TOWARDS A PHILOSOPHY OF CHEMISTRY*

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SUMMARY. The paper shows epistemological, methodological and ontological peculiarities of chemistry taken as a classificatory science of materials using experimental methods. Without succumbing to standard interpretations of physical science, chemical methods of experimental investigation, classification, reference, theorizing, prediction and production of new entities are developed one by one as first steps towards a philosophy of chemistry. Chemistry challenges traditional concepts of empirical object, empirical predicate, reference frame and theory, but also the distinction commonly drawn between natural science and technology. Due to its many peculiarities, I propose to treat chemistry philosophically as a special type of science, apart from other sciences.

Key words: philosophy of chemistry, epistemology, experiment, classification, reference, prediction, technology, matter, material properties

1. INTRODUCTION

Compared with their interest in physics, mathematics, biology, psychology and even technology philosophers of science have noticeably neglected chemistry, inspite of its vast influence on everyday life.[1] There is ample literature on the history of chemistry,[2] some of which is even enriched with philosophical considerations,[3] or otherwise motivated to emphasize a Popperian, Lakatosian, Kuhnian or other model of scientific change by using case studies from chemistry.[4] And more than once examples taken from chemistry have been used in general philosophy of science and even in the philosophy of language.[5] But one hardly finds something like a special philosophy of chemistry,[6] although several serious studies have shown that the reduction of chemistry to physics is just too problematic to justify this neglect.[7]

If the reduction of chemistry to physics is not possible, then we are faced with the philosophical task of singling out just what is actually peculiar to

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chemistry from a philosophical point of view. This task is impeded by a fundamental methodological problem: Unfortunately there is no appropriate philosophical method for isolating the peculiarities of particular scientific disciplines in a systematic way. Searching for *peculiarities* seems to be the task of historians, whereas philosophers care about *generalities*. On the other hand, ontology, epistemology, and methodology are topics of philosophy and not of history, and there is no reason a priori, why sciences should not differ in this respect. While we commonly admit some intuitive differences (say between biology and mathematics), there is no systematic method for philosophical investigations which can be used to found a philosophical classification of the sciences.

Due to this (meta-)methodological deficit, we cannot claim to have a systematic philosophy of chemistry in what follows. Instead I shall view chemistry as a *classificatory science of materials which works with experimental methods* and try to single out some ontological, epistemological and methodological peculiarities it displays when compared with other well examined sciences. Starting with the chemist's idea of empirical objects and material properties, I will one by one develop chemical methods of investigation, classification, reference, theorizing, prediction and finish by considering the affinity between chemistry and technology.

2. PRE-ONTOLOGY

Like any other empirical science, chemistry sees empirical objects from a particular view. While the physicist's perspective concentrated on classical primary qualities (nowadays partly replaced by rest mass, charge, spin, charm, color, and so on), the chemist's view in contrast abstracts from all extensive and spatial properties such as coordinates, size, structure, or absolute mass and in some respect number, just as it abstracts from personal and economical value, magical meaning and beauty. That does not mean (as it is often misunderstood) that chemistry deals with macroscopic and presupposed continuous bodies. Actually, chemistry abstracts from micro/macro and continuous/discontinuous distinctions, gives up the spatial reference frame, and even ignores *prima facie,* whether the object is separable into two, three or a thousand drops, crystals or other physical parts. As long as an object can be placed in an experimental context, chemists do not care about the size, form, physical parts, spatial coordinates or the number of its physical parts.[8]

For the chemist, to be an empirical object means only to be available for empirical investigation. The central point I want to make for understanding chemistry is that we must abandon the *a priori* assumptions and ontological commitments of traditional mechanistic epistemology and go beyond the physicalistic reference frame. To have spatial extension (Descartes), primary qualities (Locke), to be "formed" by the *Anschauungsform* space (Kant) or to be localized by spatial coordinates (Newton) – these are attributions based on epistemic results of special investigations, but they are neither *epistemological* conditions for chemical investigations nor are they of any direct interest for chemistry. On the other hand, if an abstraction from mechanistic categories is a necessary epistemical condition for chemical investigation, then mechanistic doctrine is even a barrier for understanding the epistemology of chemistry.

The one and only ontological criterion necessary for an epistemology of empirical investigation, or for being an object of empirical investigation, is the capacity to be empirically investigated, and this can easily be proven by investigation itself. If an object is capable of being investigated materially, I will call it a "material object" keeping in mind that the same object might also be called morphological, economical, astronomical, aesthetical or otherwise.

The following section gives a survey of scientific material investigations.[9]

3. MATERIAL INVESTIGATIONS AND MATERIAL PROPERTIES

3.1. *Experimental conditions and material properties*

Chemists are interested in material properties. A material property is reproducible behaviour within certain reproducible contextual (i.e. experimental) conditions. Unlike the epistemology of the empiristic tradition, in chemistry material properties are not classified according to the behaviour of objects, let alone phenomenalistic qualia, but according to experimental conditions. The conditions in question can be made explicit by listing contextual factors (cf. Schummer 1994):

(1) mechanical forces,
(2) thermodynamical conditions (temperature, hydrostatical pressure),
(3) electromagnetic fields,
(4) other material objects or chemical substances (Section 4),
(5) biological organisms,
(6) ecological systems.

According to the list of contextual factors chemists distinguish between:

(1′) mechanical properties (like elasticity),
(2′) thermodynamical properties (like specific heat capacity, melting point),

(3′) electromagnetic properties (like specific magnetic susceptibility, specific electric conductivity, optical absorption coefficient),

summing up (1′) – (3′) under the name of physical or physico-chemical properties;

(4′) chemical properties (like the capacity for oxidation or the solubility in a certain liquid),
(5′) biological or biochemical properties (like LD_{50}, antibiotic or anaesthetic effect),
(6′) ecological properties (like ozone depletion potential (ODP), greenhouse effect factor).

This list is neither systematically complete nor disjunctive. Because every context can be specified with respect to each of these factors, it is necessary to minimize or standardize the uninteresting factors for each case (working with inert container materials, minimizing electromagnetic fields, controlling thermodynamical standard conditions etc.). If two or more factors of interest are combined, it is possible to create new types of material properties (photo-chemical, thermo-electrical, thermo-electro-chemical etc.) (cf. Schummer 1997c).

3.2. *Behaviour and types of change*

Realistic epistemologies in the empiristic tradition are based on the idea of seeing things as they are in a state free from intervention (depiction-paradigm). In contrast, material investigation consists of studying the changes of material objects (or systems) by controlled intervention using the list of contextual factors (intervention-paradigm[10]). *All material properties are dynamic properties*[11]. Changes can be classified with regard to (1) the object which changes, (2) the kind or dimension of change and (3) the reversibility and repeatability of change.

Ad (1): An experiment can either be described as the behaviour of the material object under investigation in a certain unchanged context (like most physical predicates), as the interactive behaviour of the elements of a system, including the object as well as some or all contextual components (like chemical predicates), or even as the behaviour of a certain contextual component of interest (like some biological and ecological predicates: the sensitivity/immunity of an organism to chemical substances, biological requirements of oxygen etc.). Correspondingly, the predicate is attributed to one or to many objects. The choice is guided by: (a) the object(s) of interest (cf. the last example), (b) ontological customs,[12] and (c) the separability of the behaviour of the components (the reactivity of a chemical mixture is scarcely attributed to a single component). As a consequence, all material properties are dynamic *relations* in a more or less obvious way.

Ad (2): If we neglect the more intricate biological and ecological properties for the moment, the behavior can be described with regard to (a) relative geometrical form, (b) electromagnetic state, (c) thermodynamical state, (d) chemical identity (cf. Section 6). At first glance this seems to strictly correspond to the contextual factors (1) – (4), so that the classification of material properties could be achieved as well according to the behaviour. But there is no change of chemical identity in chemical contexts without simultaneous changes in (a), (b) and (c), sometimes even very obvious as in the case with chemoluminescense, which is a chemical property. And there is no change in (b) and (d) without simultaneous change in (c). On the other hand, changes of chemical identity under certain thermal or optical condition (thermal and photo-dissociation) are not chemical but thermal or optical properties. And if a material object shatters in a thousand pieces when exposed to high temperature or if it is separated by destillation, nobody would take these to be mechanical properties. Contrary to phenomenalistic intuitions material properties are classified according to contextual factors.

Although chemistry is based on the substantial differences between materials (cf. Sections 4–5), there is no reason to do without *quantitative predicates*. The widely held opinion, according to which chemistry is a science of the qualitative, is wrong. Instead, all types of behaviour capable of being grasped in qualitative terms can be grasped in quantitative terms as well. This is obviously the case with physico-chemical properties (cf. Schummer 1997c). Quantitative description of chemical change is done by giving the change of relative masses of chemical compounds during the investigation. But chemical investigations are actually more intricate, because they include a lot of experimental tests before and after the behaviour to determine the change of chemical identity according to the chemical classification (cf. Section 5). Substantial changes are different from qualitative changes and cannot be grasped in quantitative terms.

From the philosophical point of view the most striking peculiarity of material behaviour might be the *abstraction from form, size and mass* as mentioned in the last section. The three main procedures (standardization, forming intensive quantities, and relative quantities) can easily be explained with quantitative predicates. If the behaviour is described in terms of geometrical form, as for instance mechanical properties like elasticity, all material test objects must have a standard geometrical form. The behaviour is described in terms of *standardized quantities* by giving the quantitative deviation from standard form when exposed to a certain mechanical force. As an alternative, one can grasp the individual form of the test object by specific form parameters and divide the quantitative deviation of form through the form parameters. If the behaviour is described in terms of extensive quantities (depending directly on mass or size) in the first step, then one can divide through any other extensive quantity next. The second procedure yields quantities which are independent of form, size and mass and are called *intensive or specific quantities*. The third procedure is peculiar to investigations with more than one material object. If the behaviour is described in terms of mass or volume, then abstraction is achieved by dividing the masses or volumes with each other yielding *proportional or relative quantities*. There is no quantity of relevance for material classification which is not standardized, specific or relative. But sometimes the procedure of abstraction is not necessary, because the measured quantity is already intensive (e.g. phase transition temperatures and pressures).

Ad (3): Behaviour can be *reversibile or irreversible* and the investigation can be repeatable or not repeatable with the same object. From the thermodynamical point of view every real change (i.e. a finitely large step in finitely short time) of thermodynamical parameters of a thermodynamical closed system is irreversible according to the Second Law. But if we concentrate on the material object as an open system, we can make the distinction between two types of change: (a) The change is automatically reversible in the sense that the initial state is restored when the object is exposed to initial conditions. In this case the investigation is repeatable and the result is reproducible *ad libitum* (like most of the electromagnetic and thermodynamic investigations). (b) The initial state is not restored when exposed to initial conditions.

This last type of change, which is typical for chemical investigations, creates ontological, logical and methodological problems. When the result is not reproducible in the same context, at least one property of the material object has obviously changed. Consequently, one must distinguish between material objects before and after the test. This has challenged substantialistic ontology with problems of radical *coming-to-be and passing-away* since the ancient Greeks,[13] which seems to be the strongest argument for reconstructing the change on a theoretical level in substantialistic (atomistic) terms. On the logical level material predicates must be stated as complex dynamic relations with two strictly separated classes of variables. Moreover, because the object of interest vanishes during the test, the change raises the *methodological* problem that chemical investigation of a single material object is neither reproducible nor enriched by further tests.[14] In Section 4 we shall see how the methodological problem is operationally solved by sampling technique.

3.3. *Programs of property reduction*[15]

A reductive program of material properties can be defined as follows: A certain kind of material property is to be reinterpreted so that the object behaviour and all contextual conditions are described only in terms of a different kind of property. Reductive programs make an epistemological shift from the intervention-paradigm to the depiction-paradigm, from the experimenting to the supervising point of view – the act of experimental experience is described as the interaction of elements of the same type within a closed system. There is also strong tendency to postulate new (theoretical) entities, which are completely determined by a single type of property, because nobody can easily deny that material objects reveal a variety of properties.

While physicalistic programs try to reduce contextual factors and object behaviour to so-called fundamental interactions (electromagnetic, strong, weak, and gravitational) and search for a theory of unifying interaction, this is pragmatically uninteresting for chemists. Instead, there are some particular and more or less successful reductive programs:

(1) Reduction of ecological and biological properties to chemical properties of elements of ecological and biological systems;
(2) reduction of chemical properties to electromagnetical properties of certain theoretical entities;[16]
(3) mechanic, thermodynamic and electromagnetic properties in terms of electromagnetical properties of certain theoretical entities.

Theoretical entities in programs (2) and (3) belong to a proliferating bunch of models somewhere between quantum and classical mechanics with a shot of (quantum) electrodynamics and enhanced with statistics.

Program (3) is the most successful one due to the pragmatic variety of its models and the correspondence between reducing and reduced properties. The striking step for the reduction of thermodynamical properties is the equivalence postulate of temperature and mean kinetic energy. But the equivalence is challenged by the shift from classical mechanics to quantum mechanics, which implies a shift from classical to quantum statistics.[17] Anyway, temperature is no material property for classificatory purposes, because every material object reveals the same temperature under certain context conditions. Instead, phase transition temperatures are specific quantities, but these are still hard to handle in the reductive program.

Program (2) is quite less successful as it seems to be at first glance. There are actually some quantum mechanical models of the chemical bonding of isolated molecules,[18] but there is no successful *general* theory concerning the *interactive change* of chemical bonds between several molecules. The theoretical account of chemistry will be discussed in detail in Section 7.

Program (1) is challenged by the functional complexity of biological and ecological systems and the amount of chemical substances involved. A shift to laboratory contexts is necessary, because *in vivo* contexts are difficult to standardize and formalize. Some progress is made by functional analysis leading to partial processes, which can be described in (bio- or geo-)chemical terms (like enzymatic and atmospheric reactions, metabolism etc.).

3.4. *Epistemological and logical peculiarities*

Material properties bear some philosophical curiosities worth discussing in detail. In contrast to the philosophically preferred primary qualities or phenomenalistic qualia, material properties are *extrinsical* in the sense of depending irreducibly on contextual conditions. Material predicates are attributed to material objects *in relation* to certain contexts. As we have seen, predicate precision is achieved by defining the contextual factors and precisely describing the relevant components of the context. The less precise the description, the less informative the statement about material properties. Statements like “it melts”, “it reacts” or “it is red” (to say nothing about “here, now: red”) are nearly without any empirical content about the material object in question as long as we do not explicitly or implicitly know the context of experience.[19]

In ordinary language the meaning of material predicates is implicitly bound to ordinary contexts of experience. When we say that something is red, we implicitly presuppose ordinary lighting. The fallacy of phenomenalism is the neglect of implicit knowledge about the context which actually is a necessary condition of the possibility of material experience. In contrast, material sciences try to make contextual conditions explicit, precise and complete in the relevant aspects. That is why material sciences are experimental sciences in a very strict sense: Every empirical predicate must be operationally defined according to a certain experimental context including the rules to perform the experiment in question.

Context relativity of material predicates implies some very unwelcome consequences for traditional philosophy of science: (1) nonderivableness, (2) inductivity, (3) vagueness, (4) incompleteness.

Ad (1): There is no precise definition of material predicates which does not make ontological presuppositions concerning the contextual components.[20] But precise description of contextual components already requires the attribution of material predicates, as long as the components are themselves material objects. This is obviously of special importance for chemical predicates. Hence, any precise definition of dispositional predicates presupposes precisely defined dispositional predicates. In material science material predicates cannot be founded on the basis of context-free predicates, because there are no basic predicates such as were assumed in logical positivism.[21] Alternatively, a given set of vague dispositional predicates implicitly bound to ordinary contexts must be stated more precisely and enlarged in genealogical steps: Determining the context more precisely provides more precise predicates to determine the context more precisely, and so on.

Ad (2): The difference between dispositional and non-dispositional (manifest) material predicates is not based on context dependence (extrinsity vs. intrinsity); instead it is based on the pragmatical difference of intended instances of attribution. By saying "x melts under contextual conditions y" I can either (a) describe the singular behaviour of x in a certain experiment with conditions of kind y or (b) express my expectation that x will always melt whenever it is exposed to contextual conditions of kind y. The so-called theoretical or law-like character of dispositional predicates does not arise from misleading logical problems of defining them by context independant (phenomenalistical) basic predicates (Carnap 1953) but from the inductive usage which shifts from (a) to (b). If an empirical statement F(x) means that we can experience F with x, whenever we want, then there is no empirical predicate without inductive use. But that does not mean, that F is not empirical, otherwise there would be no empirical predicate and no empirical science at all. F is empirical, because the intended instances of attribution of F are empirical contexts.

Ad (3): Material predicates have an unavoidable element of uncertainty. If the precise definition of a material predicate requires the precise description of the context, this can only be achieved by giving a complete description of the actual state of the entire world. The obvious cognitive problems are joined by logical and linguistic problems. Dispositional predicates must be applicable to infinitely many situations of the same material object (induction from (a) to (b)), although the state of the world changes. They must also be useful in many other instances for many other people, otherwise it is practically worthless. The problem can be tackled by looking for those *relevant* contextual conditions on which the behaviour of the material test object significantly depends, i.e. looking for functional laws. There is no guarantee for the completeness of the relevant conditions or for the correctness of the functional laws, so there will always remain an residue vagueness.[22]

Ad (4): Material predicates are created by inventing new experimental contexts. There seems to be no limit to new experimental contexts apart from limits of our imaginations. The number of material properties suitable for characterizing a particular material object can be increased *ad libitum*. This is again of special importance for chemical predicates because of their relational structure. To create a new chemical context means to choose a new combination of chemical substances and conditions. The immense proliferation of new chemical substances (cf. Section 9) goes hand in hand with an exponential proliferation of new chemical properties. As a consequence, our knowledge about material properties will always remain incomplete; in material science, we must abandon the epistemic aim of complete knowledge. The best we can do is to consider what kind of knowledge might be relevant for special purposes and start the experimental investigation afterwards. Because one must first know, which property might be of interest, material objects turn up a lot of surprises when put into new contexts by chance. This seems to be the epistemological background for some of the unwelcome ecological surprises we have become aware of the last few decades (cf. Schummer 1996c/d).

4. MATERIAL HIERARCHY BASED ON EXPERIMENTAL OPERATIONS

By exposing a material object x_0 to certain contextual conditions it may be separated into two or more objects x_i with different material properties but not further separable under the same conditions. Experimental contexts like this are of central importance for chemistry as a classificatory science using experimental methods: (1) Material objects are operationally connected by an asymmetrical relation (classification in the vertical dimension) and one gets experimental rules to produce material objects of sort x_i from material objects of sort x_0. (2) Separability/inseparability with respect to a certain context is itself a material property which groups material objects in one of two classes according to operational criteria (classification in the horizontal dimension). If (1) and (2) are combined, an operational hierarchy of classes of material objects can be gained. We must look for an ordered *sequence of separation techniques* (T_0, T_l, ..., T_n) so that for any material object x there is a technique T_i for which holds: x is inseparable by techniques T_j if $j \geq i$ and separable if $j < i$.

In chemistry there is an ordered sequence of three groups of separation techniques according to which materials can be roughly put in a hierarchic order. (1) In contexts with mechanical forces (cutting, grinding and sorting according to density by sedimentation or centrifugation, filtration etc.) one decides between *heterogeneous* and *homogeneous* materials. (2) In contexts with thermic energy and hydrostatic pressure (both within conventional limits) homogeneous materials are divided into *mixed* and *pure* materials (distillation, condensation, melting, crystallizing, sublimation); pure materials are also called *chemical substances*. (3) In contexts with electric fields or thermic energy and hydrostatic pressure (on a higher level) pure materials are divided into *compound* and *elementary* materials (cf. Schummer 1996a).

To avoid fallacies of strict or blind operationalism we should mention some problems. First, each separation technique must be applied several (ideally infinitely many) times until there is no more separation effect noticable. Inseparability (especially pureness) is a kind of convergence point of repeated operations depending pragmatically on the standard of resolution. Second, operational criteria for chemical substances based on thermal separation technique (i.e. the so-called phase rule[23]) must sometimes be applied very carefully (thermodynamic instable compounds, azeotropic mixtures, dissociative compounds in equilibrium) and sometimes even modified or supplemented by chemical techniques (e.g. enantiomers).[24]

In spite of the development of several spectroscopic methods for purity tests, conventional techniques still remain *methodologically primary* for two reasons: First, there is no pure material object and consequently nothing to investigate in chemistry, if it is not first produced according to the corresponding laboratory rules. Second, no spectroscopic method yields information about purity as long as nobody knows what the spectra of a certain pure material looks like. There are two ways to use spectroscopic methods for purity tests: Either we produce a pure material at first, prove purity by conventional methods and then record the spectra as a fingerprint for any further spectroscopic purity test; in this case the secondary status is obvious. Or we anticipate spectroscopic results by theoretically predicting electromagnetical properties of materials which might be pure according to a certain theory. The second way obviously requires a theoretical concept of pure materials and there is indeed a theoretical account available for making predictions about electromagnetic properties. But unfortunately there is in turn no theory for the *general* distinction between spectra of pure and mixed materials from the spectrographic data alone. Whatever the theoretical concept of pure materials may be, it cannot work as a purity/impurity *criterion* for logical reasons, because there is no proof of impurity. Imagine a chemist who is investigating a material object exclusively with spectroscopic methods. His experimental result does not fit to anything that is predicted to be a result of supposedly pure materials. So he must not conclude that the material is mixed, because it might be a hitherto unknown pure material which he did not take into account in theory. The realm of pure materials is not closed *a priori*, instead chemists find about 3.000 new ones each day (Section 9). So we must take conventional purity criteria to be primary.

The way in which materials are operationally ordered has some important consequences for chemistry: (1) a methodological basis for sample technique, (2) a discontinuity within the realm of chemical substances, and (3) conclusions about the elementary basis of material classification.

Ad (1): According to the definition of homogeneous materials, homogeneous objects cannot be broken down to pieces with different material properties by mechanical methods alone. Hence, any mechanical separation of a homogeneous object yields materially indistinguishable objects. That is the justification for the *technique of sampling* which is something like the methodological basis of chemistry as a *science of changeabilities*. If the object under investigation changes (not to say: vanishes) during the first test, then there is no more experience of the same object; hence, classification according to changeabilities would be impossible. But by sampling (i.e. mechanical separation) you can make a lot of experiments with samples each giving informations about material properties of the whole object.[25]

Ad (2): From the classificatory point of view purification technique is of greatest importance for chemistry, for it reduces the classification of homogeneous materials to the classification of pure materials and their relations to mixed materials. Because the realm of homogeneous materials is continuous according to any quantitative property, direct classification would require never-ending work. Let material quantities be represented by real numbers, then any systematical classification of homogeneous materials would have to take into account non-countable infinitely many possibilities to the power of the number of material quantities. Instead, the classificatory problem is solved by picking out distinct materials in such a way that the rest of the homogeneous materials can be described by quantitative relations of them. Purification technique provides the central step from the continuous to the discontinuous realm by complying with three conditions:

The method must be able (a) to single out certain materials definitely, (b) to provide a criterion for identification, and (c) to provide a new type of classification for the remaining homogeneous materials in order to avoid the sketched classificatory effort. I claim that operational separation is the only method that complies with all three conditions simultaneously: separation singles out materials as the products of separation, separability/unseparability works as a criterion for identification, and every separable material can be classified according to the products of its separation.

Let us regard how the singling out of distinct materials is managed by purification technique. According to the thermodynamic criterion of pure materials, phase transitions (e.g. vaporization) occur without change of temperature at certain pressure,[26] i.e. pure materials have constant phase transition temperatures as a particular thermodynamic property (e.g. boiling-point) given a certain pressure. Because the phases do not differ in material properties at any time,[27] which is obviously the case with transition temperature, there is no material separation by phase transition of pure materials. If temperature continuously changes during phase transition, the material is called mixed material. Because the phase transition of mixed materials yields phases with different material properties, which is obviously the case with transition temperature, it goes along with material separation.[28] Purification is achieved by repeating material separation with one of the two phases until the criterion for pure materials is fulfilled. In the course of this procedure every value of quantitative material properties (including phase transition temperature) converges towards a certain point which is the value of the inseparable material, the chemical substance.

Ad (3): Since Lavoisier the definition of chemical elements has no longer been given by Aristotle’s substantial forms but by operational definition, i.e. the unseparability with respect to any separation techniques. Due to this definition, a material once characterized as an element can later lose its elemental status by further separation, but it will never lose its classificatory function on the vertical dimension with respect to pure, homogeneous and heterogeneous materials. *Prima facie* there seems to be no reason why the former elements cannot be separated into compound, mixed or heterogeneous materials by more sophisticated techniques which would yield circular classification structures. But such a technique would violate the norm for an ordered sequence of separation techniques (see above), because the separation products would be separable by a technique of lower order; hence, any circularity is excluded by operational definition. Moreover, we can draw rough conclusions about the relative number of elements from the ordered sequence. For the set of elements must be a subset of pure materials which is a subset of homogeneous materials being a subset of materials. But what about the proportion of elements and compounds? From the classificatory point of view it would be of special interest, that the elementary basis is smaller than the next level, as it was achieved in the Aristotelian hierarchy of materials. Can we draw similiar conclusions as we did concerning the relation of pure and mixed materials? Compounds can be classified according to the combination of kind and relative mass of their elementary separation products. From the mathematical point of view a finite set of elements allows infinitely many (quantitative) combinations. But there is no *a priori* argument for concluding how many mathematical combinations actually correspond to empirically possible compounds. One cannot even exclude that infinitely many elements do not combine to compounds at all. Hence, there seems to be no *a priori* guarantee that the number of elements is smaller than the number of compounds – as far as we know, this is the most lucky *empirical* fact for classificatory purposes in chemistry.[29]

The operational definition of chemical elements allows historical flexibility and, moreover, it allows pragmatic criteria for what might be called the *relative elementary basis for classificatory purposes*. For instance, chemical elements have been separated into isotopes by sophisticated techniques for many decades, but outside of nuclear chemistry there is no need to take isotopes as the basis of material classification. For most chemical purposes there is no gain, while the classificatory costs would rise immensely. This seems to indicate a shift from metaphysical philosophy of nature to pragmatic classificatory science.

5. CHEMICAL REACTIONS AND CHEMICAL PREDICATES

With the concepts of chemical element and chemical substance we can give a precise definition of chemical reaction. Given a sample of any kind of material (pure, mixed or heterogeneous) at time t_1 and $t_2 > t_1$ then we speak of a *chemical reaction*, if and only if there is a change of number, kind or mass of pure materials from t_1 to t_2, while number, kind and mass of elementary materials remain constant. To find out if a sample has undergone a chemical reaction, one has to analyse it at t_1 and t_2 according to the separation hierarchy and compare the results on the level of pure and elementary materials.[30]

According to the definition of chemical reaction chemical investigations can be documented by listing the pure materials including masses at t_1 on the left side and at t_2 on the right side and connecting both sides by an arrow. To give a full account, one must add a complete description of the experimental conditions from t_1 to t_2 including all operations like stirring, shaking etc. If x_i is a name of a chemical substance, m_i the detected mass of x_i and b the complete list of conditions then one can write the result in a general form:

$$(x_1{:}m_1), (x_2{:}m_2), \ldots, (x_j{:}m_j) \xrightarrow{b} (x_{j+1}{:}m_{j+1}), (x_{j+2}{:}m_{j+2}), \ldots, (x_k{:}m_k).$$

Two further steps are nesessary to design a chemical predicate, which is indeed a highly sophisticated construction. First, one must generalize the result from certain mass values to any mass values by reformulating it in terms of mass proportions or relative masses and generalized conditions B.[31] And secondly, the complex processual relation between the chemical substances in question and the experimental conditions must be remodelled into a dispositional predicate which can be attributed to a single chemical substance. Chemical substances appear on both sides, so there are exactly *two types of chemical predicates*, which are explicitly formulated for x_j and x_k, respectively:

P1: “having the potential to produce chemical substances x_{j+1}, x_{j+2}, ..., x_k in mass proportions m_{j+1}/m_j, m_{j+2}/m_j, ..., m_k/m_j under certain general conditions B by chemical reaction with the chemical substances x_1, x_2, ..., x_{j-1} in mass proportions m_1/m_j, m_2/m_j, ...,m_{j-1}/m_j”

P2: “having the potential to be produced by chemical reaction of chemical substances x_1, x_2, ..., x_j in mass proportions m_1/m_k, m_2/m_k, ..., m_j/m_k under certain general conditions B together with the chemical substances x_{j+1}, x_{j+2}, ..., x_{k-1} in mass proportions m_{j+1}/m_k,m_{j+2}/m_k, ..., m_{k-1}/m_k”

Summarizing the results of this section: (1) Chemical reactions are material changes on the level of chemical substances with conservation on the level of elements; (2) Chemical reactions can be described by complex processual relations; (3) Two types of chemical predicates can be derived for chemical substances describing either the *potential to produce or the potential to be produced*.

6. THE CHEMICAL REFERENCE FRAME: CHEMICAL IDENTITY AND TYPES OF REFERENCES

All chemical relations, drawn from chemical reactions as shown in the last section, constitute a complex chemical network. This network connects all chemical substances with each other directly or indirectly in many and distinct ways. Unlike physics the reference frame of chemistry is not a physical space-time universe but the chemical network, which can be read as "chemical space" (cf. Schummer 1996a). While in physics two objects are physically identical, if and only if they have the same space-time coordinates, two objects are *chemically identical*, if and only if they are found at the same place in the chemical network, which means that they have the same chemical properties.[32] Chemical identity ignores differences with respect to the object's shape, size and physical place as well as to the physical state of matter (gaseous, liquid, solid).[33]

In the philosophy of language the term "reference" has sometimes been used in the sense of "denotation", indicating a kind of magic relation between words and things. Meanwhile it seems to be accepted that reference is an asymmetric relation between people and objects,[34] in the sense of people's selective choice of an object, which is guided by certain selection rules embedded in language. Chemistry has three types of references: Reference guided by (1) labels, (2) chemical analysis, (3) experimental rules for production.

Ad (1): Imagine a chemist in the laboratory, who needs a certain reagent for his experiment. If the laboratory is well equipped, he grasps the bottle labeled with the name of the reagent in question. This is the trivial case of chemical reference; it illustrates, how the relation between words and objects actually works.

Ad (2): Our chemist has got a piece of material and is asked to identify it in terms of chemical substances. By the art of chemical analysis he takes the sample to pieces of different chemical substances and makes a lot of experiments to localize each in the chemical reference frame. This case corresponds to the philosophical theory according to which reference is an act of selection or recognition guided by neccessary and sufficient conditions for identification.

Ad (3): Imagine that the laboratory is not well equipped and our chemist lacks a certain reagent. To emphasize the difference between the chemical and the physical reference frame, imagine further that the reagent is sold out everywhere and that there is not a drop of this reagent in the whole (physical) world. While searching for the reagent is useless in physical space, it is not so in chemical space. Remember that there are two types of chemical properties: the potential to produce and the potential to be produced (Section 5). The first type of properties was used for references of type 2 by performing reaction tests, the second type can be used now. If the chemist really knows what he is looking for, then he also knows how to produce it. Starting with different materials he has to walk (reaction) step by (reaction) step in chemical space until he arrives at the place of the chemical substance in question. The most interesting point of the chemical reference frame is, that it provides us with reference rules for chemical substances in the sense of laboratory rules to produce them. Philosophers have overlooked this kind of experimental reference, which seems to be typical for chemistry.[35]

7. CHEMICAL THEORY: THE SIGN SYSTEM OF STRUCTURAL FORMULAE AND REACTION MECHANISMS

Chemistry is a science of dynamic relations. Therefore, any successful theoretical account of chemistry has to systematize chemical relations by mapping the chemical network. Many hopes were placed in quantum mechanics. But the obvious success in explaining electromagnetical and even thermodynamical properties made people blind for the fact that quantum mechanics is rather silent about *chemical* properties.[36]

The most successful account is the sign system of structural formulae and reaction mechanisms developed in organic chemistry. It systematically maps the chemical network of (organic) substances, it allows the prediction of new chemical substances and even provides laboratory rules to realize them. The chemical sign system has been developed since the 1860s only by chemical methods, it is methodologically independent of quantum mechanics and has been totally ignored by philosophers of science and language, although it is the key instrument for the production of millions of new chemical substances, which themselves contribute to the philosopher's world daily.

To understand this remarkable semiotic instrument, it is necessary to examine its semiotic peculiarities (cf. Schummer 1996b). But first we must clear up the widely held misconception, that structural formulae are *iconic* representations. According to Peirce an icon is related to his object by some properties in common. Because structural formulae and quantum mechanical entities do not have any (relevant) properties in common, the only objects in question are isolated classical molecules consisting of classical atoms in definite structural composition and lacking intra- and intermolecular dynamics. To shorten the argument let us ignore the varieties of pictographic styles in chemistry (cf. Hoffmann and Laszlo 1991) and take the structural formulae as exact two-dimensional portrays of classical molecules. The object relation is achieved by structural properties of the sign corresponding to structural properties of the molecule. This is supposedly the common reading of structural formulae by philosophers.

But the central problem of iconic interpretations is that the signs have lost any information about material properties. There is indeed no way to represent material properties by structural properties iconically, because both are of logically different type: extrinsic and dynamic, on the one hand and intrinsic and static on the other. There would be no reason at all to construct the complex chemical sign language, if it does not contain any information about material and especially chemical properties. But of course it does, and it does so on a highly sophisticated level enabling chemists to even grasp a lot of chemical information from a structural formula never seen before.

It would be too complex to develop the chemical sign system here, so I only make some general remarks about the semiotic strategy, how to represent dynamic relations (e.g. chemical properties) by static means of structural formulae.[37] Given a set of signs and a set of semiotic rules for allowed changes (transformations, connections, separations, exchanges, etc.) of the signs, then one can define *semiotic properties* of the sign, which have the same logical structure as chemical properties (dynamic and relational). According to the rules, the signs can be characterized by allowed semiotic changeabilities instead of structural properties by shifting from the static to the dynamic point of view. In correspondence to the chemical properties (cf. Section 5) one can make the distinction between the potential of a sign to generate new signs and the potential to be generated by different signs. To construct an ideal sign language for chemical purposes one has to transfer the chemical relations between chemical substances into semiotical relations between structural formulae, so that every chemical substance definitely corresponds to a single structural formula and every laboratory rule for chemical experiments definitely corresponds to a semiotic rule for structural formulae. The semiotic task of chemistry is, in other words, to map the chemical network by a sign system, which could be called a "super-icon" in Peirce's terminology.

In chemistry the semiotic rules are called "reaction mechanisms". The number of reaction mechanisms is ever increasing by taking into account (1) new chemical substances, (2) differences between substances of a substance class, and (3) differences between contextual conditions. The limits of sophisticating the chemical sign system are of pragmatical nature, i.e. semiotic rules must be comprehensive. If modifications according to (2) and (3) are carried to extremes, so that each rule is applicable to a single type of experiment only, then rules loose their comprehensive character. To ensure general application, it is necessary to systematize the semiotic elements according to a systematization of chemical properties and experimental operations and to modify the rules deliberately. While iconic languages are sophisticated by working out pictographic details of each sign, this would be disastrous for the chemical sign system.

Someone who does not master the reaction mechanisms will misinterpret structural formulae as icons and may draw misleading philosophical consequences. The impact of 17th century mechanical philosophy with its preference for primary qualities is still present in the "pictographic molecular paradigm" (Luisi/Thomas 1990). The development of physical techniques for structural investigation in 20th century, like x-ray diffraction and spectroscopic methods, seems to have given new support. But (by celebrating tremendous sets of physical structure data as a kind of "visual" proof for atomic structure) one easily forgets to ask what kind of information do we get by this. Indeed, the price for the metaphysical ideal of exact structural pictographs can be the total lack of chemical information. For as long as it is not integrated into the chemical sign system by semiotic rules, a structure provided by x-ray technique is chemically meaningless. And as long as nature does not speak to us, there is no apparatus that automatically provides semiotic rules.

8. TYPES OF PREDICTION

In chemistry there are at least four types of prediction. We distinguish between predictions of properties with the help of (1) sample technique, (2) classification system, (3) analogy, and (4) predictions of new entities by classification. While (1) is ensured by *a priori* reasons, predictive reasoning of types (2)–(4) is based either on empirical or on theoretical grounds.

Ad (1): Take a sample of a piece of homogeneous material and investigate some material property. Then you can predict the same property for any other sample of the same piece, if you follow the rules of sample technique. This is the trivial case of prediction, though it is of the greatest methodological importance. It is actually a peculiarity of material science, because it is guaranteed by the operational definition of pure materials (cf. Section 4).[38]

Ad (2): If a piece of material is identified as belonging to a certain chemical substance, then one can predict all properties corresponding to the chemical substance. This type of prediction implies, that identification works by investigation of a limited number of properties, which is indeed the case in chemistry. (Remember that the number of chemical properties can be increased *ad libitum*; hence, a complete chemical investigation would be

an endless enterprise). But what should we take as identifying properties? There are two alternatives:
a) Take a quite arbitrary series of properties until every other well-known chemical substance of the classification is excluded. Then you can predict any other specific property corresponding to the particular chemical substance. This type of prediction is based on the empirical classification system.
b) If the sign system of structural formulae and reaction mechanism is worked out in the sense of mapping the chemical network, then determining the structural formula is equivalent to its localization in the chemical network. In contrast to type 2a) the selection of identifying properties is not totally arbitrary now but guided by the theoretical sign system, whereas there are many ways to determine the structural formula. This type of prediction is based on theory.

Both types of prediction are peculiar to chemistry, for in contrast to other classificatory sciences there is no definite general catalogue of properties in chemistry which functions as necessary and sufficient condition for identification.

Ad (3): Chemical classification provides classes of chemical substances due to similiar chemical properties. If some new properties are discovered belonging to certain examples of a class, one can make a prediction about similar properties belonging to other examples of the same class. This is the familiar type of prediction by analogy. Analogical reasoning is possible either on the level of empirical properties or on the level of structural formulae. Analogical reasoning on the level of structural formulae, e.g. looking for structural similarities, seems to be vague, but it is one of the most powerful heuristic tools in chemistry.

Ad (4): Classificatory systems in the strict sense transcendend the empirical realm in so far as they provide criteria for still missing but possible classificatory objects according to the systematics. A well-known example from chemistry is the prediction of new chemical elements from the periodic table. A neglected but more instructive example is the prediction of new chemical substances of a class by analogy, for instance the prediction of homologues in early organic chemistry: A and B are classes of chemical substances $\{a_1, a_2, ..., a_j, ..., a_k\}$ and $\{b_1, b_2, ..., b_j\}$ respectively, r is a special reagent so that one can produce any b_i by chemical reaction with r and a_i $(1 \leq i \leq j)$. Then we can make predictions about the production of hitherto unknown chemical substances b_{j+1} ..., b_k of class B by chemical reaction with r and a_{j+1} ..., a_k.

This type of prediction is put on a theoretical basis by the system of structural formulae and reaction mechanisms. With regard to predicting new entities the chemical sign system seems to be the most powerful predictive theory in science at all, though ignored throughout by philosophers of science. By applying semiotic rules to well-known structural formulae chemists have generated millions of new structural formulae during the last hundred years. Predictions of this type concern the existence of new chemical substances and certain (identifying) properties as well as chemical properties which give information about how to produce them by experiment. To prove the prediction one simply has to translate the semiotic rules into laboratory rules.

In the philosophy of science entities which are postulated by theory are called theoretical entities. Hence, new chemical substances predicted by chemical theory are *theoretical entities*. Someone who believes that theoretical entities exist in the same sense as empirical entities is called a scientific realist with respect to theoretical entities. Compared with high energy physicists chemists seem to have much better reason to be *scientific realists*.

9. POIETICAL CHARACTER AND TECHNOLOGICAL RELEVANCE

As a classificatory science with experimental methods chemistry has an inherent poietical character and technological relevance (cf. Schummer 1995d/1996d). The poietical character was already emphasized by describing the two types of chemical properties: the potential to produce and the potential to be produced. On the very experimental level chemistry reveals a momentum to multiply the number of its objects, because every chemical experiment possibly generates new chemical substances for new chemical experiments and so on. With the help of the chemical sign system the proliferation of chemical substances can be controlled theoretically. As a result, the number of chemical substances has increased to more than 16 million in 1995 and about 1 million (!) new ones are made a year now. There is actually no comparable natural science with such a productive power concerning its own classificatory objects (cf. Schummer 1997a/b).

From a pure epistemic point of view the proliferation of chemical substances can be read as an enlargement of the empirical content of chemical theory. Chemistry as a *science of the realm of possible chemical substances* tries to give theoretically based answers to the question which chemical substances are empirically possible, i.e. experimentally realizable, and how to realize them (cf. Schummer, 1996a). Predictions are made and tested by experimental production. Unlike falsificationism, there is no need to give up chemical theory, if the experimental product has not been predicted, for there is no simple and universal theory in chemistry. In contrast, the complex sign system is modified, supplemented or refined step by step by carefully investigating the unexpected products. The procedure of exhausting refinement tends to map the whole network of possible chemical substances on a theoretical level. If perfect mapping of the chemical network were the aim of chemistry, then the tremendous production of chemical substances would just be a by-product of the exhausting method.

Based on the epistemological peculiarities of chemistry a quite unique alliance between academic science and industry began in the rise of organic chemistry of natural products about a hundred years ago. While chemical industry was looking for natural products as pharmaceuticals, dyes, pesticides etc., academic chemistry was challenged to analyse them with chemical methods. The chemical efforts of determining structural formulae for chemical identification always provided laboratory rules to produce the natural products (c.f. Section 6). As long as synthetic production was cheaper than isolation from natural sources, academic knowledge was of direct use for industrial fabrication, although academics could regard their knowledge as pure epistemic or even platonistic.

Nowadays the predictive power of chemical methods allows the production of new materials with desired properties in many areas of application. As a neccessary condition for technical applications the classificatory system of chemical substances must be enriched by the relevant properties on an empirical and a theoretical level. In the area of pharmaceutical application the systematical investigation of biological properties is still young. Some success has already been made in the (bio-)chemistry of proteins, where correlations between molecular structure and biological properties have led to some (bio-)chemical theories of biological properties. That is the theoretical basis for the so called “molecular modelling”: the production of new proteins with desired biological properties. If the methods of definite gene manipulation belong to chemistry, then chemistry has even reached a new level of productive activity, according to the common distinction which the philosophy of technology makes between the use of instruments and the production of instruments. Gene technique can be regarded as the chemical production of biological instruments to produce chemical substances with desired biological properties.

These short remarks should illustrate that the border between natural science and technology or between pure and applied science cannot easily be drawn with respect to chemistry (cf. Schummer 1997d). Poietical activity does not imply technical production, whereas poietical knowledge for pure epistemic reasons can exactly correspond to poietical knowledge for technical purposes. But if systematical research concentrates on technically relevant properties, then there seems to be little difference between natural science and technology.

10. CONCLUSION

In the course of this paper I have sketched several epistemological, methodological and ontological peculiarities of chemistry as a classificatory science working with experimental methods. From the chemical point of view we must abstract from classical primary qualities (extensive or spatial properties like coordinates, size, structure, and number) and concentrate on context-dependent dynamic properties including substantial changeabilities. Changeabilities with respect to certain experimental conditions and procedures are of central importance for classificatory purposes in two dimensions: the hierarchical order of materials and the relational network of chemical substances. In contrast to physics, the latter works as chemical reference frame or chemical space. It provides criteria for chemical identity and reference rules in an experimental sense, for chemical knowledge about a material entity implies the knowledge of how to produce it. The only theory which maps the chemical network by representing chemical relations is a semiotic system of structural formulae and reaction mechanisms being improved over the last hundred years. It is non-physicalistic, it need even not be interpreted as micro-reductive – but it is able to systematize experimental knowledge about chemical reactions and it is highly predictive. We have distinguished between different types of reference and different types of prediction, most of them being peculiar to chemistry. The methods for theory-guided prediction of new entities together with the experimental methods of reference make chemistry a classificatory science, which produces about 1 mio new classificatory objects a year now. This immense poietical activity seems to challenge the distinction made between natural science and technology.

Unlike physical interest in a few intrinsic quantities and fundamental theories, chemistry is interested in the variety of context-dependent dynamic properties with special reference to substantial changeabilities in order to improve the classification of its manifold objects. Unlike biological or geological classifications which work with phenomenal similarities or original relationships, chemical classification is based on dynamic relations performed by experiment. And unlike technology, the poietical activity in chemistry may (but need not) be read as guided by the aim of classificatory completeness on theoretical grounds. Because it seems hard to decide whether chemistry more resembles physics, biology, technology or what ever, I propose to handle it as its own type of science.

NOTES

[*] A short extract of this paper was first read at the 10th International Congress of Logic, Methodology and Philosophy of Science, Florence, August 19–25, 1995.

[1] Cf. van Brakel/Vermeeren 1981; some reasons for the neglect are discussed in Psarros et al. 1996.

[2] For a critical and complete survey of the historiography of chemistry in the last two centuries cf. Weyer 1974; an international journal for the history of chemistry is *Ambix*, annual bibliographies are prepared by *Isis*.

[3] Cf. for instance Böhm 1961, Ströker 1967/1982 or Nye 1972/1993.

[4] To give an arbitrary example for each: Le Grand (1976-77) favours the Kuhnian approach, Musgrave (1976) holds on to the Lakatosian model, and Akeroyd (1986) tries to confirm the Popperian strict falsificationsm; for some new and more sophisticated interpretations of the favourite subject, the so called “Chemical Revolution”, cf. Donovan 1989.

[5] For a survey cf. van Brakel 1993.

[6] Some older accounts are Ostwald 1907/1909 and Bachelard 1932, Caldin 1960/1961; Laitko/Sprung 1971 and Simon/Niedersen/Kertscher 1982 looked upon chemistry from the point of view of dialectical materialism (cf. Schummer 1996e); new beginnings are documented in Mittelstraß/Stock 1992 (with bibliography), Janich 1994a/b, Psarros et al. 1996, Janich/Psarros 1996, Schummer 1996.

[7] Theobald 1976, Léyy 1979, Bunge 1982, Primas 1981/1982/1985, Del Re et al. 1986, Del Re 1987, Liegener/Del Re 1987a/b, Scerri 1991.

[8] In the next section we shall see, that for some material investigations an abstraction from size, absolute mass and form is achieved by certain mathematical transformations which presuppose knowledge about size, absolute mass and form. In these cases the knowledge is only of indirect interest, namely to perform the abstraction correctly.

[9] The terms *material* and *matter* (stemming from the Latin *materia* as a translation of the Greek *hyle*) have radically changed their (philosophical) meaning since Descartes (cf. McMullin 1978) and apparently lost any contact to chemistry in favour of mechanics, cosmology and even geometry (cf. Schummer 1995b/1996c). I will reinterpret the term *material* in the next section by giving a list of properties in which mechanical properties (like elasticity) are integrated without being dominant. I prefer to avoid the term *Matter*. One should keep in mind that an expression like “the structure of matter” is suspect of being a *contradictio in adjecto* from the epistemological point of view scetched above.

[10] Cf. Hacking 1983.

[11] Notice that material changes under electromagnetic fields have been well-known long before philosophers discussed the so-called quantum mechanical measurement problem and even before the discovery of the photo-electric effect, at the latest since the invention of photography.

[12] Notice that light, heat, electricity and magnetism were counted as (imponderable) chemical substances as late as the early 19th century in the systems from Lavoisier to Berzelius and Gmelin (cf. Schummer 1997c).

[13] Cf. for instance Aristotle 1922.

[14] Popper (1959: 440; new appendix X) seems to use this problem, when he tries to argue for the circularity of operational definitions as follows: To test the water solubility of sugar

it is necessary: 1. to make the solubility test, 2. to vaporize the water after the test, 3. to identify the residue as sugar by making the solubility test inter alia, and so on. If Popper knew a chemical property with irreversible change, his judgement would have been even more devasting, I think, although his argument would not gain any plausibility from a chemical point of view.

[15] For more details concerning reductive programs cf. Schummer 1995a.

[16] It might be necessary to mention, that in modern science micro-reduction of dynamic properties like chemical reactivity or water solubility is not achieved by simply claiming a micro-structure, as some homespun "physicalistic" philosophers seem to think. In contrast to the pre-dynamic mechanistic tradition of 17th century, all contemporary reductive programs are based on electromagnetic interactions, (i.e. *dynamical relations*) on subatomic, atomic or molecular level.

[17] Notice that the temperature of electrons in a piece of metal at ordinary temperature might be of several thousands Kelvin according to kinetic energy.

[18] Notice that the concept of molecular structure is not even explicable in terms of quantum mechanics; cf. Woolley 1978, Weininger 1984.

[19] Notice that nearly every solid object melts at a certain temperature as anything seems to be red under red light.

[20] This is slightly different to Hacking's (1983: 146) statement: "We shall count as real what we can use to intervene in the world to affect something else (...)" Hacking formulates a pragmatic position for experimental realism, but leaves the question open, why scientists should change the world by intervention, as he restated Marx and Engels. More or less interested in experiments of high energy physics, he overlooks the fact that any common material experience implies intervention and that ontological commitments about experimental components are *necesssary conditions* for the scientific formation of material concepts.

[21] The problem is more basic than Carnap's (1953) logical trouble with operational definition of disposition predicates like "soluble in water" by material implication. Carnap simply presupposed that there are basic phenomenalistic predicates at all. But "being in water" is not basic, because the solvent must first of all be identified as water by material predicates. In philosophy of science it seems to be common place, that Carnap has demonstrated the impossibility of operational definition. But he actually demonstrated the inadequacy of the phenomenalistic account of basic predicates.

[22] The epistemological problem is of great practical importance in chemistry as an experimental science. For experimenting in chemistry requires a lot of implicit knowledge (cf. Polanyi 1958), i.e. the experimentor's skill for manual and instrumental operations, which is trained by practice and difficult to describe by functional laws only.

[23] Cf. Wald 1899, Ostwald 1904, Timmermans 1963, van Brakel 1986.

[24] For detailed discussion of such problems cf. Timmermans 1963.

[25] Notice that abstraction from physical reference frame implies abstraction from mechano-geometrical part-whole relations. In material sciences part-whole relations are defined with respect to each of the material separation techniques. To describe sampling in logical terms one has to turn to mereological set theory.

[26] For more details cf. Timmermans 1963, van Brakel 1986.

[27] Notice that there are no simple scientific *material* properties to distinguish between, say, liquid water and water steam. This is contrary to ordinary opinion and unfortunately to many school book texts in chemistry, which lack a consistent concept of material property (cf. Schummer 1995c). According to our definition, material properties essentially depend on contextual conditions. Therefore investigations of water at the temperature of, say, 20°C

and of steam at 120°C refer to different types of material properties. To compare objects from the material point of view it is necessary to equalize the contextual conditions like temperature and pressure, and then there is no more material difference between them. In contrast to Aristotelian chemistry, liquid water and steam are different states of the same substance and not different substances.

[28] For the exceptional azeotropes cf. Note 24.

[29] Notice that the systematical order of chemical elements, as it was achieved by Mendeleev's periodic table in the last century, is not a closed system but a structure open to systematical enlargement *ad libitum* (Ströker 1968). Here again, we meet one of the cleverest strategies in chemistry to put things in order without turning to an ideal realm with *a priori* limits.

[30] In laboratory practice the task is made easier by two steps: (1) Samples for reaction tests are not analysed but definitely composed in advance with substances of high purity, which can be bought in chemical factories. (2) One hopes that conservation on the level of elementary materials is guaranteed, if the reaction takes place in closed vessels of inert materials. Hence, the remaining task is to analyse the samples at time t_2 and compare the results with the data of the initial composing procedure.

[31] Historically this step was skipped by stating the law of constant mass proportions for all chemical reactions. But this law is challenged by the well-known counterexamples, the Berthollides (compounds with varying composition), which must be excluded by definition. Besides the logical problem of induction there is another problem of logical and practical relevance mostly forgotten: There are in fact no general rules to generalize certain experimental conditions and operations to any scale. Hence, chemical predicates imply additional vagueness, and industrial chemists are troubled by the so-called scaling-up problem, when laboratory results should be transferred to factory dimensions.

[32] In contrast to the current philosophical use of the expression "identical", I always add "physical" or "chemical" to indicate the underlying reference frame. Because there is no absolute notion of identity, the current use in philosophy seems to presuppose a physicalistic position.

[33] Cf. Note 27.

[34] Cf. Rom Harré's (1986: 124) citation of Mary Tiles: "People refer, terms denote."

[35] An exception is Harré 1986 to which I am indebted for this idea outlined in Schummer 1996a.

[36] There is actually not a single *ab initio* solution of the time-dependent Schrödinger equation for a macroscopic reaction system of several chemical substances. In kinetics, the semi-classical collision theory with the concept of potential energy surface yields some primitive models for very simple gas phase reactions, whereas the contact with quantum mechanics is hard to recognize. The Eyring theory provides some rules of thumb for reaction rates, if the reaction mechanism is known from elsewhere, but it incorrectly interprets kinetics in terms of equilibrium thermodynamics, which is reconstructed in terms of semi-classical statistical mechanics. At first glance, thermal dissociation and photo-dissociation of isolated substances seem to be successful examples of quantum mechanical treatment. But the capacities to dissociate under certain thermal and photonic conditions are actually not chemical but thermic and electromagnetic properties according to our list of material properties. The only remarkable success is made in terms of the MO-model with the approximations of pertubation theory and selection rules of orbital symmetry: the model of HOMO-LUMO-interactions. Because the model makes a lot of assumptions necessary, its application is restricted to selective cases and to more or less qualitative treatments. For more details cf. Schummer 1995a.

[37] For more details cf. Schummer 1996a, chap. 6; Schummer 1996b.

[38] Notice that the common (trivial) type of prediction (inferring F(x) for any t from finitely many determinations F(x) at t_1, t_2, ...) does not generally work with material properties, because every single test may cause material changes. While philosophers of science have discussed experimental changes as a novum of the so-called "quantum mechanical measurement", this is actually the usual case with chemical experiments (cf. Schummer 1994).

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