UB, M is not a proportionality constant. It is a defined physical quantity (see above).

About the order of n and M in the equation $m = M \cdot n$. UB says: "It is all one to me." and "...In fact, it is the most fundamental stoichiometric equation." "But then ... you identify molar mass as the constant and "amount of compound" as the unknown variable ..."
UB made a conclusion about SI at the end of the interview: "... The system is wonderful as such, but you can find some inadequacies in it like the disharmony between the mole, 'amount of compound' and mass. We shouldn´t dig into it because I think ... we should live with this system even if small inadequacies are attached to it. If you are going to change those ... we will soon have 711 different systems again within a span of time.

Personal development: Student 1952. About changes: "Nothing dramatic has happened. But ... gradually I think I have gained a concept of amount which is more transparent, one that is really amounts. That it's an amount of atoms, that it is a specified number of atoms which react with each other... (...) for me the mole concept is N pieces of hydrogen atoms or 2N, 2 times Avogadro's constant atoms of hydrogen with 1 (N)... atoms of oxygen because then I get a practical quantity. (...) I link it to number and then ... In my point of view it's a dispute 'to split hairs' if it is a continuous or discontinuous physical quantity (...) But based on the definition I think it is easy to look upon it as a number ... that it should move discontinuously one unit at a time."
This view grew out in the middle of the 1970's. UB's view of "the mole" in upper secondary school was that of gram-molecule and gram-atom but it is possible that the concept of amount came across since he had a special interest in stoichiometry at school. But, as he says, he might be mistaken, it is difficult to remember.

UH

The task: atomic weight, density, weight. Guess: Group I

The mole: "Well, we consider ... simply ... one mole to us is ... well, one could speak of one mole photons or one mole electrons ... Well, it's simply a number, which is 6 point something times 10 power to 23 pieces per mole ... (...) ... it's only an 'amount of compound' it's a method to ... make fair comparisons between different amounts of different substances instead of talking about kilograms or something else."

Amount: "Well, mole is 'amount of compound' ... but let's take amount of heat. It's less defined." UH does not use amount as a synonym of 'amount of compound' or amount of substance.

Amount of substance: "Amount of substance, 'amount of compound' well, ... it's equivalent to number of moles, well e.g. the 'amount of compound' is two moles."

Relationships: "I demand ... or at least a personal demand is to use quantity calculus ... I look upon the situation ... much the same as the demand to use grammar correctly in normal language, to use the correct grammar in this physical/mathematical language. (...) I don't link ... volume to amount of substance (...) Because ... one mole ... one mole water ... it's a specified amount of substance. (...) Its volume is very different. It's a factor of one thousand, if it's a liquid or a gas, but it's still one mole."
Relationships mentioned and written by UH: $m = M \cdot n = M \cdot N/N_A$, $PV = nRt$, $V = V/n$.
Personal development: Student 1952."I can't remember any problems or that I didn't understand... now one uses carbon-12 instead of oxygen ... otherwise I don't know (...) one only said: atomic weight ... of copper is 64 ... in fact a wrong expression, I think ... due to quantity calculus ... now I write molar mass Cu = 64 grams per mole (...) But ... the number, I think I know it quite well ... that connection, so to say, to Avogadro's number. That it's .... the weight ... it's the mass of ... roughly 6 isotopes ... nuclide [laughing].
Textbook at upper secondary school: Böös & Lundberg;
Textbook at university Sillén, Lange & Gabrielsson.

UJ

The task: molar mass (molar weight), density, volume. Group I

The mole: "...We look upon it as a number (...) The mole ... 6,022 · 10^{23} pieces of something. It can be atoms and molecules. It can be electrons." "Then ...(...) we speak about the definition as it is formulated in many text-books ,... it starts from carbon-12, etc. ... but ... but ... we consider it to be a number. As well as I have one dozen apples I can have one mole of atoms of sulphur."

Avogadro's number, Avogadro's constant: UJ doesn't make any difference between Avodagro's number and Avogadro's constant. "...Avodagro's number but ... it ought to be Avogadro's constant ... this is the present denotation as far as I know."

Amount of substance: "We use 'amount of compound' (...) We are a bit conservative ... (...) but I must confess that we are gradually turning over to call it only amount, because amount can hardly be anything else." "... perhaps you feel the whole situation to be very vague when you begin to talk about 1/12th of the mass of one atom carbon-12 and things like that. It ... it is long and troublesome and you can only scarcely sort out the concepts. Suddenly you discover that it is a number. The only thing is that there are too many to count, but it is a number. (...) .... it is an amount ... it is a number ..."

Molar mass: "... we define it as the mass of 1 mol of a substance ... e.g. the mass of 6.022· 10^{23} pieces of atoms or molecules or whatever it is..."
Molar volume "... it is the volume of one mole of a substance..."

Relationships: UJ dislikes formalised relations between the physical quantities. "... we are not so very fond of making formulas ... we don't like learning a formula by heart and not really comprehending its meaning ... only inserting something ... (...) huge mistakes can be made if you learn a formula by heart and don't understand the components and in what contexts they are applicable." About $N = N_A \cdot n$: "In fact, I think it is too elementary."

UJ about proportionality: "... it is unfamiliar to me ... to ... to say that the physical quantity mass equals a proportionality constant times a physical quantity of a different kind, viz. amount of substance, where we are saying ... density ... that volume can be converted to a mass with a factor of proportionality ... and ... and ... it ... it ... it is strange in my opinion ... yes... purely mathematical I realise that but ... but ... but I mean ... it is two totally separate physical quantities ... mass is one thing ... volume another ...."
When the interviewer proposes that the proportionality constant is derived from the other physical quantities in the proportionality UJ says: "Well ... but ... then ... it isn't a factor of proportionality - any longer ... but I think it is to simplify too much if (the factor of proportionality) can be used to convert one quantity into another ... to make volume to mass ... it is a manner of thinking and ... I don't think like that."
UJ accept proportionality between the numerical values but not between physical quantities. "Yes, purely mathematically it is like that ... proportionality between the numerical values for those quantities ... as far as that I agree."
The interviewer asks about the units ... are they excluded in this discussion? "In fact, I haven't made up my mind ..."
UJ recommend dimensional analysis because it is good to make an additional control to find out that you have got the right dimension at the end of a calculation.

Personal development: At upper secondary school UJ was taught the gram-molecule and gram-atom, but he can't tell when he changed his conception of the "mole". "In fact, it was more or less a mass ... at that time." "It shifted by ... me using the [mole] concept in calculations to ... teaching what it really was."
UJ assumes that the shift is connected to the demands in teaching. Then you must be able to explain things, you are forced to think a little deeper into the concepts you are teaching.

UK

The task: molar mass, volume, density. Group II

The mole: "Number ... atoms ... yes or formula units. In fact I really feel it as a mass ... containing..."

Avogadro's number: "It is something tied to the reflexive nervous system..."
When the interviewer asks if it is possible to put a sign of equality between 1 mol and 32 grams: "I think it is common, when you are calculating. When you are careless, you do, I think. Even if I am fully conscious that it isn't correct."
UK agrees that it is possible to put a sign of equality between 1 mol and Avogadro's number. "Yes, we begin it that way when we start teaching (the mole) (...) Although ... then, you turn in a direction of praxis, more of everyday manipulation."
UK is not teaching the mole himself to students nowadays.
About the definition of 1 mol in SI: "Well, it is not good. Well, not good ... it is clear! Perhaps it's good as a scientific definition. But it is lacking, in a general sense, practical importance, because in my own view one uses this definition, ... you take ... the formula weight and put the unit gram to the numerical value. And that goes for practical life. And everyone is content."
The definition is not so important even in scientific contexts: "No, but ... I mean, seconds, we are measuring with a watch, we don't bother about ... some oscillation in some crystal ... I fully comprehend that there must be a sophisticated definition of every physical quantity in the background. But then you create a handy praxis, usable in practical life. And I ... I am not capable to judge if ... if the definition of the physical quantity 'amount of compound' or amount of substance, if it is good or bad. One could say that it is bad as far as it is not included in ... the units of the SI-system. It would have been kilomoles then."
In UK's opinion methodological simplifications are necessary: "Yes, it is really true. The scientific definition ... Yes, I ask if you at all ... Yes, at the university level you perhaps ought to ... show it. But you never use it in practice. It is bad ... it is simply not usable. I think very few students care, or they ... they don't try to understand it, simply. They need more concrete elements in their calculations."

Amount of substance: "I am not sure if we use the expression amount of substance at all. I think it is ... a little bit ridiculous ... to introduce that concept. We use 'amount of compound'.
UK considers the genuine Swedish word 'ämne', here translated 'compound' to be more well-defined than 'substans' which is equivalent to the English word substance. "We have always stressed that 'ämne' in a chemical context is well defined. I can't really understand what's gained by using amount of substance instead of 'amount of compound'. I ... we can't really catch the finesse..."

UK uses 'amount of compound' as a synonym of 'number of moles'. According to UK 'amount of moles' is another expression, which is used by the students,. UK has never succeeded in defining molar weight (he prefers that expression rather than molar mass.) "... but in pure practice ... When I do that, then it is clear that I ... change u to g. (...) but if I am forced to give a definition then I would certainly not define it in that way. Then I would say, that it is the mass of that number of elementary particles ... which corresponds ... to as many particles as in 12 grams of carbon -12, this is what I have learnt, ha, ha.

Personal development: Student 1951. UK's earliest conception of the mole was a mass, with some connection to Avodagro's number. Gram-molecule and gram-atom and gram-equivalent were used at the gymnasium. He used the textbook Sillén, Lange & Gabrielsson around 1955, but that book has not made any impression on him regarding the mole. He taught stoichiometry at a university in 1964-70, in agreement with the current text-books. His own conception of the mole has developed in the sense that the definition has been made more precise. But his conception of the mole has, broadly speaking been the same all the time, he says.

UL

The task: molar weight, molar volume, density. Group I

The mole: "I think of the mole as a number. Exactly as dozen and score and things like that ... (...) As many as Avogadro's constant." "If I say that this is one mole, as many as ... in 12 grams of carbon-12, but you must also say that ... that Avogadro's constant is as many as there are in 12 grams carbon-12 so it becomes ridiculous, if it isn't the same."
UL dislikes the SI-definition of 1 mol because it includes another SI basic unit, the kilogram, however as gram. "Well this is also only to ... mark words and philosophy, how you define it. It must be like it is in practice ..."

The Avogadro constant, Avogadro's number: About the difference between Avodagro's number and the Avogadro constant UL says: "Well, there is no (difference). It's purists, who say that it's not a number but a constant, but it is only like ... marking words..." (...) "In fact, the constant is a number but it is defined as a number per mole."

Molar mass: UL does not make any distinct separation between atomic weight, formula weight and molar weight. "... it is a question of definition ... (...) atomic weight and formula weight don't have any units, in fact. But then, to make it easier to ... remember, then you can put on grams per mole." "Molar weight and formula weight are synonyms ... molar weight is the weight of one mole ..." But when UL uses mass instead of weight, then there is a difference. Then you must use the unit gram.
UL uses the word 'amount of compound' instead of 'amount of substance', but the words are synonymous. The latter you can use if you are a purist.

Relationships: UL uses "rules of three" in stoichiometry. He finds it convenient. He has used that method since the 1950's when he learnt it at grammar school.

Personal development: Student 1960. UL was taught to identify the mole as a number at upper secondary school. "... and then the ratio of the masses ... should equate with the ratios of the formula weights. No changes have occurred during his career, he says.
Textbook at upper secondary school: Böös, Leden, & Lundberg.

UM

The task: molar mass, density, volume. Group II or Group III (definitely not Group I!)

The mole: "... more like a number because we use it in other contexts, in physical chemistry, we have a mole of electrons too ... and things like that, ... it is practical to work with that ... (...). But it is practical to *convert* [my emphasis] it to a mass ..." "Well I know the definition ... I always have it in my mind ... it should be so many elementary entities as there are in 12 grams of the nuclid carbon -12 ... But ... it is easier to say, that one mole is 6.0, what is it, 22 or 23, power to 23 pieces ..." (...) "The mole is comparable to a dozen and a score.... In fact, they are ... In practice you must use masses ... one mole ... it is the same as ... yes the value of the atomic weight ... but generally one mole is a number." UM agrees that $1 \text{ mol} = 6.02 \cdot 10^{23}$. The SI definition is not good because: "... you could have said that one mole is 6,022, whatever it is, times 10 power to 23 ... pieces, and there's an end of it! (...) Because it is not good ... to relate it to the kilogram. I think this is a weakness."

Avogadro's number, the Avogadro constant: "... as the chosen definition, ... it is a constant ... so it's nicer. A number should be without units. This (The Avogadro constant) has got a unit, in fact mol to the minus one (mol^{-1}) , ... and then it is not acceptable to use Avogadro's number ... it is a bit careless ...". Comment on the unit mole to the minus one: "It's practical, when you are making calculations and *conversions* [my emphasis] . Then you make calculations with the dimensions. And the right things appear ... (...) to make sure that you haven't forgotten anything or made any mistake." UM uses "rule of three" in stoichiometry.

Amount of substance: "In fact ... it is simply ... a number, in fact, of small units of substances ..." "It ... it is a very peculiar .. unit in a way. But it is practical, so you can't be without it, evidently."
UM dislikes the expression 'amount of substance'. "I am used to 'amount of compound'. UM discusses the importance of using the right words in the right situations and stresses the importance of being aware of precise meanings of words in scientific language. The use of a word in everyday life with an uncertain meaning is something different to the use of the same word in science with a definite meaning.

Personal development: Student 1963. "... I remember the rule of thumb that you should translate it directly to atomic-weight or formula-weight ... (...). But ... Yes, that it is a number .... Well, I think ... I don't know, if I had that in mind from the beginning."
Textbooks: Böös, Leden, & Lundberg, 9th edition (1958).

US

The task: molar mass, mass, volume. Group I

The mole: "Well, I am thinking of the chemist's dozen. (...) ... I have heard about these discussions ... about the mole ... as a unit or ... But ... practically I look upon the mole as a unit of an amount. (...) ... and I think it is a handy and useful way of looking upon the whole thing and it works, you don't need to use a lot of time to repeat ... if you are allowed to say "the mole concept", perhaps it is not proper ... "the unit ..."

She is very surprised about the ongoing discussion about mole, and that a lot of papers have been written about the mole issue. "Yes, my first reaction was ... in fact, why create problems, when there aren't any."

In a way she can understand why the discussion has started, but: "... I ignore that discussion, because I think there are so many other things which are more urgent to ... (...) I don't think the students will improve ... if we change this ... concept."

After a seminar we had at her department in 1983 she had discussed the mole issue with one of her own children. The child (between 13-16 years old) thought the whole thing was ridiculous. "What is the problem?" was the child's reply. The mole had been presented to the pupils as a unit of number in secondary school. By the way it is very uncommon to teach the mole at that age-level in the Swedish school-system. US considers this statement from her own child as a confirmation that the mole issue is a field with no problems.

Amount: "Yes, what do I mean by mass, what do I mean by volume? ... (...) if I speak about a specified amount ... sulphur, then I can see sulphur in front of me and ... I must have something more ... to ... or otherwise I look upon it as a number ... of particles of some kind."(...)"Amount is like the mole, comprehended as the chemist's dozen." "I think ... it is a practical use ..."

Amount of substance: "Yes, well, amount of substance and 'amount of compound' and amount, if we compare them, then you can say that you are twisting your tongue if you ... if you ... are going to use ... if you are using ... it often ..., amount, is shorter." (...) "And then I must confess that I am saying 'number of moles' too." "How many moles have we got here, but I can also say ... how many dozen oranges ... or how many scores of ... eggs ... I think it is OK linguistically. I think that some persons dislike it, linguistically and then ... then you can discuss it. I accept that point of view, but I don't think you make a big mistake, at the beginning ... because it is so handy. How many moles have you got at the beginning and where are they now?" The later statement was related to chemical reactions.

She cannot remember when she first heard the expression "amount of substance". She assumes that it must have been after her own basic education, probably when she started to teach at the department of Chemistry (1960?) "It wasn't so precise in those days ..." when she studied, she says.

Molar mass: "Yes, it, it is simply the mass of one mole."

Relationships: About the relation between amount of substance and number: "Yes, I consider it ... as a number ... but also a mass, and amount of substance has also a, a volume exactly as..."

She doesn't use any quantitative relationships. It is unnecessary because they don't have that kind of problems in the curriculum. If there had been an experiment to determine Avogadro's number then they could perhaps have used the symbol N_A.

About the relationship between amount of substance and mass. The expression $n = n/M$ is used, and she thinks that the students insert the units in the relation, but she is not sure, perhaps they use the units only when they have got numerical values. Her opinion is that the students are drilled to use the formula, and that is good. About M as a proportionality constant and the proportionality $y = k \cdot x$ in the equation $m = M \cdot n$ "Well, if you were going to write a paper on the concept then you would go for that. (...) Then you must reconstruct it yourself in that way. (...) Well, as a chemist I would permute those (the variables) arbitrarily."

After she has been presented the equations in agreement with F3 (SI and quantity calculus) she says: "... I would have done it in this way (like you), ... and then one must do it in a consistent way ... You have got another aim with this. I ... eh ... eh ... I, never, never think so far ... and I never think so accurately. Perhaps I should but ... but ... eh ... eh ... it ... I, I don't think that would increase it in any way ... increase. Yes, you should be a purist and make the perfect ... (...)." "Well. But it is excellent that this is dealt with thoroughly ... then ... because I agree on this. It is evident that it is correct. And I am negligent here, but ... but ... you can say consciously ... negligent because I think that ... that ... it isn't so important. (...) I don't think it will change anything regarding our students conceptions of ... these properties and the reactions."

It is evident that the respondent is not susceptible to call in question. She is content with her view of the mole as a number unit, because it is so handy, and it works when she solves stoichiometric problems. It is evident that she is not aware of the conceptual problems connected to the mole issue and consequently her attitude to the discussion is comprehensible.

Personal development: Student 1953. She cannot remember any change in her own conceptualisation of the mole during her career. Her present view is so settled that she cannot recall anything from her own conceptual development. All earlier conceptions have faded away. When the interviewer asks her if she was confronted with the gram-atom in her studies at upper secondary school in the early 1950's she says: "Yes, it is possible. It ... it ... it is possible. I don't know. I really don't know."

Referring to Segal (1985, p. 28) where 1 mol is said to *contain* Avogadro's number of particles she says: "So, this is the practical definition... which the purists dislike. But it is useful."

When the students begin university she controls if they know the meaning of the word (amount of substance) through solving some 'practical applications' (exercises, problems). "And ... as it is so many things that they (the students) don't know ... from the upper secondary school you leave everything that is unstable (!) very soon. So ... I can't afford to use ... one hour to discuss the mole concept."

She is showing a text-book and says: "... here ... and I have decided to accept the chemist's dozen. ... I want to present those relations (formulas on page 13 in Stomberg) so they can use them ... and most of them (the students) include the units ... which they are used to from school."

Her educational policy is: what she teaches must be practical, must be applicable (useful). ("... you must go to the chemicals themselves ...") "... basically you have got a conceptualisation, I think, ... about atoms ... I mean ... atoms can only change places with each other ... And then you look upon them as balls or ... or whatever you want ... And then it is, ... natural to tie the mole to a chemical equation ... And then it is a handy unit to use in calculations."

As a comment to the SI definition of the mole she says: "Yes, I know that, I know, I know that, I ... eh ... eh .... Yes, of course (...) Yes, or, or well, we have only paid a slight attention to that ... I must confess that. If, if we shouldn't do that, then it means, well, ... then it means several hours less to other parts of chemistry. In fact I close my eyes and ... Well they learn what I want them to learn. They get more hours to learn about chemical reactions between elements and chemical compounds. This is my goal, and that's my destiny. If I stop at every crossroad, then I will never get there. (...)" (...) "... a lot of us think that the most important thing is the basics. A solid base to stand on ... eh ... if you have got that, then you can manage by yourself."

UX

The task: Density, molar mass, volume. First choice, Group III, eventually Group I

The mole: "... a number. $6 \cdot 10^{23}$ pieces. ... There is a discussion going on about the mole ... if it has any meaning of it's own. I don't think it has. And I have never realised that this concept is anything other than a quantity of bookkeeping."
The mole is denoted by UX as a pseudo-quantity which should be excluded from SI. UX dislikes SI and want to re-establish MKSA and CGS. UX is critical toward the unit kilogram because it include a prefix (kilo-).

Amount of substance: Amount of substance has no significance to UX.

Molar mass: "... the mass ... of a specified number of particles ..(...) ... kilograms."

Personal development: "... I have always considered it as numbers of atoms." "... but ... I linked it rather early to the mass ... of a number of atoms ..." "... it was connected to the definition of the atomic mass unit ... dividing an atom of carbon in twelve parts ... or was it oxygen? ... "
Textbook at upper secondary school: Böös, Leden, & Lundberg.

UY

The task: Molecular weight, mass, (volume). Group I

The mole: 'First I think of Avogadro's number, and that is an enormous number (...)... and then I think of perhaps...water... 18 grams...(...) so I know approximately how much it is.
About the definition of mole: ' To me it is as many particles of that substance as Avogadro's number...
About the scientific definition: '... as many grams as what is given in the table of atomic weights.

Amount: "...to me, the border between amount and mass, probably..."

Amount of substance: " ... if I'm dealing with the definitions of these things, then perhaps, I use it (...) but otherwise I'm not sure that I use amount so much, in fact..."

Molar mass: "the mass of one mole of different substances...(...) ... the unit is unit of mass per mole.(...)... so it's grams per mole..."

Relationships: Data missing in the interview.

Personal development: "...in fact, an excellent teacher in Chemistry at Upper Secondary School (...) it was at Upper Secondary School (...) I grasped it.(...) he (the teacher) made a lot of calculations, it was very boring, I had a great advantage when I entered university...". UY doesn't remember how he learnt 'the mole'. He had identified 'the mole' with Avogadro's number as long as he could remember, and had connected it to some known substance. "Well, for instance, I have got an idea of how much 18 g water is (...). Well it's both mass and volume, I think. (...) Because, I mean,... it's totally impossible to understand

the magnitude of Avogadro's number. I have to remember this number... It's like Planck's constant and all these natural constants (...) they exist whether you want them or not."

Textbook at Upper Secondary School :Böös, Leden, & Lundberg.

Appendix IV

Swedish quotations in chapter 4 in original:

> ... voro till ziffran noggrannare än någon annan samtida kemists, och hafva till större delen blivit bekräftade av de bästa sednare analyser.(Berzelius, 1818, p. 3)

> Lavoisier har ingenting positivt yttrat rörande detta ämne. Han anmärkte endast, att det gafs en förening som alltid sker i bestämda oförändeliga förhållanden och en annan, som kan ske i alla proportioner. (Berzelius , 1818, p. 6)

> Elementen, sade han, hafva ett maximum och minimum, som utgöra yttersta gränsorna för möjligheten av deras föreningar; utom dessa kan ingen förening äga rum, men mellan dessa två punkter äro föreningar möjliga i alla förhållanden, utan några bestämda mellangrader. Då sådana inträffa, bero de af andra tillkommande omständigheter, som vanligast äro antingen cohæsion, hvarigenom en förening stäfvar att antaga fast form, eller expansion, som uppjagar den i gasform. Då elementen i förenings-ögonblicket undergå en stark condensering, sker föreningen alltid i oförändeliga förhållanden, och af denna orsak förenas alltid gasformiga ämnen endast i bestämda förhållanden, t.ex. syrgas och vätgas, qväfoxidgas och syrgas, o.s.v. Men då föreningen befinner sig i samma täthetstillstånd som elementen förut innehade, kunna föreningarna ske i alla förhållanden emellan maximum och minimum. (Berzelius, 1818, p. 7)

> (...) så väl genom sin grundlighet, som genom sin värdighet i stil och fullkomliga frihet från all personlighet, förtjenar att vara en modell för det sätt, varpå stridiga meningar böra framföras. (Berzelius, 1818, p. 9)

> ... att njuta den ärofulla bekräftelse hans ideer vunnit genom Gay-Lussac's upptäckt...och sökte istället ... bevisa att Gay-Lussac misstagit sig... (Berzelius, 1818, p. 14)

A Swedish quotation in chapter 5 in original:

> När missförstånd inte befaras kan kortformen mängd användas. Vid behov kan precisering ske med ord som elektronmängd, fotonmängd osv. (SIS 01 61 74 3.2, SIS handbok, 1982, p. 129)