A Preliminary Application of Frame-Theory to the Philosophy of Science: The Phlogiston-Oxygen Case[1]

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Abstract. In the first part of this paper we investigate how scientific theories can be represented by frames. Different kinds of scientific theories can be distinguished in terms of the systematic power of their frames. In the second part we outline the central questions and goals of our research project. In the third and final part of this paper we show that frame-representation is a useful tool in the comparison of the theories of phlogiston and oxygen, despite those theories being traditionally conceived as incommensurable. The frame-theoretic representation reveals common attributes, values and ultimately structural correspondence relations between the two theories. In our view this outcome lends credence to a structural realist view of science.

Keywords: frame theory, phlogiston theory, oxygen theory, scientific realism, structural realism, incommensurability, structural correspondence relations.

1. Introduction: Representing Theory Structure by Means of Frames

A frame represents a super-ordinate category by a (recursive) system of (functional) attributes. Every *frame*, and even more so every *net of frames*, defines a *system of classification* for the objects of the underlying super-category. Therefore, frames are an excellent tool for the investigation of conceptual frameworks underlying scientific *theories* and their respective *ontologies* (cf. Chen & Barker 2000, Chen 2003). 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*.

The examples contain all the intended properties that frames should possess, something which accords well with the theoretically central project B1 of the FOR 600 (cf. Petersen 2007). Concerning Figure 1, the first thing worth noting is that the values of most attributes of the super-ordinate frame for the category mammal are not specified. Such values are specified in sub-categories (such as zebra). Although "viviparous" is often regarded to belong to the *meaning* of "mammal", strictly speaking it is only correct to regard it as a *default* value of the attribute "reproduction" in the frame for mammal because there are some species of mammals which are non-viviparous. However, in the frame for the subcategory of zebra "viviparous" becomes a fixed value of the attribute "reproduction". The same is true of the value "four-legged locomotion". 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 Figure 2 below instantiates the empty slots of all (or at least most) of the remaining mammal-attributes with values. Crucially, the zebra-frame also *imports*

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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*.

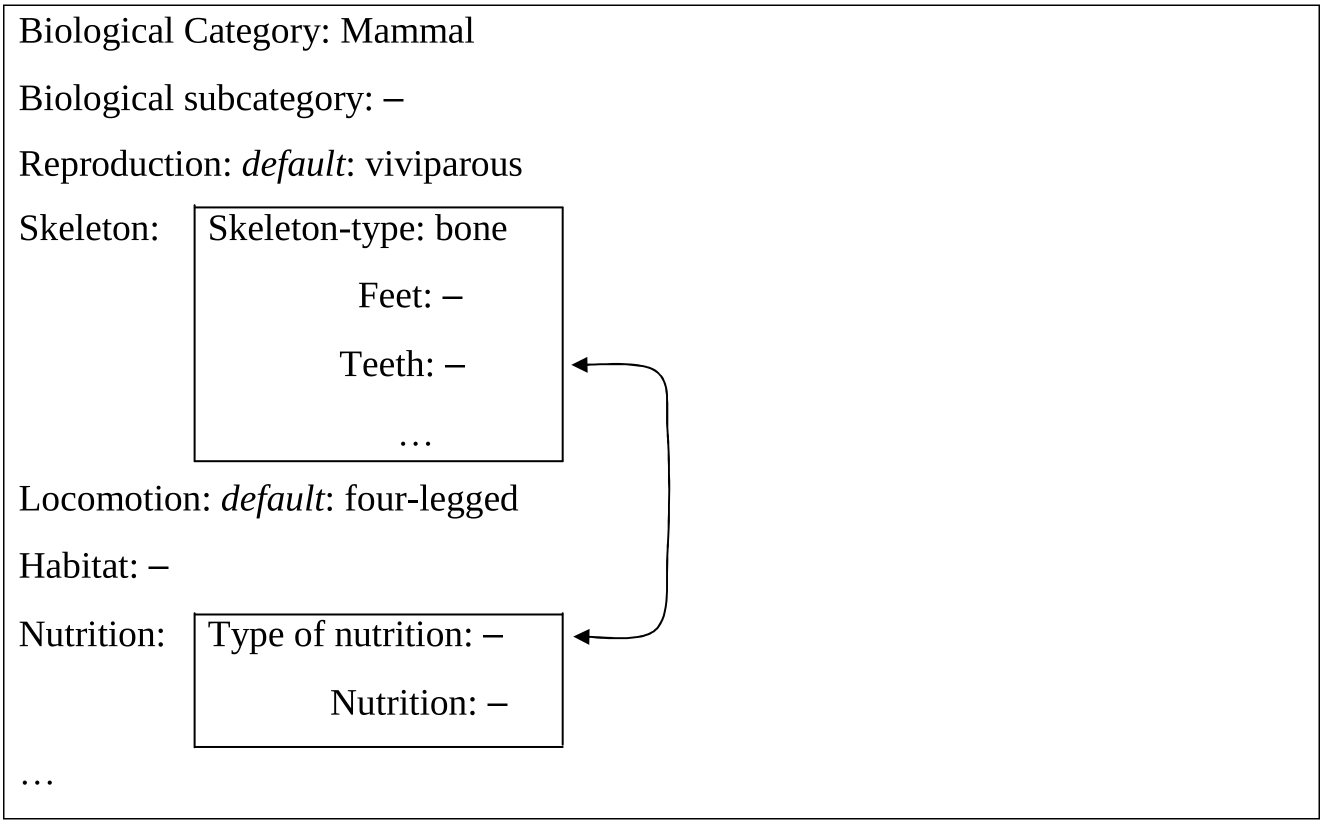

Figure 1. Frame for the biological super-category “mammal”.

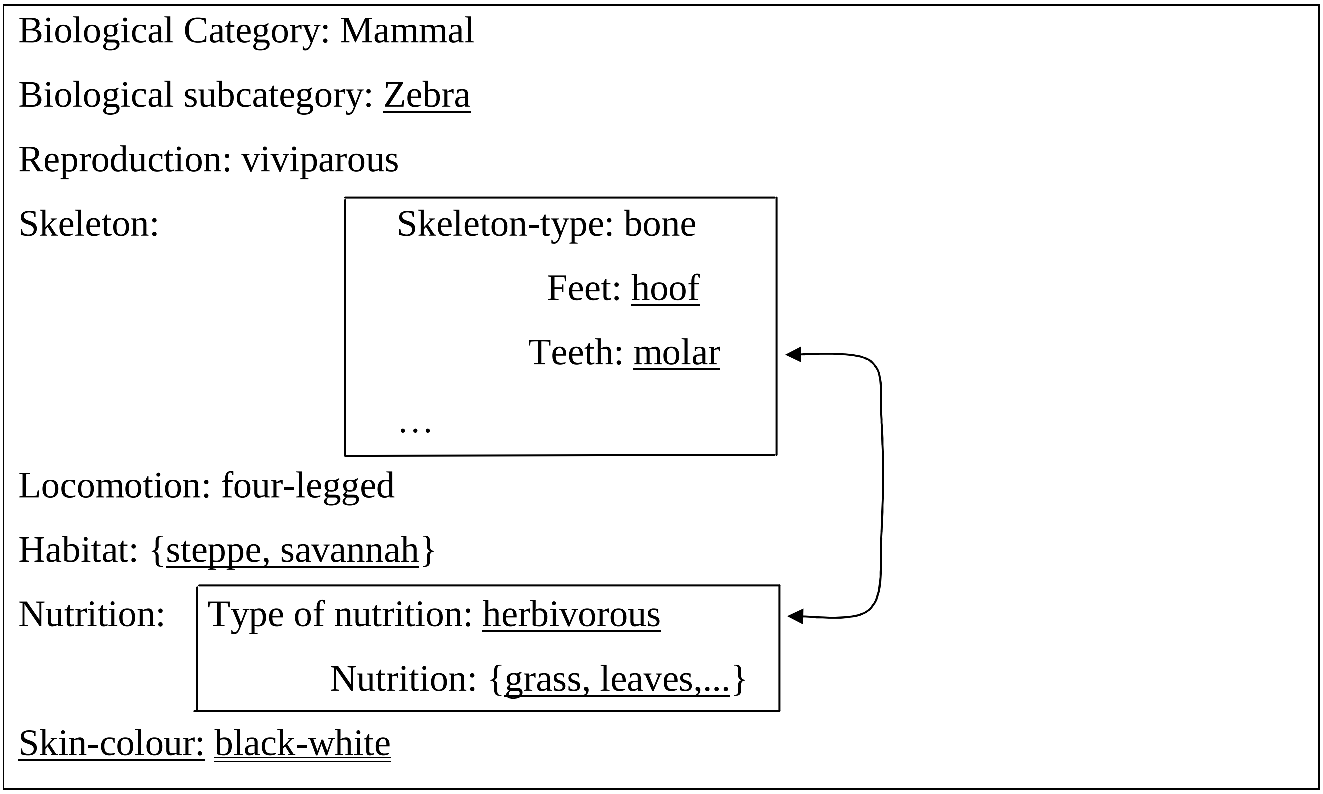

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Figure 2. Frame for the subcategory “zebra”. The new entries instantiated by the zebra-frame are underlined.

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 concepts* such as “zebra” do not count as proper attributes, because they determine the values of all of the relevant proper attributes on trivial 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 sub-frame of zebra, for example, do not determine many of the values of the other attributes. For instance, 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) determines all further attributes and their values. This takes the form of a strictly general value-attribute and value-value constraint – see Figure 3.

Chemical category: element

Chemical subcategory: – [name of element]

Atomic number (= number of protons): –

Mass number (= number of protons and neutrons): –

Various further attributes, all of which are strictly determined by atomic (and mass) number e.g.:

Melting point: –

Boiling point: –

Electronegativity: –

Character: (metallic or semi-metallic or non-metallic): –

If metallic character: solubility in different kinds of acids;

If non-metallic character: solubility in different kinds of bases; etc.

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

2. Central Questions and Goals of our Research Project (B6 of FOR 600):

Goal 1: The first goal of the project is the frame-theoretic investigation of theory-transitions, onto-logical change and structure preservation in the development of chemistry and biology. In particu-lar, we intend to find plausible answers to the following questions:

- Which historical and epistemological conditions must be fulfilled in order for an attribute to become a *central dimension* (*node*) in a scientific classification frame?
- What is the (hidden) *role* of conceptual frames in the *dynamics* of theories?

- How can conceptual frames coming from competing (even: incompatible, incommensurable) scientific theories or research programs be *compared*? We have the following *conjecture:* Frame-representation can reveal *structural correspondence relations* between different frames, which can be regarded as *invariances* in the sense of structural realism (see Worrall 1989).

Goal 2: Our second goal is the development of criteria for the ontological interpretation of frames. The central questions to be answered while working on this goal are the following:

- Which nodes of a frame can be regarded to possess *realistic reference*, and which nodes have merely an *instrumental value*? Our *conjecture* is the following: Nodes which figure as causal unifiers of correlated dispositional properties are genuinely referential (Schurz 2008)

Goal 3: Finally, the third goal is the development of evaluation criteria for (a) the *theoretical unification* and (b) the *diagnostic effectivity* of frames. We *conjecture* that dimensions (a) and (b) may sometimes come into conflict (e.g. in biology)

3. A Preliminary Reconstruction of the Correspondence Relations between Rival Frames: The Phlogiston-Oxygen Case

The theory of phlogiston 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 or 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 *dephlogistication*. It is widely known today that phlogiston theory had difficulty explaining a number of phenomena – in Kuhnian terms it faced a number of anomalies. What is not so widely known is that the theory of phlogiston was empirically quite successful (cf. Carrier 2004, Schurz 2004, 2009) – examples of this success 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. in modern terms its forming a polarized bond with oxygen. In the modern generalized oxidation theory, the oxidizing substance need not be oxygen but another strongly electronegative substance, e.g. a halogen. Thus, according to the 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*.

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

In Schurz (2009) it is argued that the theoretical term "phlogiston" was empirically underdetermined. The theoretical expressions which performed the empirically relevant work for the theory of phlogiston and thus were *not* empirically underdetermined were *phlogistication* and *dephlogistication*. These concepts of phlogiston theory stand in the following relation of correspondence (C_i) 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 Figure 4.

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

Figure 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 FOR 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 in future case studies.

Interestingly, the understanding of chemical reactions according to the proposed frame, together with its intra- and inter-theoretic constraints, was *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 rival 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 (i.e. salt-formation) 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. Underlining indicates 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 metal calx + phlogiston, 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. Items in brackets denote residuals. Finally, "H" stands for "hydrogen".

Calcination of metals:
Oxygen theory: Metal + Oxygen → Metal$^+$–Oxide$^-$ [+ HotAir ↑]
Phlogiston theory: Metal (= MetCalx–Phlog) → MetCalx + Phlog–Air↑

Salt-formation of metals in acids:
Oxygen theory: Metal + H$^+$–X$^-$ (=Acid) → Metal$^+$–X$^-$ (=Salt) + Hydrogen (H_2)↑
Phlogiston theory: MetCalx–Phlog + Acid → MetCalx–Acid (=Salt) + Phlog (inflammable air)↑

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

Inversion of salt-formation:
Oxygen theory: Metal$^+$–Oxide$^-$ + Hydrogen → Metal + Water (= Hydrogen$^+$–Oxide$^-$)
Phlogiston theory: MetCalx + Phlog [+ Water-in-Air]) → Metal [+ Water-in-Air]↑

Note that the identification of phlogiston with 'inflammable air' (i.e. hydrogen) did not work in all domains. Moreover, 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. This was unconvincingly explained by different ad-hoc assumptions, e.g. by postulating that phlogiston had negative weight. 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.

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 salification frame of Figure 5. Here the oxygen theory's condition of being electropositive but in neutral-bond translates into the phlogiston theory's condition of being rich in phlogiston. Acid is primitive in phlogiston theory but consists of hydrogen ions plus a negative oxydans in oxygen theory. Metal is primitive in oxygen theory but analysed as metal calx-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 salt-formation, acid is the second input substance in both theories.

Chemical Reaction Category:	General Oxidation	Dephlogistication

Input 1: Condition: Is-Electropositive, Is-in-Neutral-Bond	Rich-in-Phlogiston
Substance: X = Metal	Metal calx–Phlogiston
Input 2: Condition: Is-Electronegative, Is-in-Neutral-Bond	Poor-in-Phlogiston
Substance: Z: {Oxygen:Y, Acid H^+–Y^-}	{Pure Heat, Acid}
Special and Catalytic Conditions: Heat	
Output 1: X^+–Y^- If Z = Oxygen: XCalx	If Z = Acid: XCalx–Acid
Output 2: If Z = Oxygen: none, If Z = Acid: H_2	Phlog
Residuals: None (exception: Hot Air in combustion)	

Figure 5. The chemical reaction frame for the process of combustion and salification in the theories of phlogiston and oxygen.

The inverted processes of reduction are displayed in the frame of Figure 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	Phlogistication
Input 1: Condition: Is-in-Electropositive Bond	Poor-in-Phlogiston
Substance: X^+–Oxide^-	XCalx
Input 2: Condition: Is-Electropositive, Is-in-Neutral Bond	Rich-in-Phlogiston
Substance: Y {Coal, Hydrogen}	Y {Coal = Ash–Phlog, Phlog}
Special and Catalytic Conditions: Heat	
Output 1: X	
Output 2: If Y = Coal: Coal^+–Oxide^- If Y = Hydrogen: Water (=Hydrogen^+–Oxide^-)	
If Y = Coal: Ash If Y = Phlog: none	
Residuals: If Y = Coal: Ash Phlog-Air If Y = Hydrogen/Phlog: none / Water	

Figure 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 tell 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 are underlined once and those that are underlined twice). On the basis of these and other reasons we are confident 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 frame-theory itself can be sharpened and further developed by its application to this field.

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