

An Examination of Quality in Patents

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The generation of one or more systematic names associated with the submission of a patent is generally a time-consuming and challenging process requiring nomenclature skills and much rigor. Even though IUPAC rules are well defined, the final systematic name generated can often be the result of a subjective decision. Unfortunately, such a path will not necessarily lead to success and the resulting names will not only be incorrect according to a well-defined rule set but provide an ambiguous name which cannot be reversed to the correct chemical structure. The reverse process of converting the name to the chemical structure(s) referred to in a patent is obviously even more time consuming and challenging under these conditions.

Fortunately, software offers an objective, facile, and fast manner by which to generate high quality systematic names. In particular, ACD/Name (<http://www.acdlabs.com/name/>) offers the possibility to generate systematic names according to both IUPAC and CAS-based Index rules. Rather than belabor the capabilities of this software package in this document, the reader is referred to a technical overview (http://www.acdlabs.com/products/name_lab/name/tech.html), to an analysis with alternative software packages also offering systematic naming support (http://www.acdlabs.com/products/name_lab/name/competit.html), and to the feedback obtained from a series of unbiased and independent reviewers (http://www.acdlabs.com/products/name_lab/name/reviews.html), as well as a summary of features relevant for patent experts (<http://www.acdlabs.com/solutions/chempatent>).

The purpose of this document is to focus specifically on examples of how the subjective, manual generation of systematic names can impact the quality of information contained within a patent. Resulting errors could potentially lead to delays during the filing process and create ambiguity in the coverage. As an example of the typical quality of names contained within patents, let us consider two patents available online at

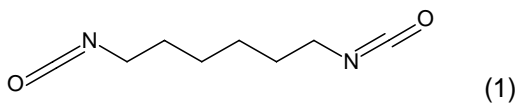
Patent 1 <http://l2.espacenet.com/espacenet/viewer?PN=US5085725&CY=gb&LG=en&DB=EPD>
and
Patent 2

<http://l2.espacenet.com/espacenet/viewer?PN=US2002111519&CY=gb&LG=en&DB=EPD>

Patent 1 describes a **“Method of chemical bonding of solid propellant grains to the internal insulation of an interceptor motor”** and the patent abstract includes the following statement, *“The trimer of 1,6-hexanediiisocyanate, which has the chemical name in accordance with International Union of Pure and Applied Chemistry (IUPAC) nomenclature of 7-aza-8-oxo-7[1-isocyanato-6-oxohexyl]pentadecanediiisocyanate, is employed in a method of chemical bonding of solid propellant grains to the internal insulation of an interceptor motor.”*

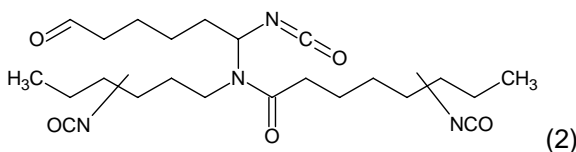
To understand the nature of a patent, we need to conclude what substances are used. This task can be rather simple using the listed chemical names and especially those that are systematic in nature according to either IUPAC or CAS Index rules.

Considering the monomer name of **1,6-hexanediisocyanate**, we can comment that it is **not** possible to confidently reverse this name to the chemical structure using ACD/Name name-to-structure functionality. We assume that compound (1) is the proposed monomer.

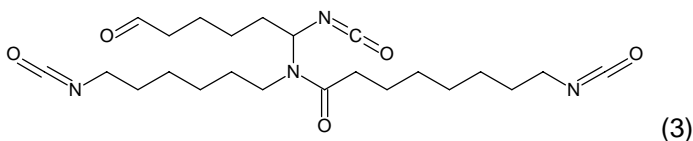


According to strict IUPAC nomenclature, the actual systematic name should be 1,6-diisocyanatohexane or hexane-1,6-diyl diisocyanate. Less strict variations include 1,6-hexanediyl diisocyanate, 1,6-Hexamethylene diisocyanate, 1,6-Hexylene diisocyanate, or Hexamethylene diisocyanate. So, the structure of the monomer can be simply concluded from the name. The trimer structure is far less clear.

The trimer is listed in the patent as **7-aza-8-oxo-7[1-isocyanato-6-oxohexyl]pentadecanediisocyanate**. This name has a number of significant errors including the fact that it violates the order of the citation of modifications, has a missing dash, and does not indicate the positions for the two "isocyanate" groups on the 15-atom chain. The lack of the positional information results in the ambiguous structure shown below (2), with a molecular formula of $C_{23}H_{36}N_4O_5$.



Assuming that the isocyanate groups are terminal, we will obtain the following structure (3).



The molecular formula of the monomer is $C_8H_{12}N_2O_2$, and by definition a true trimer must have a molecular formula of $C_{24}H_{36}N_6O_6$, which this does not. Chemical sense also suggests that such a structure cannot be formed from the monomer at least due to the presence of a seven carbon chain in the structure.

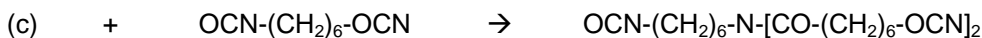
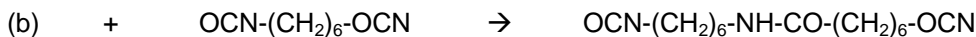
To determine whether this questionable substance is used or not, we can investigate the full patent information found at the same website. You may find that the Summary of the Invention section provides the necessary details and clarifies the situation.

The conversion of 1,6-hexanediisocyanate into its trimer involves three steps. These are:

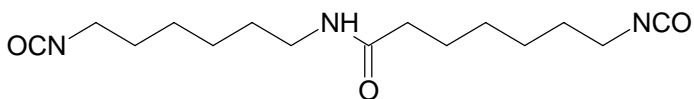
- Reaction of **1,6-hexanediisocyanate** with water to form **1-amino-6-hexaneisocyanate**
- Reaction of an additional molecule of 1,6-hexanediisocyanate with 1-amino-6-hexaneisocyanate to form **7-aza-8-oxo-1,6pentadecanediisocyanate**
- Reaction with another molecule to form triisocyanate whose chemical name, (according to the International Union of Pure and Applied Chemistry) is **7-aza-8-oxo-7[1-isocyanato-6-oxohexyl]pentadecanediisocyanate**

Once again, the same strange names are given but the patent includes chemical reactions that clearly describe the process:





It seems clear that the substance described in step (b) is:



with the correct IUPAC name being:

7-isocyanato-N-(6-isocyanatohexyl)heptanamide

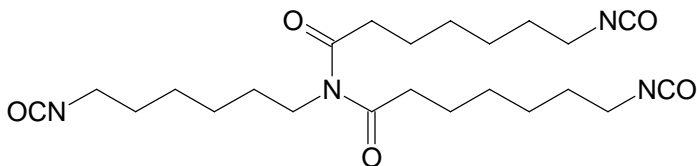
Alternatively, using the "patent way of naming", the name would be:

7-aza-8-oxo-1,14-tetradecanediisocyanate

which is very different than the given name:

7-aza-8-oxo-1,6-pentadecanediisocyanate

Now we also have the described structure of trimer:



with the correct IUPAC name being:

7-isocyanato-N-(7-isocyanatoheptanoyl)-N-(6-isocyanatohexyl)heptanamide

Alternatively, using the "patent way of naming", the name would be:

7-aza-8-oxo-7-[6-isocyanato-1-oxoheptyl]-1,14-tetradecanediisocyanate

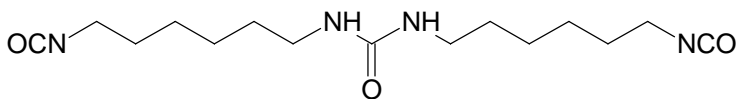
which is also very different than the given name:

7-aza-8-oxo-7-[1-isocyanato-6-oxohexyl]pentadecanediisocyanate

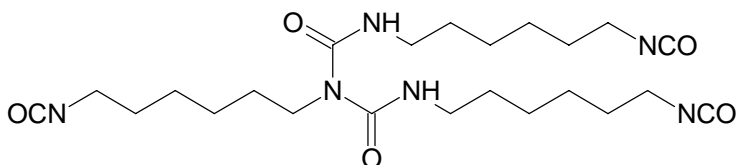
Everything should now be clear with respect to the differences between IUPAC names and the names used in this patent nomenclature. However, there are additional factors to consider.

Even minor chemical sense leads to the question of how two seven carbon bonds may be formed from a structure that only has a six carbon chain? We may even ignore the well known fact that isocyanates react with amines to form urea derivatives.

If we change the college level reactions so that they lead to the correct urea derivatives, we will have the following, **finally correct**, structures for (b) and (c) correspondingly:



N,N-bis(6-isocyanatohexyl)urea

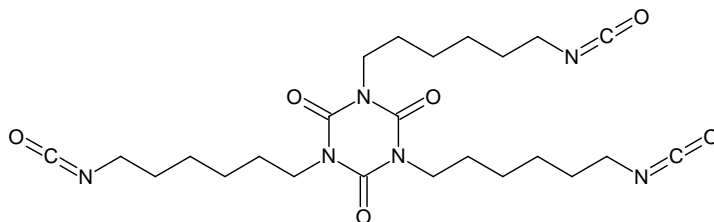


1,3,5-tris(6-isocyanatohexyl)biuret
(or *N,N',N''*-tris(6-isocyanatohexyl)dicarbonimidic diamide)

To be absolutely certain of our conclusions, the paper "Urethane Acrylates from Oligomeric Hexamethylene Diisocyanate Derivatives", by Dr. Thomas Fäcke, Dr. Wolfgang Fischer, Diethelm Rappen, Dr. Frank Richter, and Dr. Jan Weikard, can be found at:

<http://www.radtech-europe.com/download/weikardpapermay2004.pdf>

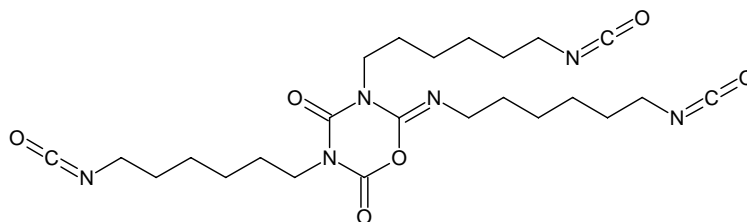
This article describes the structures that can exist in oligomeric diisocyanate products including those that can form due to the presence of water. The biuret structure concluded above is given in this article along with the true trimeric structures below (4).



Symmetric trimer

Correct IUPAC name: 1,3,5-tris(6-isocyanatohexyl)-1,3,5-triazinane-2,4,6-trione

Index name: 1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione, 1,3,5-tris(6-isocyanatohexyl)-

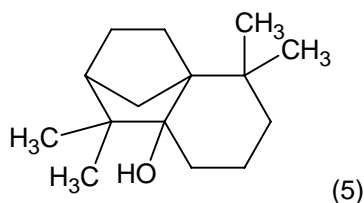


Asymmetric trimer

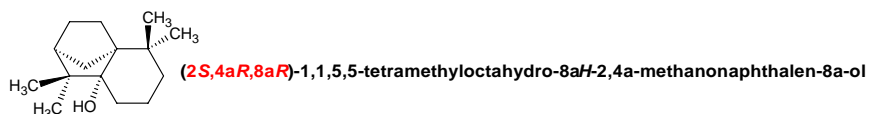
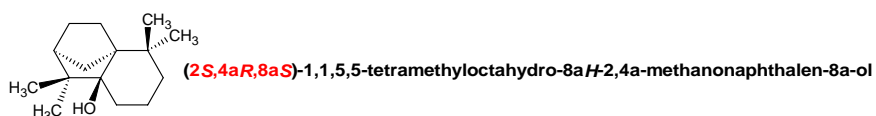
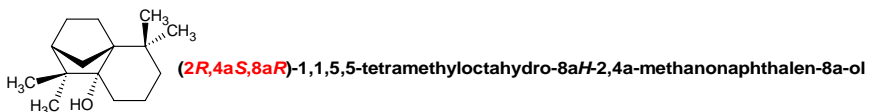
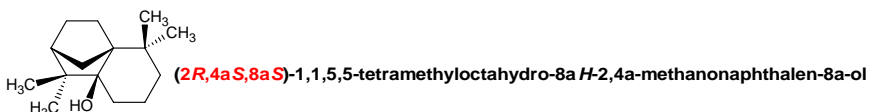
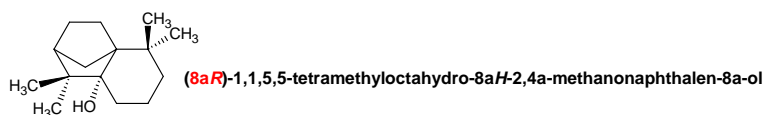
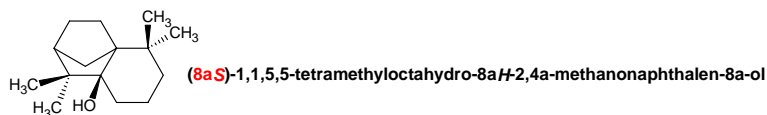
3,5-bis(6-isocyanatohexyl)-6-[(6-isocyanatohexyl)imino]-1,3,5-oxadiazinane-2,4-dione
2*H*-1,3,5-oxadiazine-2,4(3*H*)-dione, dihydro-3,5-bis(6-isocyanatohexyl)-6-[(6-isocyanatohexyl)imino]- (4)

Patent 2 describes a "Process for the preparation of isolongifolanol" and the patent abstract includes the statement "The invention relates to the preparation of the compounds isolongifolanol (IUPAC name: 2,2,7,7-tetramethyltricyclo[6.2.1.0^{1,6}]undecan-6-ol) and isolongifolenol (IUPAC name: 2,2,7,7-tetramethyltricyclo[6.2.1.0^{1,6}]undec-4-en-6-ol) and to the use thereof as fragrance or aroma substance."

We are uncertain whether this is an error due to the web-based display, but the original name is listed online as 2,2,7,7-tetramethyltricyclo[6.2.1.0^{1,6}]undecan-6-ol, while it probably should be 2,2,7,7-tetramethyltricyclo[6.2.1.0^{1,6}]undecan-6-ol in order to allow conversion of the name to the chemical structure shown below (5).



However, the name is ambiguous in terms of stereochemistry and the resulting chemical structure is simply a connection diagram. Since the stereochemistry is not defined, all of the structures drawn below (6) are consistent with the name in terms of connectivity. The actual IUPAC Name generated using ACD/Name is listed adjacent to the corresponding chemical structure with the differences in stereochemistry highlighted in red.



ACD/Name offers powerful visualization tools displaying the association between a substructure and a portion of the name as shown below in Figure 1.

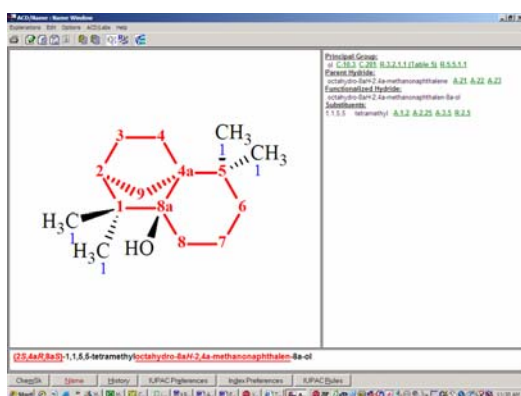


Figure 1

Stereochemistry is obviously complex to assign manually. ACD/Name not only correctly assigns the stereocenters, but also provides a map of the stereochemical tree, as shown in Figure 2, which is used to generate the correct stereochemistry label.

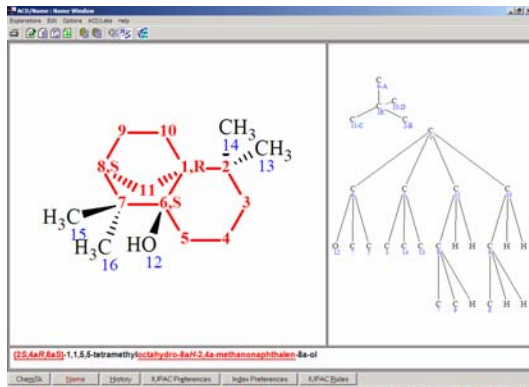
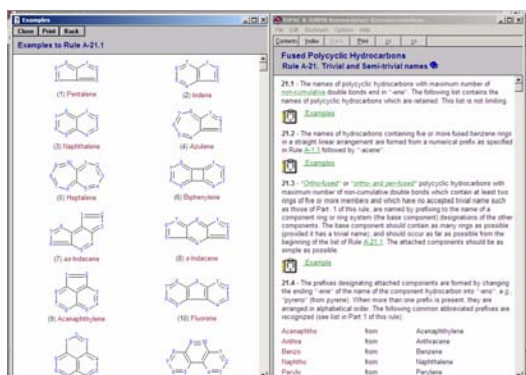


Figure 2

ACD/Name also provides direct links to the IUPAC rules which were used to generate the systematic name. In Figure 1 above, the links on the right side can be selected to highlight the appropriate rules as shown below in Figure 3.



Examples to Rule A-21.1

(1) Pentalene (2) Indene
(3) Indolizene (4) Azulene
(5) Heptalene (6) Dphenylene
(7) Anthracene (8) Indolene
(9) Acenaphthylene (10) Fluorene

Fixed Polycyclic Hydrocarbons
Rule A-21.1. Trivial and Semi-trivial names

A-21.1 - The names of polycyclic hydrocarbons with maximum number of non-cumulative double bonds end in "ene". The following list contains the names of polycyclic hydrocarbons which are retained. This list is not binding.

A-21.2 - The names of hydrocarbons containing five or more fused benzene rings in a straight line arrangement are formed from a numerical prefix as specified in Rule A-21.1 followed by "acene".

A-21.3 - "Ortho-fused" or "ortho and para-fused" polycyclic hydrocarbons with maximum number of non-cumulative double bonds which contain at least two rings of five or more members and which have no accepted trivial name such as those of Rule 1 of this rule, are named by prefixing to the name of a component ring or ring system (the base component) designations of the other components. The base component should contain as many rings as possible (provided it has a trivial name), and should occur as far as possible from the beginning of the list of Rule A-21.1. The attached components should be as simple as possible.

A-21.4 - The prefixes designating attached components are formed by changing the ending "ene" of the name of the component hydrocarbon into "ene" or "ylene" (from "ylene"). Other more than one prefix is present, they are arranged in alphabetical order. The following common abbreviated prefixes are recognized (see list in Part 1 of this rule).

Acenaphtho	from	Acenaphthylene
Anthra	from	Anthracene
Benz	from	Benzene
Indaph	from	Indaphthalene
Phenyl	from	Phenylene

Conclusion

High quality systematic nomenclature is a necessary part of communicating details regarding chemical structures, especially during a patent filing. The ability to generate names in a manual fashion has been surpassed by the development of systematic naming software. Access to convenient methods by which to generate names and reverse names is available through ACD/Name, and includes comprehensive features that facilitate manual inspection and review. ACD/Name occupies a unique space in being able to generate IUPAC and CAS-Index type systematic names, as well as reverse these names to their associated chemical structures. Predictably, this software suite is already the preferred choice of chemical and pharmaceutical companies who produce and patent novel chemical compounds on a regular basis. It has become increasingly popular among patent agents and attorneys whose reputation depends on the quality of their generated patent applications, prior art searches, and litigation documents.