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How Terms Meet in Small-World Lexical Networks: The Case of Chemistry Terminology

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Abstract

We present a new type of terminological model based on formal network structures called lexical systems. Those are non-hierarchical lexical graphs where the bulk of lexical relations is formally encoded by means of Meaning-Text lexical functions. This paper describes how this approach to lexical structuring can be applied to the modeling of terminologies, more specifically, to the French and English terminology of chemistry. The first section explains the importance of terminology in chemistry and introduces the aim of our project. Section 2 is a brief presentation of formal characteristics of lexical systems. Section 3 illustrates the type of terminological descriptions we are implementing with the specific case of the chemical term catalysis.

1 Structuring the Lexicon of Chemistry

1.1 Key Role of Terminology in Chemistry

Terminology plays a key role in chemistry research. For instance, chemical terms, by their very morphological structure, are closely related to the behavior and properties of substances they designate. As noted by R. Hoffmann1 and P. Lazlo (1991), the knowledge of the name of a chemical compound, that strictly reflects the compound structure, gives the chemist the “control” over the molecule. Additionally, the terminology of chemistry is extremely vast and fluctuant. The importance of using a proper terminology in chemistry has lead to the creation, in 1919, of the IUPAC: International Union for Pure and Applied Chemistry. IUPAC elaborates rules for the nomenclature of molecules, in order to avoid definitional ambiguities and ensure harmonization of terminological proposals when new molecules are discovered. It has made available on-line for chemists the so-called Gold Book (McNaught and Wilkinson, 1997): an extensive dictionary-like description of English chemistry terms.

In spite of such efforts, the terminology of chemistry is loosely normalized. There is also a lack of multilingual perspective as most scientific papers are written in English, which can lead to serious problems in the context of the teaching of this discipline in schools and universities.

1.2 Terminological Networking

In the on-line IUPAC Gold Book, term descriptions are eminently relational, as illustrated by the entry for the nominal term bond below.2

(1) bond
There is a chemical bond between two atoms or groups of atoms in the case that the forces acting between them are such as to lead to the formation of an aggregate with sufficient stability to make it convenient for the chemist to consider it as an independent ‘molecular species’.
See also: agostic, coordination, hydrogen bond, multi-centre bond

The definition (There is a chemical bond …) in this description is doing its job of establishing connections between bond and related terms such as force, aggregate, etc. It is however an unstructured and non-formalized model for such connections. A greater applicative potential could

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1Nobel Prize in Chemistry 1981.

2http://goldbook.iupac.org/B00697.html
be achieved by explicitly encoding the linguistic structure of a term definition. If such structure mirrors the logical organization of concepts in the corresponding scientific domain, the lexical definition can be an efficient tool for the understanding of scientific texts, for scientific writing and for teaching chemistry.

Additionally, as illustrated by terminological pointers at the end of (1) – agostic, coordination, hydrogen bond, multi-centre bond – the mastering of a chemistry term and of the corresponding notion depends on the ability to position this term within the network of other terms that gravitate in its semantic space.

Polysemy is another acute problem in the terminology of chemistry, that is generally ignored in existing resources. Polysemy manifests itself in two ways.

A) It can occur within the terminology itself, when a single form is used to denote different terminological notions – for instance, to catalyze as ‘[for a substance] to cause a certain type of chemical reaction’ in (2) vs. ‘[for a chemist] to make this reaction take place’ in (3).

(2) These fiber catalysts can efficiently catalyze the Knoevenagel condensation of benzaldehyde and ethyl cyanoacetate in water (yields: 95-98%).

(3) These Ta2O5-T samples were characterized by TG / DTA, XPS, nitrogen adsorption, XRD, and UV-Raman, and were employed to catalyze the gas-phase dehydration of glycerol (GL) to produce acrolein (AC) at around 315 degrees C.

B) Polysemy can also spread over both chemistry terminology (2)-(3) and general language (4).

(4) Cities are always building new stadiums with the justification that they’ll catalyze the local economy.

All these observations show that it is necessary to organize the terminology of chemistry according to rigorous theoretical and descriptive principles.

The project we are presenting has a very practical aim: the design and construction of a terminological database in chemistry, for both the English and French languages. It also has theoretical implications as it explores a new approach to the structuring of terminologies based on non-hierarchical graph structures (see lexical systems, section 2 below), where each term is an element in a global lexical network in which it is related to the rest of the domain terminology, as well as to general language lexicon, by means of Meaning-Text lexical functions (Mel’čuk, 1996).

Lexical functions have already proved to be an efficient tool to model relations between terms (L’Homme, 2002). In our project, however, the recourse to lexical functions is embedded within a formal proposal for the graph structuring of lexical knowledge – lexical systems – that we believe is particularly suited to account for the interaction between terminologies of different domains – e.g., chemistry terms used in physics – as well as between “purely” terminological units and units that belong to the general language – e.g. water as a type of molecule and water as a substance.

2 Terminologies as Lexical Systems

The terminological models we are elaborating are grafted on two general language lexical resources: the English and French Lexical Networks (Gader et al., 2014; Lux-Pogodalla and Polgëre, 2011), respectively en-LN and fr-LN.

The design of the en- and fr-LNs is based on a new type of lexical model called lexical system (Polgëre, 2014). From a formal point of view, a lexical system is a graph whose vertices are lexical units of the lexicon under description and whose edges are lexical relations of essentially two types:

1. semantic relations – (chemical) bond is linked to to bond, interaction, compound . . . ;

2. combinatorial relations – (chemical) bond combines with covalent, ionic . . .

Both types of relations are modeled by means of lexical functions (section 1.2 above): paradigmatic lexical functions in the first case and syntagmatic lexical functions in the second case. Though lexical functions provide the bulk of graph structuring in lexical systems, other types of relations are also implemented. For instance,
semantic embedding is implemented via links weaved within lexical definitions: cf. the definition of CATALYSIS I.1, section 3.3 below, that formally links this term to two semantically embedded terms: REACTION 1 and GIBBS ENERGY.

Such graphs belong to the family of so-called small-world networks (Watts and Strogatz, 1998) and their topological properties allow for the automatic identification of semantic spaces through clusterization. Figure 1 illustrates the semantic space of BONDN I.2 – the chemistry sense of the noun BOND in the current version of the en-LN.

Beside being computer-tractable structures, lexical systems are equivalent to “virtual dictionaries”, as all properties of lexical units are encapsulated in graph vertices – lexical definitions, grammatical information, citations from corpora (i.e. contexts), etc. Thanks to a specially designed lexical graph editor, it is possible to build a lexical model and, thus, a terminology, by methodically weaving lexical systems (Polguère, 2014). In the specific case of the work presented here, we are describing the terminology of chemistry by weaving the terminological network of this discipline directly on top of the general language en- and fr-LNs. This will allow not only for the proper connection of terminologies in both language, but also for the “interpretation” of chemical terms relative to the non-specialized lexical stock, with which these terms naturally interact in standard research activity as well as in scientific texts.

3 Example: The Case of CATALYSIS I.1

We now illustrate our approach with the en-LN description of the noun CATALYSIS. It possesses the same polysemic structuring as the corresponding verb CATALYZE – see (2), (3) and (4), section 1.2. Therefore, two chemistry senses have to be distinguished within the nominal vocable:

- CATALYSIS I.1 [The catalysis occurred via the formation of a chloromethylated triflate complex, and electrophilic addition to an aromatic hydrocarbon.]
- CATALYSIS I.2 [Were they doing catalysis, and if so, how did they recover the catalyst?]
core structuring element of our model: the multidimensional system of lexical function relations that connects lexical units.\footnote{The distinction between article-view and lexical graph perspectives on the en-LN bears some similarity with written vs. graph information modes in Pram Nielsen (2013).}

3.2 Web of Lexical Function Relations

The structurally most relevant information in Figure 2 appears in the lexical function zone \([\text{LF}]\). It corresponds to the set of paradigmatic links that originate from the CATALYSIS I.1 headword and connect it the rest of the lexical system. (At present, no syntagmatic link has been encoded for this specific term.) It is this information, together with incoming lexical function links, that position the term in the global structure of the en-LN and defines its semantic space.

In our terminology, the semantic space of a lexical unit such as CATALYSIS I.1 is much more than just the subgraph constituted of all outgoing and incoming lexical function links. It is the topologically significant cluster of semantically-related nodes that gravitate around CATALYSIS I.1, as illustrated in Figure 3.

This semantic space features not only lexical units that are directly connected to CATALYSIS I.1 – e.g. CONTACT ACTION or CATALYST I –, but also indirectly connected terms – e.g. GREEN CHEMISTRY or CHEMICAL CHANGE – that entertain significant semantic proximity with this headword.

At present, semantic space clustering is based

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Figure 2: Current en-LN article-view for CATALYSIS I.1.

Figure 3: Semantic space of CATALYSIS I.1.
of Proxemy analysis (Gaume, 2008). It is optimized by taking into consideration the semantic weight of each individual lexical function. For instance, a paradigmatic lexical function such as $S_1$ possesses the maximal semantic weight “2” in the en-LN model of lexical functions, while the $\text{Oper}_1$ lexical function denoting support verb collocates possesses the minimal semantic weight “0”.  

We believe that lexical systems – small-world graphs of lexical units connected by paradigmatic and syntagmatic relations – are powerful alternatives to more traditional taxonomic models for at least two reasons: (i) they favor semantic space connectivity over a more restricted class-based organization and (ii) they unite both semantic and combinatorial connections within the same formal apparatus (lexical functions).

3.3 Definitional Embedding of Notions

To conclude, we wish to say a few words about definitions and their role in the structuring of terminological knowledge. As indicated in section 2, lexical definitions also participate in the weaving of lexical systems, though to a lesser extent, by implementing semantic embedding. In the specific case of CATALYSIS1.1, two lexical units appear in the article-view as clickable targets of definitional embedding links: REACTION1 and the terminological idiom GIBBS ENERGY. This is made possible by the formal encoding the definition: an XML-like tagging of the definitional text, that we will not detail here for lack of space.

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