## Chapter-13

# IUPAC Nomenclature of Higher Alkanes – Innovative Method

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IUPAC nomenclature of lower alkanes (1C to 10C) is quite common and digestible. But students face problems remembering and predict IUPAC word-root during IUPAC nomenclature of higher alkanes (C >11). Here in this innovative article, I have tried to focus IUPAC nomenclature of higher alkanes (11C to 90C) through the prediction of IUPAC word root by using innovative mnemonics to make the concept unambiguous, simpler, time-economic, and interesting.

#### 1. Introduction

Anatomy of hydrocarbon unit constitutes of carbon and hydrogen. In alkane, bond order is always one. In hydrocarbon, IUPAC nomenclature of alkane should be carried out by counting the total number of carbon atoms present in the longest continuous carbon chain. Alkane is nothing but the conjunction of 'alk' and 'ane', where 'alk' is treated as *prefix* and 'ane' is treated as *suffix*. Conventional methods<sup>1,2,3,4,5</sup> that have been used to predict IUPAC nomenclature of higher alkanes are limited in numberandare arranged for sets of tens over twenty. As per conventional method<sup>1,2</sup>IUPAC word-root for sets of tens over twenty are formed by adding the ending "-conta-" to the name of the corresponding units, with insertion of an "a" for thirty like as 3 tri -30 triaconta; 4 tetra- 40 tetraconta; 5 penta- 50 pentaconta-, etc. If we want to extend the list by sets of 10, we shall need a specific ending for hundreds and for thousands.

In this present article, IUPAC word-root of higher alkanes (11C – 90C) have been illustrated in detail including intermediate higher alkanes along with alkanes having sets of tens over twenty by innovative way using useful mnemonics. Here, higher alkanes are divided into two series 'odd'and'even' for which two different prefixes 'alka' and 'alk' should be used respectively.

<sup>1.&</sup>quot;Extension of Rules A-1.1 and A-2.5 concerning numerical terms used in organic chemical nomenclature (Recommendations 1986)", Pure & Appl. Chem., Vol. 58, No. 12, pp. 1693—1696, 1986.

<sup>2.</sup> S.C.Pal, "Nomenclature of Organic Compounds", Revised ed., Narosa Pub., p-30, 2008.

<sup>3.</sup> T.W. Graham Solomons and C.B. Fryhle, "Organic Chemistry", Wiley: India 10<sup>th</sup>ed., p142, 2012. 4. A. Bahl and B.S.Bahl, "A Text Book of Organic Chemistry", 22<sup>nd</sup>ed., S.Chand, p155, 2015.

<sup>5. &</sup>quot;Nomenclature of Alkanes", Jonathan Mooney, McGill University, chem.libretexts.org, University of California, Davis,

UShttps://chem.libretexts.org/Bookshelves/Organic\_Chemistry/Supplemental\_Modules\_(Organic\_Chemistry)/Alkenes/Naming\_the\_Alkenes

# 2. Methodology

#### 2.1. Classification of higher alkanes

First of all classify the higher alkanes (11C-19C), (21C-29C), (31C-39C), (41C-49C), (51C-59C), (61C-69C), (71C-79C), and (81C-89C) into two series 'odd number' and 'even number' based on nature of initial numerical (natural number) present in each series.

In (11C-19C) series, initial numerical '1' falls in 'odd number', so, it is treated as 'odd number series'. Same track should be followed for (31C-39C), (51C-59C), and (71C-79C) series of higher alkanes.

In (21C-29C) series, initial numerical '2' falls in 'even number', so, it is treated as 'even number series'. Same track should be followed for (41C-49C), (61C-69C), and (81C-89C) series of higher alkanes.

### 2.2. Usage of convenient prefixes based on classification of higher alkanes

Among higher alkane series, for 1C to 4C convenient *prefixes* will remain same irrespective of classification of series. For 1C, 2C, 3C, and 4C useful *prefixes* are 'un', 'bi', 'tri', and 'tetra' respectively. But only in case of 12C (2C+10C), useful prefix for 2C is 'do' instead of 'un'.

For higher alkanes suitable *prefixes* are used based on application of classification of series and application of classification of series should be started from 5C and carried out up to 9C. For 'odd no series' convenient *prefix* will be 'alka' and for 'even no series' convenient *prefix* will be 'alka'.

# 2.3. Usage of convenient *format* in writing IUPAC word-root of higher alkanes containing natural number multiple of ten

IUPAC nomenclature for 10C and 20C will be 'decane' and 'icosane' respectively where, 'dec' and 'icos' will be the word-root for 10C and 20C respectively. But for the IUPAC word-root of 30C, 40C, 50C, 60C,70C,80C, and 90C convenient *format* will be 'alkacont' irrespective of the classification of higher alkanes. So, for 30C, 40C, 50C, 60C, 70C, 80C, and 90C IUPAC word root will be triacont, tetracont, pentacont, hexacont, heptacont, octacont, and nonacont respectively.

# 2.4. Usage of convenient *format* in IUPAC word-root of rest intermediate higher alkanes other than alkanes having natural number multiple of ten

In the IUPAC word-root, convenient *format* used for higher alkanes (other than alkanes having natural number multiple of ten) based on 'odd number series',15C-19C will be 'alkadec' and that for (35C-39C), (55C-59C and (75C-79C) will be 'alkaalkacont'.

During writing IUPAC word-root, convenient *format* used for higher alkanes (other than alkanes having natural number multiple of ten) based on 'even number series', 25C-29C will be 'alkicos' and that for (45C-49C), (65C-69C), and (85C-89C) will be 'alkalkacont'.

For 11C to 14C convenient format will be 'prefixdec'; for 21C to 24C convenient format will be 'prefixicos'; for 31C to 34C convenient format will be 'prefixtriacont'; for 41C to 44C convenient format will be 'prefixtetracont'; for 51C to 54C convenient format will be 'prefixpentacont'; for 61C to 64C convenient format will be 'prefixhexacont'; for 71C to 74C convenient format will be 'prefixheptacont'; and for 81C to 84C convenient format will be 'prefixoctacont'.

#### 3. Results and Discussion

In phase I, for the classification of 'odd number' and 'even number' of series, divides the higher alkanes into two parts. During this division, sum up the natural number with 10 (for 11C to 19C) or with multiple of 10 (for 21C to 29C, 31C to 39C, 41C to 49C, 51C to 59C, 61C to 69C, 71C to 79C, 81C-89C) before placing them into suitable IUPAC format to write the appropriate IUPAC word-root.

In phase II, use suitable 'prefixes' for the first part of the divided natural number as per the classification of higher alkanes based on 'odd number' and 'even number' of series except 1C, 2C, 3C and 4C.

By combining *phase I* with *phase II*, formulate suitable format and thus we can easily predict word-root of higher alkanes (11C to 90C) described in **Table-1a**, **Table-1b**, and **Table-1c**.

IUPAC nomenclature should be achieved by adding 'ane' after the word-root like triacontane (triacont + ane) for 30C, tetracontane (tetracont + ane) for 40C, pentacontane (pentacont + ane) for 50C, hexacontane (hexacont + ane) for 60C, heptacontane (heptacont + ane) for 70C, octacontane (octacont + ane) for 80C, and nonacontane (nonacont + ane) for 90C.

Table-1a: IUPAC word-root of higher alkanes (11C to 40C)

Carbons	Division	Classification	Suitable	Suitable	IUPAC	IUPAC Name
in Higher	Outline	of series	prefix	format	word-root	(word-root
Alkanes		(even or odd)	('alka'-odd	(prefix suffix)		+ ane)
		w.r.t. initial	& 'alk'-	,		,
		numerical	even)			
11C	(1C+10C)	odd (w.r.t. 1)	un	'prefixdec'	undec	undecane
12C	(2C+10C)	odd	do	'prefixdec'	dodec	dodecane
13C	(3C+10C)	odd	tri	'prefixdec'	tridec	tridecane
14C	(4C+10C)	odd	tetra	'prefixdec'	tetradec	tetradecane
15C	(5C+10C)	odd	penta (alka)	'alkadec'	pentadec	pentadecane
16C	(6C+10C)	odd	hexa (alka)	ʻalkadec'	hexadec	hexadecane
17C	(7C+10C)	odd	hepta (alka)	ʻalkadec'	heptadec	heptadecane
18C	(8C+10C)	odd	octa (alka)	ʻalkadec'	octadec	octadecane
19C	(9C+10C)	odd	nona (alka)	ʻalkadec'	nonadec	nonadecane
20C	-	-	-	-	icos	icosane
21C	(1C+20C)	even (w.r.t. 2)	un	'prefixicos'	unicos	unicosane
22C	(2C+20C)	even	bi	'prefixicos'	biicos	biicosane
23C	(3C+20C)	even	tri	'prefixicos'	triicos	triicosane
24C	(4C+20C)	even	tetra	'prefixicos'	tetraicos	tetraicosane
25C	(5C+20C)	even	pent (alk)	'alkicos'	penticos	penticosane
26C	(6C+20C)	even	hex (alk)	ʻalkicos'	hexicos	hexicosane
27C	(7C+20C)	even	hept (alk)	'alkicos'	hepticos	hepticosane
28C	(8C+20C)	even	oct (alk)	'alkicos'	octicos	octicosane
29C	(9C+20C)	even	non (alk)	'alkicos'	nonicos	nonicosane
30C	-	-	-	'alkacont'	triacont	triacontane
31C	(1C+30C)	odd (w.r.t. 3)	un	'prefixtriacont'	untriacont	untriacontane
32C	(2C+30C)	odd	bi	'prefixtriacont'	bitriacont	bitriacontane
33C	(3C+30C)	odd	tri	'prefixtriacont'	tritriacont	tritriacontane
34C	(4C+30C)	odd	tetra	'prefixtriacont'	tetratriacont	tetratriacontane
35C	(5C+30C)	odd	penta (alka)	ʻalkatriacont'	pentatriacont	pentatriacontane
36C	(6C+30C)	odd	hexa (alka)	'alkatriacont'	hexatriacont	hexatriacontane
37C	(7C+30C)	odd	hepta (alka)	'alkatriacont'	heptatriacont	heptatriacontane
38C	(8C+30C)	odd	octa (alka)	ʻalkatriacont'	octatriacont	octatriacontane
39C	(9C+30C)	odd	nona (alka)	'alkatriacont'	nonatriacont	nonatriacontane
40C	-	-	-	'alkacont'	tetracont	tetracontane

Table-1b: IUPAC word-root of higher alkanes (41C to 70C)

Carbons	Division	Classificatio	Suitable	Suitable <i>format</i>	IUPAC	IUPAC Name
in Higher	Outline	n of series	prefix	(prefix suffix)	word-root	
Alkanes		(even or odd)	(ʻalka'-odd	,		
		w.r.t. initial	& 'alk'-			
		numerical	even)			
41C	(1C+40C)	even (w.r.t.4)	un	'prefixtetracont'	untetracont	untetracontane
42C	(2C+40C)	even	bi	'prefixtetracont'	bitetracont	bitetracontane
43C	(3C+40C)	even	tri	'prefixtetracont'	tritetracont	tritetracontane
44C	(4C+40C)	even	tetra	'prefixtetracont'	tetratetracont	tetratetracontane
45C	(5C+40C)	even	pent (alk)	'alkalkacont'	penttetracont	penttetracontane
46C	(6C+40C)	even	hex (alk)	'alkalkacont'	hextetracont	hextetracontane
47C	(7C+40C)	even	hept (alk)	'alkalkacont'	heptetracont	heptetracontane
48C	(8C+40C)	even	oct (alk)	'alkalkacont'	octtetracont	octtetracontane
49C	(9C+40C)	even	non (alk)	'alkalkacont'	nontetracont	nontetracontane
50C	-	-	-	'alkacont'	pentacont	pentacontane
300				amacom	ренцеон	pentacontane
51C	(1C+50C)	odd (w.r.t. 5)	un	'prefixpentacont'	unpentacont	unpentacontane
52C	(2C+50C)	odd	bi	'prefixpentacont'	bipentacont	bipentacontane
53C	(3C+50C)	odd	tri	'prefixpentacont'	tripentacont	tripentacontane
54C	(4C+50C)	odd	tetra	'prefixpentacont'	tetrapentacont	tetrapentacontane
55C	(5C+50C)	odd	penta (alka)	ʻalkaalkacont'	pentapentacont	pentapentacontane
56C	(6C+50C)	odd	hexa (alka)	ʻalkaalkacont'	hexapentacont	hexapentacontane
57C	(7C+50C)	odd	hepta (alka)	ʻalkaalkacont'	heptapentacont	heptapentacontane
58C	(8C+50C)	odd	octa (alka)	ʻalkaalkacont'	octapentacont	octapentacontane
59C	(9C+50C)	odd	nona (alka)	ʻalkaalkacont'	nonapentacont	nonapentacontane
60C	-	-	-	'alkacont'	hexacont	hexacontane
		I			1	
61C	(1C+60C)	even (w.r.t. 6)	un	'prefixhexacont'	unhexacont	unhexacontane
62C	(2C+60C)	even	bi	'prefixhexacont'	bihexacont	bihexacontane
63C	(3C+60C)	even	tri	'prefixhexacont'	trihexacont	trihexacontane
64C	(4C+60C)	even	tetra	'prefixhexacont'	tetrahexacont	tetrahexacontane
65C	(5C+60C)	even	pent (alk)	ʻalkalkacont'	penthexacont	penthexacontane
66C	(6C+60C)	even	hex (alk)	ʻalkalkacont'	hexhexacont	hexhexacontane
67C	(7C+60C)	even	hept (alk)	ʻalkalkacont'	hepthexacont	hepthexacontane
68C	(8C+60C)	even	oct (alk)	ʻalkalkacont'	octhexacont	octhexacontane
69C	(9C+60C)	even	non (alk)	ʻalkalkacont'	nonhexacont	nonhexacontane
70C	-	-	-	'alkacont'	heptacont	heptacontane

Table-1c: IUPAC word-root of higher alkanes (71C to 90C)

Carbons in	Division	Classification	Suitable	Suitable <i>format</i>	IUPAC	IUPAC Name
Higher	Outline	of series	prefix	(prefix suffix)	word-root	
Alkanes		(even or odd)	('alka'-odd	,		
		w.r.t. initial	& 'alk'-			
		numerical	even)			
71C	(1C+40C)	odd (w.r.t. 7)	un	'prefixheptacont'	unheptacont	unheptacontane
72C	(2C+40C)	odd	bi	'prefixheptacont'	biheptacont	biheptacontane
73C	(3C+40C)	odd	tri	'prefixheptacont'	triheptacont	triheptacontane
74C	(4C+40C)	odd	tetra	'prefixheptacont'	tetraheptacont	tetraheptacontane
75C	(5C+40C)	odd	penta (alka)	ʻalkaalkacont'	pentaheptacont	pentaheptacontane
76C	(6C+40C)	odd	hexa (alka)	ʻalkaalkacont'	hexatheptacont	hexatheptacontane
77C	(7C+40C)	odd	hepta (alka)	ʻalkaalkacont'	heptaheptacont	heptaheptacontane
78C	(8C+40C)	odd	octa (alka)	ʻalkaalkacont'	octaheptacont	octaheptacontane
79C	(9C+40C)	odd	nona (alka)	ʻalkaalkacont'	nonaheptacont	nonaheptacontane
80C	ı	-	-	'alkacont'	octacont	octacontane
81C	(1C+80C)	even (w.r.t. 8)	un	'prefixoctacont'	unoctacont	unoctacontane
82C	(2C+80C)	even	bi	'prefixoctacont'	bioctacont	bioctacontane
83C	(3C+80C)	even	tri	'prefixoctacont'	trioctacont	trioctacontane
84C	(4C+80C)	even	tetra	'prefixoctacont'	tetraoctacont	tetraoctacontane
85C	(5C+80C)	even	pent (alk)	ʻalkalkacont'	pentoctacont	pentoctacontane
86C	(6C+80C)	even	hex (alk)	ʻalkalkacont'	hexoctacont	hexoctacontane
87C	(7C+80C)	even	hept (alk)	ʻalkalkacont'	heptoctacont	heptoctacontane
88C	(8C+80C)	even	oct (alk)	ʻalkalkacont'	octoctacont	octoctacontane
89C	(9C+80C)	even	non (alk)	ʻalkalkacont'	nonoctacont	nonoctacontane
90C	-	-	-	'alkacont'	nonacont	nonacontane

It may be expected that this time-economic innovative mnemonics on IUPAC word-root of higher alkanes (11C to 90C) would go a long way to help to the students of chemistry at undergraduate, senior undergraduate and post-graduate level who would choose the subject as their career.

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