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White Paper

# An Examination of Quality in Patents

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## Introduction

The generation of systematic names for the submission of a patent is a time-consuming and challenging process requiring much rigor. While IUPAC rules are well defined, when manually naming compounds the final systematic names generated can often be the result of a subjective decision. Unfortunately, this means that the names may be ambiguous or incorrect, and reversing chemical names to the correct chemical structure can be an impossible task under these conditions.

Fortunately, existing software offers an objective, facile, and fast manner by which to generate high quality systematic names, and provides a way to check the accuracy of given names. ACD/Name[1] offers the possibility to generate systematic names according to both IUPAC and CAS-based Index rules together with an ability to generate chemical structures from names.

In this white paper, we discuss how subjective, manual generation of systematic names can impact the quality of information contained within a patent. Errors could potentially lead to delays during the filing process, create ambiguity in the coverage, and lead to patent vulnerability and invalidation.

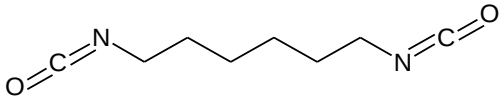
## Examination of US Patent 5,085,785

As an example of the, unfortunately, typical quality of chemical names in patents, let us consider US Patent 5,085,785 available online[2]. This patent claims the "Method of chemical bonding of solid propellant grains to the internal insulation of an interceptor motor". The abstract begins with the following statement describing the main part of this patent,

*"The trimer of 1,6-hexanediisocyanate, 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]pentadecanediisocyanate, 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 first need to understand the substances described within. This task should be easy enough, particularly if systematic names are provided as stated above; simply identify the listed chemicals.

Let's begin with the monomer named **1,6-hexanediisocyanate**. While a nomenclature expert will likely deduce the intended structure, this name is incorrect according to nomenclature rules. The correct structure of the monomer described in the patent is shown as entity (1).



(1)

According to chemical nomenclature rules, a correct systematic name would be **hexane-1,6-diyl diisocyanate** or **1,6-diisocyanatohexane**, with the traditional name **hexamethylene diisocyanate**.

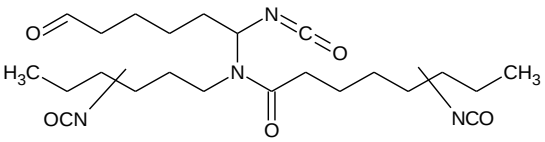
Variations in the names described above may seem innocuous, but a quick Google search shows the problems such differences raise, for example, in a prior art search.

| Name | Hits in Google Search |
|---|---|
| **1,6-hexanediisocyanate** | 7,230 |
| 1,6-diisocyanatohexane | 38,500 |
| hexane-1,6-diyl diisocyanate | 22,200 |
| hexamethylene diisocyanate | 310,000 |

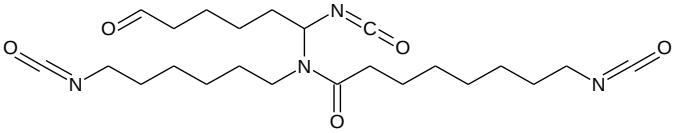
It is not surprising that the traditional name, **hexamethylene diisocyanate**, gives the largest number of hits. It still appears on bottle labels today containing this substance, often alongside the systematic name **1,6-diisocyanatohexane**. The most important result in this table is the number of hits produced by the incorrect name provided in the patent—**1,6-hexanediisocyanate**—by far the smallest number.

Having concluded the structure of the monomer, along with an understanding of the importance of good quality names, we proceed to the mysterious "trimer" described in the patent, listed as **7-aza-8-oxo-7[1-isocyanato-6-oxohexyl]pentadecanediisocyanate**. This name contains a significant number of nomenclature errors and cannot claim to have been generated according to IUPAC rules. Further, the correct chemical structure cannot be generated from this name.

Keeping in mind that the position of attachment of isocyanate groups is not indicated in the name, we might deduce the structure to be (2). Alternatively, assuming terminal isocyanate groups, we would obtain structure (3).




(2)




(3)

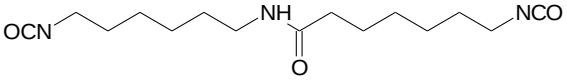
The molecular formula of the monomer is $C_8H_{12}N_2O_2$, and by definition a true trimer must have a molecular formula of $C_{24}H_{36}N_6O_6$, which neither of these structures does. To determine the structure of the mysterious "trimer", we can follow the chemical reactions described within the patent that explain how the substance is formed:

(a) $OCN\text{-}(CH_2)_6\text{-}NCO + H_2O \rightarrow OCN\text{-}(CH_2)_6\text{-}NH_2 + CO_2$

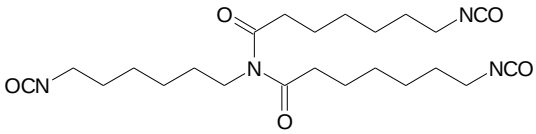
(b) $+ \; OCN\text{-}(CH_2)_6\text{-}NCO \rightarrow OCN\text{-}(CH_2)_6\text{-}NH\text{-}CO\text{-}(CH_2)_6\text{-}NCO$

(c) $+ \; OCN\text{-}(CH_2)_6\text{-}NCO \rightarrow OCN\text{-}(CH_2)_6\text{-}N\text{-}[CO\text{-}(CH_2)_6\text{-}NCO]_2$

The product of reaction step (b) is (4), and the resulting structure of the "trimer" product in step (c) is (5), as described in the patent.




(4)




(5)

The correct IUPAC name of the final product (5) is

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

Alternatively, using this patent's method of naming, the name should have been

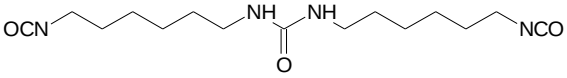
**7-aza-8-oxo-7-[6-isocyanato-1-oxoheptyl]-1,14-tetradecanediisocyanate**

which is still very different to the name provided in the patent (**7-aza-8-oxo-7-[1-isocyanato-6-oxohexyl]pentadecanediisocyanate).**

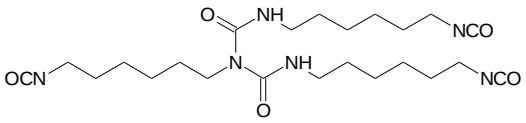
This exercise shows very clearly the difference between correct IUPAC names and the type of nomenclature that often appears in patents, and highlights some of the problems incorrect names can cause.

There are, however, additional factors to consider. Even a little chemistry knowledge leads to the question of how two seven carbon chains can be formed from a structure with only a six carbon chain.

Remembering college level chemistry—isocyanates react with amines to produce urea derivatives. We can correct the reactions so that they lead to the corresponding urea derivatives resulting in the following, **correct**, structures for (4) and (5):




(4)




(5)

Finally, we determine the correct structure of the product, and using ACD/Name (IUPAC rules) produce the correct systematic name: ***N*,*N*′,*N*″-tris(6-isocyanatohexyl)dicarbonimidic diamide** (with a more traditional name of **1,3,5-tris(6-isocyanatohexyl)biuret**). This must be the final product that the patent was supposed to cover.

In this example, we began with suspicious chemical names, and with some basic chemical sense and the help of expert naming tools, concluded the correct chemical substances implied by the patent, and arrived at the unfortunate conclusion that this patent is not really worth very much. The chemistry AND nomenclature are incorrect. One may argue that this patent, dated 1992, is rather old and the quality of current chemical names in patents is far better. Unfortunately the situation is still far from encouraging.

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# ACD/Name for Nomenclature Generation

High quality systematic nomenclature is a necessary part of communicating details regarding chemical structures, especially during patent filing, and in the analysis of existing patents or prior art searches.

Access to algorithmic tools to generate names and reverse names into chemical structures has now become absolutely necessary in all areas where chemical entities are involved, particularly where legality is an issue. Not only is ambiguity removed when using a well-built tool, but mistakes are reduced, and a systematic method for naming of chemical entities is provided. An expert may still manually re-check generated names, but the tedium of systematic naming is vastly reduced.

With a focus on providing unambiguous and correct nomenclature, ACD/Name remains a unique solution providing systematic chemical names according to both IUPAC and CAS-Index type rules. The reversal of name to structure is also provided with confidence, and alerts are issued where ambiguity may exist. Further, where a re-check of the name is required, the software provides links between structure and elements in the name, and also provides links to the specific IUPAC recommendations applied in name generation.

We offer an expert easy-to-use nomenclature software package with Name-to-Structure tools for the preparation of patent applications; a structure and text-searchable library, and Structure-to-Name capabilities to help with prior art searches; and explanations of the rules applied in name generation with links to IUPAC recommendations to address examiner disagreements.

This software is already the preferred choice of global 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.

## References


1. ACD/Name http://www.acdlabs.com/name, Advanced Chemistry Development, Inc. (ACD/Labs), Toronto, ON, Canada 29 April 2011.
2. US Patent 5,085,785 http://www.freepatentsonline.com/5085725.pdf