

On the Nomenclature of Toxaphene Congeners

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1. Introduction

Last decade brought dramatic changes into the environmental analytical chemistry of Toxaphene :

- Toxaphene was found to be more important class of chloroorganic pollutants, than it seemed before
- The need in congener-specific analysis has been realized
- The great number of chlorinated terpenes was synthesized or isolated from technical Toxaphene or environmental samples (about 50 compounds with full or partial structure elucidation)

Unfortunately, all Toxaphene congeners (like Polychlorinated Biphenyls) have very long and difficult-to-pronounce IUPAC chemical names. Naturally, people would like to have an opportunity to use short numbers instead - since it is proved to be suitable for Polychlorinated Biphenyls

This article is an attempt to introduce nomenclature of Polychlorinated Bornanes, representing the main part of Toxaphene - nomenclature, based on IUPAC principles and binary system of counting.

2. Toxaphene congeners/PCB congeners : Differences and Similarities

PCB systematic numbers have had a great success over the years and it is interesting to compare PCBs and Chlorinated Bornanes from the "classifier"s point of view.

Similarities

- 1) for both classes chemical names are long and "difficult-to-pronounce"
- 2) both classes contain a great number of compounds(209 and 32767)with different number of Cl atoms
- 3) for both classes unknown peaks on chromatograms appeared before analytical standards

Differences

- 1) Retention times for Chlorinated Bornanes are less predictable
- 2) the number of possible Chlorinated Bornanes is much higher than that of PCBs
- 3) while all PCB congeners have been isolated in pure state and properly characterized, all Chlorinated Bornanes will never be isolated

The first classification was based on toxicity(Toxicants A₁ & A₂, Toxicant A_c, Toxicant B, Toxicant C). Then, for many years scientists used to mark peaks on a chromatogram in order of elution. This practice leads, in case of coeluting compounds, to one number for several different compounds and in general to

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non-reproducibility of the numbers. For instance, you can find at least 7 different names for 2-endo,3-exo,5-endo,6-exo,8,8,9,10,10-Nonachlorobornane (T12, T9, Tox Ac, #4, #10, #17, #50)...

It is possible to put all Chlorinated Bornanes on the list in IUPAC order (like PCBs) and use the resulted numbers. The main problem is a number of congeners - 32767 ! The list would be a book and the numbers would be 5-digit for most environmentally relevant compounds.

Now we present a nomenclature of Chlorinated Bornanes, which :

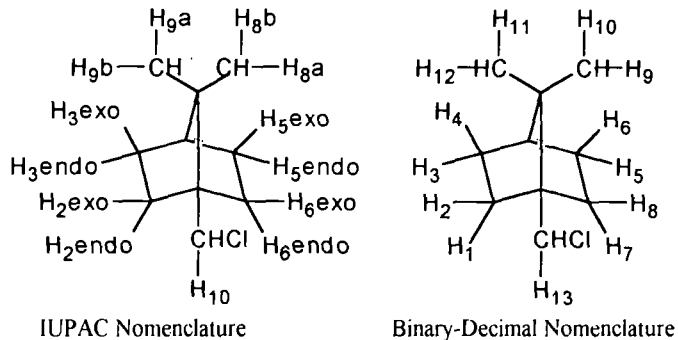
- is in accordance to IUPAC principles
- keeps any number only 4-digit
- allows to give numbers to "just identified" compounds and to decode numbers easily - there is no need in having a long list (a thick book).
- is a dream of computers (if computers are able to dream)

3. Binary-decimal nomenclature of Chlorinated Bornanes

The use of the nomenclature is based on several assumptions :

- environmentally important congeners have one or two Chlorines at C-10
- environmentally important congeners have not more than two Chlorines at C-8 or C-9
- environmentally important congeners have no Chlorine at C-4

Therefore, one can see 13 hydrogens, which could be substituted by chlorines. We mark these hydrogens consecutively, according to IUPAC order of preference).



We create 13 digit binary number - write 1 if corresponding hydrogen is substituted, write 0 - if not. Then convert it into 4-digit, easy-to-remember, decimal number.

Example : 2-endo,3-exo,5-endo,6-exo,8,8,9,10,10-Nonachlorobornane (Toxicant Ac).

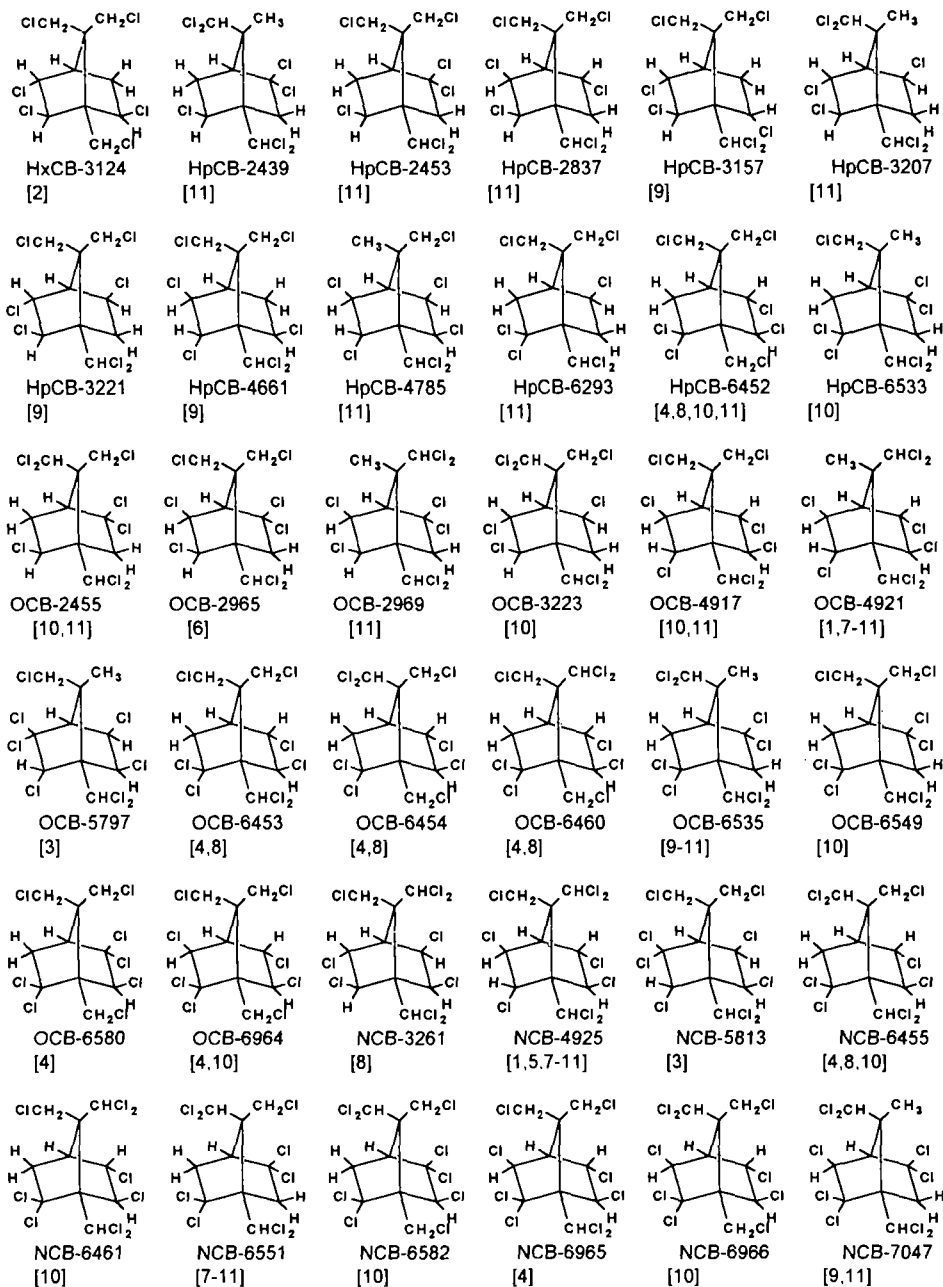
Binary number - 1001100111101

Decimal number - 4925

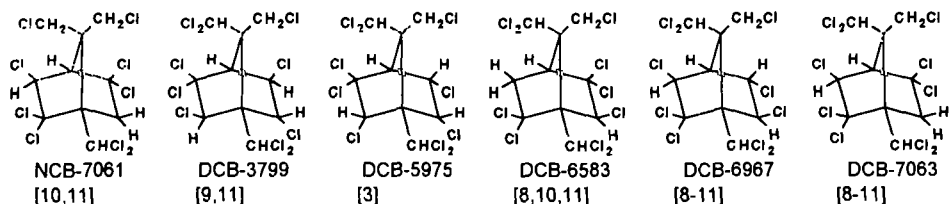
Toxicant Ac is NCB4925

Chemical structures and new numbers of 42 Chlorinated Bornanes (1 HexaCB, 11 HeptaCBs, 14 OctaCBs, 11 NonaCBs and 5 DecaCBs) reported in literature up to date are given on the next page

in order of increase of the numbers, references to the literature are given in brackets:



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We decided to accept structure elucidation from original papers. In some cases we changed the names, according to IUPAC (this problem was discussed¹⁾). It is necessary to mention, however, that reported NMR data for NCB-5813, also known as Toxicant C and for DCB-5975³⁾, are very similar to that of NCB-7061 and DCB-6967⁸⁻¹¹⁾.

4. Advantages and Disadvantages of Binary-Decimal Nomenclature of Chlorinated Bornanes

The disadvantages are :

- it is not a nomenclature for all classes of Toxaphene congeners (however, the same principle can be easily applied to Camphenes, Camphanes, Bornenes, Pinenes, etc.)
- very similar congeners may have absolutely different numbers (however, you will soon start to see some rules)
- a number of higher chlorinated congener is not always higher, than that of lower chlorinated one (however, it is usually higher)

The advantages are :

- definiteness : one number corresponds to one and only one congener
- easy coding and decoding
- computer compatibility

It will take some time for scientists to study this nomenclature, to play with it, to make improvements and corrections and to accept or reject it. It is just an attempt to put Toxaphene congeners into order...

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