B6 A frame-theoretic investigation of the dynamics of scientific theories, their conceptual systems and their realistic reference.

1 General information

1.1 Applicant

Univ.-Prof. Dr. SCHURZ, Gerhard

1.2 Topic

Frames as means for an investigation of the dynamics of scientific theories, their conceptual systems and their realistic reference

1.3 Scientific discipline and field of work

Philosophy of Science & Frame-Theory

1.4 Scheduled total duration

Six years

1.5 Application period

Three years

1.6 Summary

In this project, frame-theory shall be used to investigate the historical transition between (partially incommensurable) theories, with particular focus on the consequences such transitions have on scientific concepts, classificatory systems and ontologies. Frames are especially suited for this purpose because they explicate the central categories and concepts which underlie scientific theories in the form of recursive system of attributes (cf. Chen and Barker 2000, Chen 2003). Several case studies from the development of chemistry in the 17th and 18th century (for example, the comparison of phlogiston versus oxygen theories of combustion), and from the development of biology (from Linnean to Darwinian classification systems) shall be conducted. We will investigate the historical and epistemological conditions which must be satisfied in order for an attribute to become a central dimension (or node) in a scientific classification system – such as mole number becoming central in the classification of chemical substances and reactions after Avogadro and Dalton, or descendance become central in classification of biological kinds after Darwin.

Three related goals are central to this the project. The first goal concentrates on the question of how can competing (and in some cases incommensurable) theories or research programs be *compared*? We *conjecture* that frame-representations are especially suited to

reveal *structural correspondence relations* between different theories. Such relations can be construed as *invariances*, as the structural realists call them, that disclose objective information about the world (Worrall 1989, Votsis 2005, Schurz 2006b).

The second goal will focus on the question of which concepts or nodes of a theory frame can be regarded to successfully refer to entities in the world as opposed to merely having an *instrumental value*. We conjecture that typically we can identify successfully referring nodes of a frame when at least part of their content survived theory change in the form of structural correspondence relations between the frames of the consecutive theories.

The third goal in this project concerns the development of *evaluation criteria* for scientific classification. Two evaluation dimensions will circumscribe the discussion: (a) the degree of *theoretical unification* provided by a classification frame, and (b) its *diagnostic efficiency*. It will be asked whether there are cases in which the aim of theoretical unification and the aim of diagnostic efficiency come into conflict. For example, certain tensions of this sort seem to exist between a classification of biological kinds in terms of *attributive similarities*, and in terms of their *evolutionary ancestry* (cf. Ridley 1993, 358f, 369f). Where conflicts exist, we will try to develop strategies to resolve them.

2 State of the art, preliminary work

2.1 State of the art

According to Barsalou (1992), *frames* are a unified cognitive format for the representation of the conceptual structures underlying different kinds of knowledge. A frame represents a super-ordinate category (e.g. *mammal*) by a recursive system of (functional) attributes (e.g. *nutrition*, *habitat*, way of *reproduction*, etc.). In the frame which represents the super-ordinate category, the values of most attributes are left unspecified, but some of the values are assigned by default or specified by constraints (e.g. reproduction: *viviparous*). Special sub-categories or kinds of the respective super-category are characterized by more specific value assignments to the attributes of the frames (e.g. *zebra,* with nutrition: *herbivorous*, habitat: *steppe* or *savannah*, etc.). Some sub-categories override default value assignments in the super-category and thus constitute exceptions in the sense of non-monotonic logic (e.g. *bird* vs. *penguin*; cf. Schurz 2001a,b). Attributes do not only characterize the *individual* members of the super-ordinate category, but may also express properties of *systems* of such individuals (e.g. *populations* in biology).

Since each attribute corresponds to one *dimension of classification*, it is obvious that every frame, and also every *net of frames*, represents a *conceptual system* which defines eo ipso a *system of classification* for the objects of the underlying super-category. Therefore, frames are expected to be an excellent tool for representing scientific classifications and ontologies.

In this project, the theory of frames shall be applied to two domains, chemistry and biology, in order to answer central questions in the contemporary philosophy of science. We conjecture that there exists an *intrinsic* relation between the classificatory system or ‘ontology’ of a theory and its theoretical and causal-explanatory structure, because the central nodes of the frame which underlies a theory’s ontology consist exactly of those attributes which according to the theory occupy a causally primary role in a network of 'natural kinds'. We share the perspective of those philosophers who understand the concept 'natural kind' not in an ahistoric-essentialist way, but rather as theory and background dependent (cf. Laudan 1997, Bird 1998; Carrier 2004, Schurz 2006a, ch. 5).

That frames are an excellent tool for the representation of scientific taxonomies has been demonstrated by Chen and Barker (2000) and Chen (2003), but only in respect to a few specifically selected examples. Chen's analysis focuses on Kuhn's (1962) thesis of *incommensurability*, according to which the concepts of competing theories are incomparable. This project follows up on Chen's analysis by concentrating on Laudan's thesis of *pessimistic meta-induction,* which emerged as a successor problem to Kuhn's incommensurability thesis. A central concern of the project will be to find out how we can compare conceptual systems of successive scientific paradigms or theories which are separated by a scientific revolution.

Laudan's thesis is a counter-argument to Putnam's well known *no-miracle-argument* (e.g. Putnam 1978, 18f). According to the no-miracles argument, scientific realism - the view that the theoretical terms of our best theories designate real though unobservable constituents of the world and that such theories are at least approximately true - offers the only plausible explanation of a theory's empirical success. In other words, unless we assume that scientific realism holds, we will have to suppose that a scientific theory's empirical success is miraculous. So according to Putnam, we should all be scientific realists. Laudan (1981) counters this claim with a seemingly equally strong argument: in the history of science, theories judged to be empirically quite successful have repeatedly been overthrown by theories with radically different conceptual structures (and corresponding ontologies). Laudan concludes that on simple inductive grounds it is therefore unreasonable to expect that the currently accepted theories will escape this fate. We should rather expect that the conceptual structure and stipulated ontology of present theories are likewise far away from the 'real world' and will be radically overthrown in the future. In short, pessimistic meta-induction motivates a non-realist attitude towards science: the central concepts or *nodes* of scientific frames are at best useful tools.

A widely discussed example is the *phlogiston theory* of combustion, which at the time of its reign achieved significant empirical success (Carrier 2004). After the chemical 'revolution' initiated by Lavoisier, combustion was understood as a type of *oxidation*, and from this time on, nobody believed further in the existence of 'phlogiston' as a special substance bearing the capacity of combustion. One of the most intriguing questions that arises is the following: How can a theory, now considered to be false, have enjoyed such empirical success?

As a reaction to Laudan's challenge, Worrall (1989) developed an influential position called *structural realism*. Worrall demonstrates that certain *structural relations* between mutually corresponding concepts are preserved in the *transition* from one theory to its successor. His case study involves Fresnel's theory of light and its successor, namely Maxwell's theory of electromagnetism. Although partially incommensurable, the two theories are connected via structural relations. To be precise, Fresnel's equations for the reflection and transmission of light as it passes through different media survive into Maxwell's theory intact.

2.2 Preliminary work

Gerhard Schurz (2004, 2006b) has provided a logically generalized version of Worrall's argument which allows it to deal with more complex cases such as the phlogiston-oxygen example. He has argued that although nothing real corresponds to the concept 'phlogiston', the concept of 'dephlogistication' (the release of phlogiston) corresponds to the modern chemical concept of electrons being released to the bonding partner (generalized oxidation). This structural correspondence explains the phlogiston theory's empirical success in spite of the referential failure of its central conceptual node 'phlogiston'. Based on this observation, a restricted version of the inference from a theory's empirical success to the approximate truth of some of that theory's parts can be justified (cf. also Schurz 2008a).

Gerhard Schurz has a background relevant to conducting the historical case studies in chemistry and biology. Among other degrees, he holds a Masters degree in chemistry. Moreover, he is currently conducting research in evolution theory (writing up a book). It is also worth noting that Gerhard Schurz has a long-standing collaboration with Werner Kunz from the *Biology department* of the University of Duesseldorf. For more details see curriculum vitae and preparatory works.

Ioannis Votsis (designated as research personnel for this project) has written his doctoral dissertation on scientific theories and structural realism (2004) at the London School of Economics under the supervision of Professor John Worrall, who is one of the leading experts in the field. Dr Votsis has some relevant experience in the fields of chemistry and biology, having conducted research on the transition from the caloric theory of heat to thermodynamics and on evolutionary psychology for the project Darwin@LSE. He has also taught a Master's seminar in the Philosophy of Biology at the University of Bristol. His work has been presented in conferences around the world and has culminated in a number of publications, including two papers in the internationally leading journal *Philosophy of Science* (2003, 2005). He is thus especially suited for the work in this project.

Quoted publications of Gerhard Schurz and Ioannis Votsis

Schurz, G. (2001a). What is „Normal“? *Philosophy of Science*, 28, 476-497.

Schurz, G. (2001b). Normische Gesetzeshypothesen und die wissenschaftsphilosophische Bedeutung des nichtmonotonen Schließens. *Journal for General Philosophy of Science, 32*, 65-107.

Schurz, G. (2004). Theoretical Commensurability By Correspondence Relations. In: D. Kolak, & J. Symons (Eds.), *Quantifiers, Questions, and Quantum Physics* (pp. 101-126). Berlin: Springer.

Schurz, G. (2006a). *Einführung in die Wissenschaftstheorie*. Darmstadt: Wissenschaftliche Buchgesellschaft.

Schurz, G. (2006b). When Empirical Success Implies Theoretical Reference: A Structural Correspondence Theorem. TPD-Preprints 2006/1.
An extended and improved version will appear in *British Journal for the Philosophy of Science* 2008.

Schurz, G. (2008a). Patterns of Abduction. *Synthese*. Printed version to appear. Web site: http://dx.doi.org/10.1007/s11229-007-9223-4

Schurz, G. (2008b). Common Cause Abduction and the Formation of Theoretical Concepts. To appear in: C. Dégremont et al. (Eds.), *Essays in Honour of Shahid Rahman*. London: College Publications.

Schurz, G. (2008c). Abductive Belief Revision. To appear in E. Olsson (Ed.), *Science in Flux*. New York: Springer.

Votsis, I. (2003). Is Structure Not Enough? *Philosophy of Science*, *70*(5), 879-890.

Votsis, I. (2004). *The Epistemological Status of Scientific Theories: An Investigation of the Structural Realist Account*. Dissertation at the *London School of Economics* (so far unpublished).

Votsis, I. (2005). The Upward Path to Structural Realism. *Philosophy of Science 72*(5), 1361-1372.

Votsis, I. (2007). Uninterpreted Equations and the Structure-Nature Distinction. *Philosophical Inquiry*, *29*(1-2), 57-71.

3 Goals and work schedule

3.1 Goals

Our project consists of three central objectives:

Objective 1 – The frame-theoretic investigation of theory-transitions, structure preservation and change in the development of chemistry and biology.

To successfully pursue this objective, answers must be found to the following four questions:

(1.1) What historical and epistemological conditions (e.g. the state of empirical knowledge and of measurement technologies) must be satisfied in order for an attribute to become a *central dimension* in a scientific classification system – such as *mole number* becoming central in the classification of chemical substances and reactions after Avogadro and Dalton, or *ancestry* becoming central in the classification of biological kinds after Darwin?

(1.2) What is the *role* of conceptual and classificatory systems in the *dynamics* of theory (r)evolution? To what degree do they restrict the space of possible theories which are conceivable at the respective historical period?

(1.3) How can conceptual frames from competing (even incompatible or incommensurable) scientific theories or research programs be *compared*?

(1.4) Can relations of *structural correspondence always* be found between theories which are separated from each other by a paradigm shift?

It is a *conjecture* of this project that frame-representations can indeed reveal *structural correspondence relations* between different frames (for examples see §3.2.3 below).

Objective 2 – The frame-theoretic investigation of the conditions under which theoretical terms can be deemed referentially successful.

Which nodes of a frame can be regarded to successfully *refer* to things in the world, and which have merely an *instrumental value*? Are there relevant differences between central and peripheral nodes in the conceptual frame underlying a given theory?

One guiding conjecture is that those nodes of a frame that successfully refer stand in structural correspondence relations to successor (or predecessor) theories. Typically, the attributes or nodes of a frame that correspond to real world features figure as causal unifiers of correlated dispositional properties in the sense of Schurz (2008a, 2007b).

Objective 3 – The frame-theoretic investigation of scientific classification systems.

There are two central dimensions for the evaluation of scientific classification frames, namely (a) the degree of theoretical unification provided by the theory frame, and (b) their diagnostic efficiency. In terms of these two dimensions, what are the main evaluation criteria for scientific classification systems? We *conjecture* that there are cases in biological classification systems in which these two main families of evaluation criteria come into conflict (see §3.2.1, objective 3, below). In such cases we consider possibilities of how such conflicts can be reconciled.

Objectives 2 and 3 would also constitute a long-term perspective of this project. That is to say, research conducted towards these objectives can, and will be, extended in case the project's lifespan would be prolonged for more than three years.

3.2 Methods and work schedule

The methodology will primarily consist of logical and philosophical analysis of the historical development of theories in chemistry and biology in the past three centuries. The main objectives as explained in §3.4.1 and 3.4.2 shall be achieved according to the following programme and time schedule:

3.2.1 Programme and time schedule

Objective 1

Years 1-2: Frame-theory shall be used for the investigation of the historical transition between (partially incommensurable) theories and their underlying conceptual and classificatory systems or *ontologies*. Among other things, we shall examine the hidden role of frames in the historical development of theories by revealing how these frames *constrain* the (possible or actual) conceptual developments within a theory-paradigm.

Years 1-3: We shall conduct several case studies in the development of modern chemistry and biology to test the conjecture that frame-representations can reveal structural correspondence relations between the frames of successive theories. For example, it will be asked whether pre-Lavoisierian explanations survived the 'chemical revolution', i.e. the transition from early to modern chemistry. This question is difficult to answer as pre-Lavoisierian explanations were typically qualitative in character, citing special 'essences' (such as phlogiston) to explain phenomena (such as combustion). The 'chemical revolution' replaced them with combinatorial explanations of chemical reactions, explanations that eventually developed into modern molecular chemistry (with significant contributions by Avogadro, Proust and Dalton).

It is expected that successful answers to these questions will shed new light on four eminent topics in philosophy of science which were explained in §2.1 above: Kuhn's incommensurability thesis, Putnam's no-miracle argument, Laudan's pessimistic meta-induction and Worrall's structural realism.

Objective 2

Years 1-2: Our research into the second objective will in the first instance go hand in hand with an investigation of the *theoretical and technological background-dependence* of scientific frames and classifications (see question 1.1 above). For example, while in pre-modern chemistry qualitative properties (colors and forms) were primary, mole and electron numbers took on that role in modern chemistry. Similarly, while attributive similarities were primary for Aristotelian and Linnaean biology, evolutionary ancestry became primary after Darwin. The development of new measurement technologies and the exploration of new domains of phenomena plays a crucial role in this process. By analyzing these transitions we expect to shed new light on the conceptual developments that underlie theory change. We are particularly interested in what constitutes a barrier to the formation of new concepts such as atomic weight or mole number in chemistry, or natural selection in evolution theory.

Years 2-3 (possible long term perspective): Recall the pivotal question tied to the second objective: 'Which nodes of a frame can be regarded to successfully refer, and which have merely an *instrumental value*?' Answering this question will require the elucidation of the role which conceptual nodes play in a network of frames. For example, the underlying conceptual system of phlogiston theory will have to be reconstructed as a frame whose central node, phlogiston, does not have a corresponding referent, although two other special nodes of this frame, phlogistication and de-phlogistication, can be assigned an indirect reference relation via their correspondence to two central nodes of the currently accepted combustion frame (electron acceptance and donation respectively). This is explained in more detail in §3.2.3 below. According to our guiding conjecture, i.e. that those nodes of a frame that successfully refer stand in structural correspondence relations to successor (or predecessor) theories, research into objective 2 will be intimately connected with our search for structural correspondence relations (objective 1, years 1-3). In Schurz (2008a,b,c) it was suggested that often the attributes or nodes of a frame that successfully refer figure as causal unifiers of correlated dispositional properties. This hypothesis will be further investigated in our work.

Objective 3

Years 1-2: In the first stage of our investigation of scientific classification we will focus on the problem of the 'naturalness' of biological kinds. One pertinent issue that has recently been intensely debated concerns the tensions and in some cases inconsistencies between a classification of biological kinds in terms of *attributive similarities*, and in terms of their *evolutionary ancestry* (cf. Ridley 1993, 358f 369f; Nichols 2001). With the help of frame theory we will attempt to explain the root of these tensions and inconsistencies. Among other things, we will seek to explain why a classification based exclusively on relations of ancestry like that of Henning (1950) may be at the cost of that classification's *diagnostic efficiency* (cf. Hull 1997, Mayr 1982, 230f).

Years 2-3 (possible long term perspective): The results of our investigation into biological classification will then be compared with classification in three domains of chemistry: (a) the classification of atoms, which is straightforwardly given by the periodic table); (b) the classification of molecules, which in areas such as organic chemistry is often diagnostically difficult, and (c) the classification of chemical bonding, which is theoretically difficult. Based on our overall results, general criteria for the diagnostic efficiency and theoretical unification of scientific classificatory systems shall be developed.

In the remainder of this section we offer a few instructive examples that bring out: (1) how the objectives of this project are expected to be met and (2) how the expected achievements may relate to the central questions and problems of the broader research group (Forschergruppe FFF600).

3.2.2 The power of frames as means of reconstructing scientific theories

Figures 1 and 2 illustrate a frame-theoretical reconstruction of two categories of present biological classifications: the super-category *mammal* and the sub-category *zebra*.

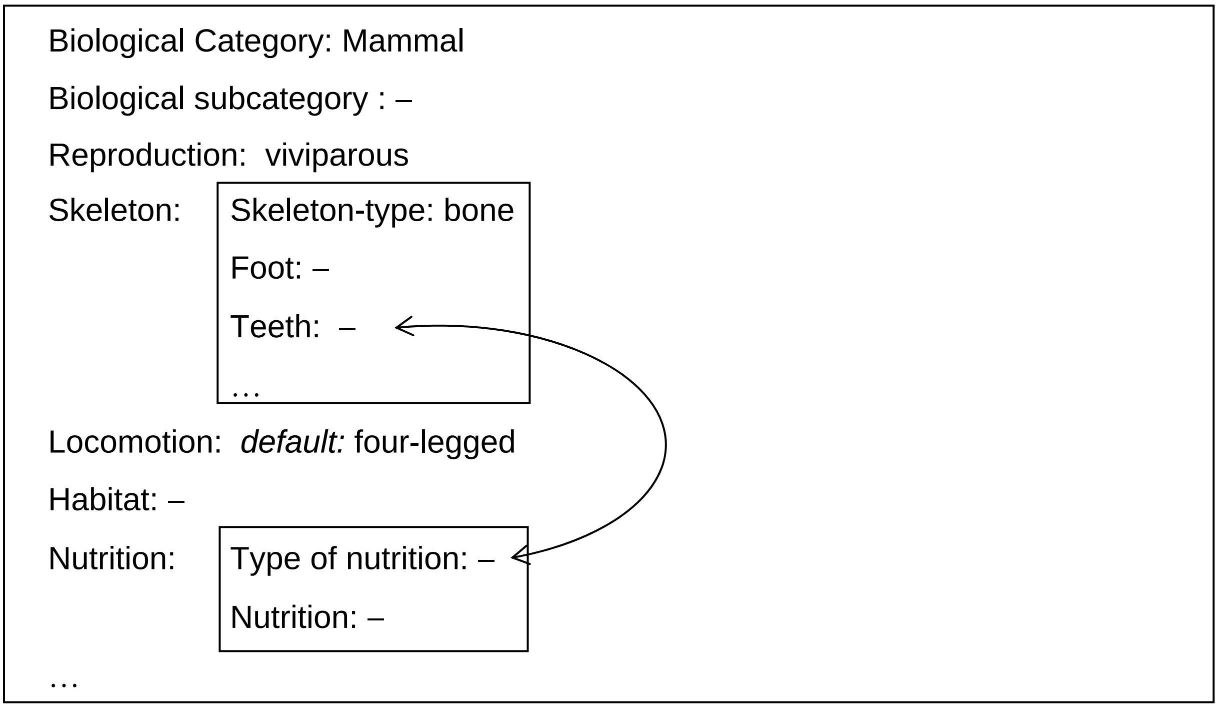

Fig. 1: Frame for the biological super-category “*mammal*”.

The examples contain all the intended properties that frames should possess something which accords well with the theoretically central project B1 of the FFF 600 (cf. Petersen 2007). Concerning fig. 1, the first thing worth noting is that the value of most of attributes of the super-ordinate frame for the category mammal is not specified. Such values are specified in subcategories (such as zebra). “Viviparous” is a strictly fixed value of the attribute *reproduction* of mammals and indeed belongs to the semantic *meaning* of “mammals”. Four-legged locomotion, by contrast, is only specified *by default*. The second thing worth noting is the recursive character of frames. This is evident by the fact that the values of certain attributes correspond to (nested) frames. For example, the skeleton type is of high classificatory importance and possesses its own characteristic attribute space, i.e. its own frame. The third thing worth noting is the constraint between the values of (type of) nutrition and that of (type of) teeth. Such a constraint relates the values of these two attributes in a non-strict empirical correlation (or uncertain biological law): herbivorous nutrition correlates well with (but does not necessitate) molar teeth, carnivorous nutrition correlates well with (but does not necessitate) fang teeth, etc.

The frame for the sub-category zebra in fig. 2 below instantiates the empty slots of all (or at least most) of the remaining mammal-attributes with values. Importantly, the zebra-frame also *imports* some *new* attributes which are central only for zebras, e.g. their black-white skin-colour. This is called a "value-attribute-constraint": the value "zebra" for the biological sub-category imports the new attribute "skin-colour". One also sees that sometimes the values of an attribute are specified only *partially* – by assigning to the attribute a *set* of values – e.g. {steppe, savannah} to *habitat*.

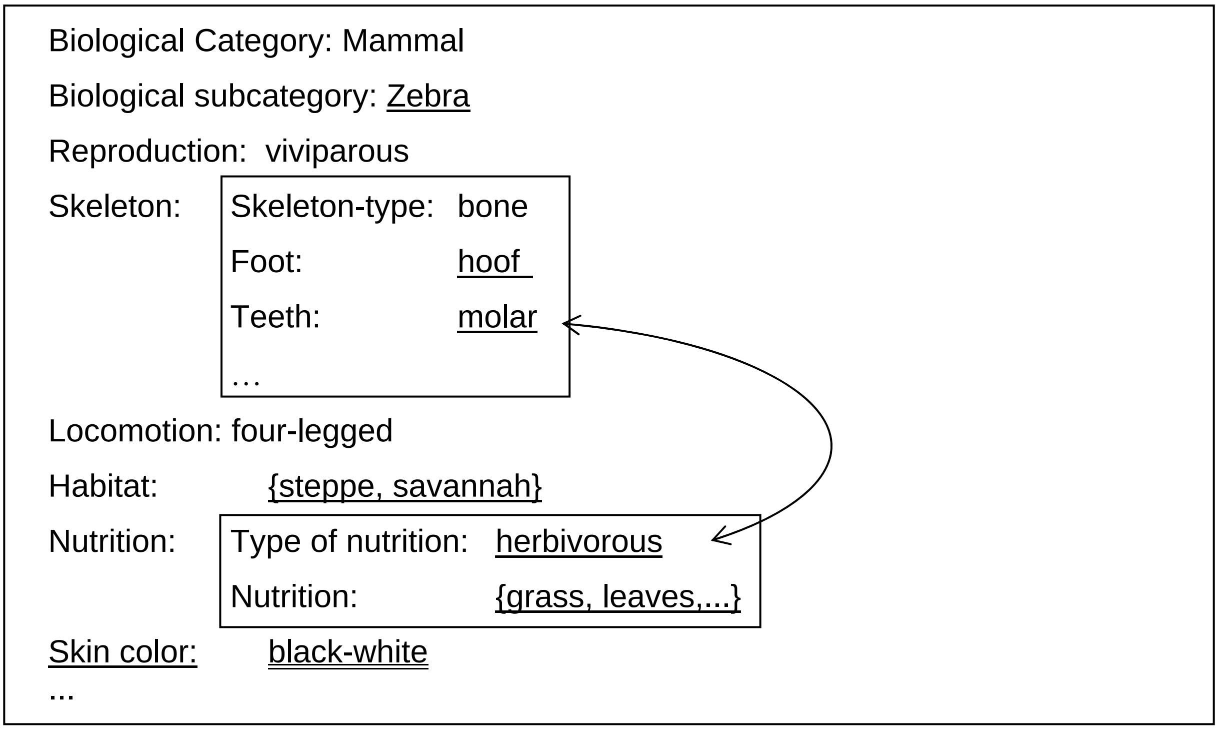

Fig.2: Frame for the biological sub-category "*zebra*". The new entries instantiated by the zebra-frame are underlined.

The degree to which the values of all attributes of a frame are determined by the values of one or only a few attributes is called the *systematic power* of a frame. Thereby, *subcategory names* such as "zebra" must be excluded from the range of predictive attributes, because they determine the values of all other attributes on trivial definitorial reasons. The diagnostic efficiency of a frame is intimately connected with its systematic power. Biological classification frames such as the zebra-frame have low to moderate systematic power because the values of the skeleton-subframe of zebras, for example, do not determine many of the values of the other attributes. For example, hoofed animals need not live in the steppe or the savannah, as they can also be found living in the mountains.

An example of a frame with an extremely high systematic power is the frame of the *periodic table* in chemistry: here, the atomic number (and concerning nuclear stability and decay properties also the mass number) determine all further attributes and their values. This takes the form of a strictly general value-attribute and value-value constraint – see fig. 3.

Chemical category: element

chemical subcategory: – [name of element]

atomic number (= number of protones): –

mass number (= number of protones and neutrones): –

Many further attributes which are strictly determined by atomic (and mass) number:

(melting point, boiling point, electronegativity,

metallic/semi-metallic/non-metallic character;

if metallic: solubility in different kinds of acids;

if non-metallic: solubility in different kinds of bases; etc.)

Fig. 3: Frame of the periodic table – the values of all additional attributes are determined by atomic (and mass) number.

3.2.3 First steps in the reconstruction of correspondence relations between incommensurable frames: The case study of phlogiston-oxygen.

Phlogiston theory goes back to Johann Becher and Georg Stahl (who coined the term ‘phlogiston’ in 1723), and was developed, among others by Henry Cavendish and Joseph Priestley (cf. McCann 1978, ch. 2). According to this theory, combustible substances contain *phlogiston*, which is the bearer of combustibility. When combustion or calcination (roasting) of a substance X takes place, X delivers its phlogiston in the form of a hot flame or an evaporating inflammable gas, leaving behind a dephlogisticated substance-specific residual (a so-called ‘calx’). This process was called *phlogistication*, and the inverted process called *dephlogistication*. It is widely known today that Phlogiston theory did not work for certain applications. What is not so widely known is that in spite of these problematic cases, Phlogiston theory was empirically quite successful (cf. Carrier 2004, Schurz 2004, 2006b), examples are given below.

In the 1780s Antoine Lavoisier developed the *oxygen theory* of combustion. The generalised form of this theory is now part of modern chemistry. According to Lavoisier’s oxygen theory, combustion and calcination of a substance X consists in the oxidation of X, i.e. its forming a polarized bond with oxygen. In the modern generalized oxidation theory, the oxidizing substance need not be oxygen but can be another strongly electronegative substance, e.g. a halogen. Thus, according to modern oxygen theory, the *oxidation* of a substance X consists in the formation of a polarized bond between X and an electronegative substance Y, in which the X-atoms become electropositive and donate electrons to their electronegative neighbour-atoms of type Y. The inversion of this chemical process is called *reduction*.

In oxygen theory, the assumption of a special bearer of combustibility was recognized to be explanatorily superfluous. Phlogiston simply *does not exist*. But how can we then explain the strong empirical success the phlogiston theory enjoyed at its historical time?

In Schurz (2006b) it is argued that the theoretical term "phlogiston" was empirically underdetermined. The theoretical expressions which did the empirically relevant work for phlogiston theory and thus were *not* empirically underdetermined were *phlogistication* and *dephlogistication*. These concepts of phlogiston theory stand in the following relation of correspondence (Ci) with central concepts of modern chemistry: (C1) Dephlogistication of a substance X corresponds (and hence implicitly refers) to the donation of electrons of X-atoms to the bonding partner in the formation of a polarized or ionic chemical bond. (C2) Phlogistication of X corresponds (and hence implicitly refers) to the acceptance of electrons from the bonding partner by positively charged Y-ions in the breaking of a polarized or ionic chemical bond. These correspondence relations *explain* the strong empirical success of phlogiston theory.

In order to reconstruct the structural correspondence between phlogiston theory and generalized oxygen theory in a frame-theoretic manner, one has first to develop a *general classification frame for chemical reactions*. A first approximation takes the following form: A chemical reaction consists of one or two input substances under certain conditions (relating to the substances as well as the circumstances of the reactions), together with one or two output substances and possibly some residuals. The general chemical reaction frame is illustrated in fig. 4.

Chemical Reaction Category: –
Input 1: Condition: –
Substance: –
Input 2: Condition: –
Substance: –
…
Special and catalytic conditions depending on inputs:
(e.g. heat, presence of catalysator,…)
Output 1:
Output 2:
…
Residuals: (incomplete reaction, catalysator-residuals,…)

Fig. 4: The general classification frame for chemical reactions.

Two constraints govern chemical reaction frames. First, the chemical *law of equal proportions* requires that for all atoms (elements) of kind *i* involved in the reaction, the number of moles of atom *i* among the input substances equals the number of moles of atom *i* among the output substances. Second, the *reaction-inversion principle*, according to which for every reaction, there exists one and only one inverse reaction. The reaction-inversion principle is important for the general frame theory as developed in project B1 of the FFF 600, for it is not an *intra*-frame, but an *inter*-frame constraint which connects frames of different chemical reactions. This principle demonstrates the need of extending the theory of frames to a theory of *nets of frames*. We expect to discover many more examples of this sort.

Interestingly, the understanding of chemical reactions according to the proposed frame, together with its intra- and inter-theoretic constraints, was be *commonly accepted* by both phlogiston and oxygen theorists. This shows how frame-theory can be useful in revealing the hidden common principles shared by otherwise ontologically incommensurable theories What was different in phlogiston and oxygen theories was not the general understanding of chemical reactions, but the *theoretical decomposition* of the empirically given substances and the observed chemical changes into unobservable components and component-changes. In particular, what was understood as pure in one theory was understood as compound in the other theory, and vice versa. This different theoretical decomposition of substances on conjectured parts is illustrated by the following major chemical reactions: the calcination (or roasting) of metals; the salification of metals through their dissolution in acids, and the inversion of these two processes.

The following schemata present four chemical reaction types as analyzed by Phlogiston and by Oxygen theory. The underlinings indicate intertheoretic correspondences: substances which are underlined in the same way correspond to the different theoretical decompositions of the same empirically given substance. For example, the pure chemical substance metal was understood as a non-compound by the oxygen theory, but as a compound, namely metacalx + ash, by the phlogiston theory. Henceforth, "phlog" stands for "pure phlogiston". "X–Y" stands for a combination of X and Y", for example, "Phlog-Air" stands for "phlogisticated air", "ash-phlog" for "combination of ash and phlogiston", etc. The symbol "↑" indicates that the substance is an evaporating gas. The symbols "$^{+}$ " ("$^{-}$ ") designate electropositivity and electronegativity Respectively. Finally, "H" stands for "hydrogenium".

Calcination of metals:
Oxygen theory: $\underline{\text{Metal }}$+ Oxygen → $\underline{\underline{\text{Metal}^{+}\text{–Oxide}^{-}}}$ [+ $\underset{\cdots\cdots}{\text{HotAir}}$ ↑]
Phlogiston theory: Metal (= $\underline{\text{MetCalx–Phlog}}$) → $\underline{\underline{\text{MetCalx}}}$ + $\underset{\cdots\cdots\cdots}{\text{Phlog–Air}}$↑

Salt-formation of metals in acids:
Oxygen theory: Metal + $\text{H}^{+}\text{–X}^{-}$ (=Acid) → $\underline{\underline{\text{Metal}^{+}\text{–X}^{-}}}$ (=Salt) + $\underset{\cdots\cdots\cdots}{\text{Hydrogenium}}$ (H_2)↑
Phlogiston theory: Metal + Acid → $\underline{\underline{\text{MetCalx–Acid}}}$ (=Salt) + $\underset{\cdots\cdots}{\text{Phlog}}$ (‘inflammable. air’) ↑

Inversion of calcination – reduction with coal:
Oxygen theory: $\underline{\underline{\text{ Metal}^{+}\text{–Oxide}^{-}}}$ + Coal → Metal + $\underline{\text{Coal}^{+}\text{–Oxide}^{-}}$↑ [+Ash]
Phlogiston theory: $\underline{\underline{\text{MetCalx }}}$+ Coal (=Ash–Phlog) → Metal + Ash [+ $\underline{\text{Phlog–Air}}$]↑

Inversion of salt-formation:
Oxygen theory: $\underline{\underline{\text{Metal}^{+}\text{–Oxide}^{-}}}$ + $\underset{\cdots\cdots\cdots}{\text{Hydrogenium}}$ → Metal + Water (= $\text{Hydr}^{+}\text{–Oxide}^{-}$)
Phlogiston theory: $\underline{\underline{\text{MetCalx}}}$ + $\underset{\cdots\cdots}{\text{Phlog}}$ [+ Water-in-Air]) → Metal [+ Water-in-Air]

Note that the identification of phlogiston with inflammable ‘air’ (i.e. hydrogenium) did not work in all domains. Moreover, the phlogiston theory did not work well across the board. For example, it failed to explain why after combustion the weight of some substances increased, instead of decreasing (which was explained by different ad-hoc assumptions). Nevertheless, phlogiston theory was strongly empirically successful with respect to the domains of oxidation and salification of metals and the retransformation of metal calxes into pure metals. Although Lavoisier’s oxygen theory surpassed the success of the phlogiston theory, it also had to face severe difficulties of its own: for example, Lavoisier assumed that the salification of metals through acid is always due to effects involving oxygen; but oxygen is contained only in some but not in all acids.

Using our chemical reaction frames, we can now express the relations between the theoretical analysis of combustion and salt-formation by means of the following special chemical reaction frames. The values of general oxygen theory are underlined once and those of phlogiston theory are underlined twice. Consider the combustion and saltification frame of fig. 5. Here, the oxygen theory's condition of being electropositive but in neutral-bond translates into phlogiston theory's condition of being rich of phlogiston. Acid is primitive in phlogiston theory but consists of hydrogenium ions plus a negative oxydans in oxygen theory. Metal is primitive in oxygen theory but analysed as metalcalx-plus-phlogiston in phlogiston theory (as explained above). In the case of combustion, phlogiston theory does not require a second input substance, but merely pure heat (because the phlogiston is already contained in the first input substance). In the case of dissolution in acid, the acid is the second input substance in both theories.

Chemical Reaction Category: General Oxidation Dephlogistification
Input 1: Condition: Is-Electropositive, In-Neutral-Bound Rich-of-Phlogiston
Substance: X = Metal
Input 2: Condition: Is-Electrogenative, In-Neutral-Bound Poor-in-Phlogiston
Substance: {Oxygen: Y, Acid $H^+–Y^–$} {Pure Heat, Acid}
Special and Catalytic Conditions: Heat
Output 1: $X^+–Y^–$ If Y = Oxygen: XCalx If Y = Acid: XCalx–Acid
Output 2: If Y = Oxygen: none If Y = Acid: H_2 Phlog
Residuals: None

Fig. 5: The chemical reaction frame for the process of combustion and salification (dissolution in acid), in the theories of phlogiston and oxygen.

The inverted processes of reduction are displayed in the frame of fig. 6. Here, the different analysis of the residuals of the reactions is of special interest: ash, which is a residual for oxygen theory, is a proper output substance for phlogiston theory, while water, which is a residual for phlogiston theory, is a proper output substance for oxygen theory.

Chemical Reaction Category: General. Reduction Phlogistification
Input 1: Condition: In-Electropositive Bound Poor-in-Phlogiston
Substance: X^+–Oxide$^-$ XCalx
Input 2: Condition: Is-Electropositive, In-Neutral Bound Rich-of-Phlogiston
Substance: Y {Coal, Hydrogenium} Y {Coal = Ash–Phlog, Phlog}
Special and Catalytic Conditions: Heat
Output 1: X
Output 2: If Y = Coal: Coal$^+$–Oxide$^-$ If Y = Hydrog: Water (= Hydrog$^+$–Oxid$^-$)
If Y = Coal: Ash If Y = Phlog: none
Residuals: If Y = Coal: Ash Phlog-Air If Y = Hydrog/Phlog: none Water

Fig. 6: The chemical reaction frame for the inverse process of reduction, in the theories of phlogiston and oxygen.

These examples elucidate the central advantage of the frame-theoretic analysis of competing theories: the frames tells us, first, what was common to both theories (those entries of the two frames which are not underlined) and second, how the two theories' different ontological frameworks correspond to each other (in our examples they are given by the structural relations between those entries that underlined once and those underlined twice). On the basis of these and other reasons we are convinced that the frame-theoretical analysis of the structure and dynamics of scientific theories and their ontologies promises to be a very powerful tool for finding plausible answers to problems in philosophy of science. At the same time, our examples show how the frame-theory itself can be sharpened and further developed by its application to the field of philosophy of science.

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3.3 Experiments involving humans or human materials

☐ **yes** ☒ **no**

3.4 Klinische Studien

☐ **yes** ☒ **no**

3.5 Experiments with animals

☐ **yes** ☒ **no**