

Nomenclature of Organic Compounds

@yang-z Revision 2

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1 Contribution

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Install TexLive parameters `apt-get install: texlive-latex-base latex-cjk-all texlive-latex-extra`

2 Number Prefix

Table 1: Universal Number Prefixes

Index	Expression	Index	Expression	Index	Expression
1	(mono)	2	di	3	tri
4	tetra	5	penta	6	hexa
7	hepta	8	octa	9	nona
10	deca	11	undeca	12	dodeca

For carbon atoms in a chain less than 10:

Table 2: Table of Carbon Number Prefixes

Index	Expression	Index	Expression	Index	Expression
1	meth	2	eth	3	prop
4	buta	5	penta	6	hexa
7	hepta	8	octa	9	nona
10	deca	11	undeca	12	dodeca

When there are more than 10 carbon atoms in a chain, the ones place of the number is expressed first, then the tens place. There are minor changes to the expression for digits at ones place (Table 2), and for those on tens place (Table 3). However, it is exceptional for number 11 (as undeca).

Table 3: Digits at Ones Place in Numbers Greater Than 10

Index	Expression	Index	Expression	Index	Expression
1	hen	2	do	3	tri
4	tetra	5	penta	6	hexa
7	hepta	8	octa	9	nona

Table 4: Digits at Tens Place

Index	Expressing Itself	Prefix	+1	+2	+3
1	deca	deca	undeca	dodeca	trideca
2	eicosa	cosa	heneicosa	docosa	tricosia
3	triaconta	triaconta	hentriaconta	dotriaconta	tritriaconta
4	tetraconta	tetraconta	hentetraconta	dotetraconta	tritetraconta
...

3 Relative Positioning

Some prefixes are used to identify the relative position of specified functional groups, spatial isomers, and common names for organic compounds

4 Hydrocarbons

4.1 Acyclic Hydrocarbons

Get the number of carbon atoms in the hydrocarbons, and check for its number prefix. Alkane names are the number prefixes (or with their modifiers) plus -ane. Alkene name suffix is -ene, and alkyne name suffix is -yne. You should omit the last letter **a** if the prefix ends with one.

For compounds with more than one double bonds or triple bonds, the corresponding alkenes and alkynes have suffixes like **Universal Number Prefix (Mono omitted) - Functional Group Suffix**.

Table 5: List of Relative Positioning

Prefix	Descriptions
iso	Isotetraene: $CH_3CHCH_3CH_3$
neo	Neopentane: $C(CH_3)_4$
Relative Positions	
ortho (o-)	Indicating the two functional groups are adjacent in a ring
meta (m-)	The two functional groups was separated
para (p-)	The two functional groups are at their opposite, especially in an aromatic compound
primary	An atom connecting to just one carbon atom
secondary (sec-)	An atom connecting to two carbon atoms
tertiary (tert-)	An atom connecting to three carbon atoms
quaternary	An atom connecting four carbon atoms
Geometric Isomerism	
cis	
trans	

Table 6: Naming Main Chains of Hydrocarbons

Carbon Numbers	Prefix	Alkanes	Alkenes	Alkynes
1	Meth-	Methane	-	-
2	Eth-	Ethane	Ethene	Ethyne (Common Name: Acetylene)
3	Prop-	Propane	Propene	Propyne
4	Buta-	Butane	Butene	Butyne

Table 7: Hydrocarbons with Multiple Functional Groups

Functional Groups	Alkenes	Alkynes
1	-ene	-yne
2	-diene	-diyne
3	-triene	-triyne
...

4.1.1 Chirality Isomerism

Given that a carbon atom is connected to four groups of atom R_1, R_2, R_3, R_4 . The chirality of that carbon is determined using the following technique.

- If none of the groups are identical, the carbon is chiral carbon atoms, otherwise it is not.
- Look at the carbon atom in a position that the smallest of the four groups is hidden from you, and you are faced with three groups.
- Make an arrangement according to the size of the three groups, count them from the largest to the smallest. If the sequence is **clockwise**, the carbon is a **R**(rectus) carbon, if **counterclockwise**, **S**(sinister) carbon.

It is essential to know the relative size of each functional group, it is assessed and compared using the **Cahn-Ingold-Prelog Sequence Rule**. This rule is rather complex in order to achieve completeness and correctness, you can see Common Functional Group Section for a brief introduction of this rule.

4.1.2 Geometry Isomerism of Ethenes

Arrange the two groups connecting to the either side of the ethene C=C, if the two larger ones are at the same side of linear core, they are called **Z(zusammen)** isomers, otherwise, they are called **E(entgegen)** isomers.

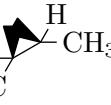
They are marked in the beginning of the name, using Z-n-nomenclature, E-n-nomenclature, or (nZ,mZ, ..., kE,pE, ...)-nomenclature. For example, butene has two isomers **Z-2-butane**, **E-2-butane**

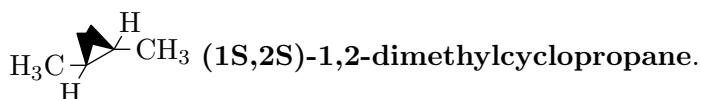
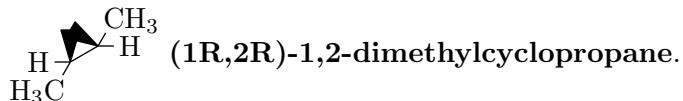
4.2 Alicyclic Hydrocarbons

Alicyclic hydrocarbons are named with prefix cyclo- plus the name of the corresponding acyclic hydrocarbons. For example, C_6H_{14} **Hexane** becomes C_6H_{12} **Cyclohexane**.

4.2.1 Geometry Isomerism of Alicyclic Hydrocarbons

If the molecule has symmetrical properties over an axis, simply name the geometry isomer by **cis** and **trans** prefix, otherwise, specify all the chiral carbon atoms using its index and **R/S** types.

For example,  CH₃ **cis-1,2-dimethylcyclopropane** or **(1S,2R)-1,2-dimethylcyclopropane**.



4.3 Hydrocarbons as Functional Groups

Replacing the -ne ending of hydrocarbons to -yl to express hydrocarbons as functional groups, and to express hydrocarbons with branched chains. For example, **CH₄ Methane** becomes **CH₃- Methyl-**, **CH₂ = CH₂ Ethene** becomes **CH₂ = CH- Ethenyl**, and **-yne** becomes **-ynyl**.

4.4 Hydrocarbons with Branched Chains

Make the longest branch as the main chain, and to choose the orientation to mark The index of carbons in the main chain, which makes the sum of all branched chain index to be smallest. (**The same as Chinese nomenclature**)

Note that **the arrangement of the functional groups and branched chains are according to the ascending alphabetical order, but not the size of the chain which applied in Chinese nomenclature.** (When evaluating the sequence, we should not take number prefixes into consideration, so **-Ethyl** is previous than **-Dimethyl**)

Table 8: List of Sample Branched Hydrocarbons

Chemical Structure	Nomenclature
(CH ₃) ₂ CH ₂ CH ₂ CH(C ₃ H ₇)CH(C ₂ H ₅)CH(CH ₃) ₂	3-ethyl-2,7-dimethyl-4-propyloctane
C(CH ₃) ₄	2,2-dimethylpropane (or neopentane)
Nested Structures	
CH ₃ (CH ₂) ₂ CH(CH ₃)CH(CH(CH ₃) ₂)(CH ₂) ₂ CH ₃	4-isopropyl-5-methyloctane 4-methyl-5-(1-methylethyl)octane

Branched alkenes and alkynes are marked in a way that the double bond and triple

bond index is smallest. For example $CH_2 = C(CH_3)CH = CH_2$ is named as **2-methyl-1,3-butadiene**

When the compounds have both double bonds and triple bonds, its name should contain both alkene endings -en and alkyne ending -yne. if there is no ambiguation, one can use -enyne instead of the two endings with their positions specified explicitly.

Table 9: List of Sample Branched Hydrocarbons

Chemical Structure	Nomenclature
$HC \equiv C - CH = CH_2$	butenyne
$CH_3CH = CHC \equiv CH$	3-penten-1-yne

If the compounds have alicyclic hydrocarbonyl components, other branches should be seen as branched chains, naming before the cyclic hydrocarbons. For example, there is a legal name: **2-methyl-1-(3-methylbutyl)cyclohexane**, which is a derivative of cyclohexane.

5 Aromatic Hydrocarbons

The basis of aromatic hydrocarbones are C_6H_6 **Benzene** and other condensed aromatic hydrocarbons. $C_{10}H_8$ **Naphthalene** $C_{14}H_{10}$ **Anthracene** These cores are usually placed at the end of the word.

The differences in geometry formed geometric isomerism in aromatic hydrocarbons, for example, $Ph-(CH_3)_3$ has three isomers, **1,3,5-trimethylbenzene** or para-trimethylbenzene, **1,2,4-trimethylbenzene** or meta-trimethylbenzene, and **1,2,3-trimethylbenzene** or ortho-trimethylbenzene. (Table 5).

6 Halogenides

Table 10: Halogens and Halides

Chemical	Halo	Halide
<i>F</i>	Fluoro	Fluoride
<i>Cl</i>	Chloro	Chloride
<i>Br</i>	Bromo	Bromide
<i>I</i>	Iodo	Iodide

Table 11: List of Common Names

Chemical	Nomenclature
$CHCl_3$	Chloroform
$CHBr_3$	Bromoform
CCl_2F_2	Freon

The table **Halogens and Halides** and **List of Common Names** of halogenides listed some basic naming principles, in another circumstance, the halogen atom replace the groups directly linked to a carbonyl group. C^{O} . They are regarded as a derivative of carboxylic acids, and are named by replacing the **-ic acid** ending to **-yl halide**. For example **Propanoic acid** became **Propanoyl chloride**.

7 Alcohols and Phenols

A hydroxyl functional group attached to a chain is called alcohols, and to name it, Put an -ol ending to the original name of **hydrocarbons**, and omit the last letter e if there is any. For compounds that have more than one hydroxyl groups, the ending becomes **-diol**, **-triol** and so forth. (Do not omit the e when there are multiple hydroxyl groups.)

Phenols are those with hydroxyl groups attached directly to an aromatic hydrocarbon ring. and exceptionally, the simplest phenol $Ph-OH$ is nicknamed **Phenol**, while other derivatives are named using the rules above. For example, $HO-C_6H_4-OH$ is named **Benzenediol**

When naming the alcohols, we selects the main chain that:

- The hydroxyl function group is **directly linked** to one of the chain's carbons.
- The chain which match the rule above is longest.
- Mark the index of carbons from the hydroxyl group.

Table 12: Alcohols and Phenols

Chemical	Nomenclature
$C(CH_3)_3OH$	2-methyl-2-propanol (derived from propane)
$CH_3CH = C(C_2H_5)CH_2OH$	2-ethyl-2-butenal
$CH_2OH - CHOH - CH_2OH$	1,2,3-propanetriol (glycerin)

Notice that if there are more than 3 hydroxyl functional groups, (a chain can have at most 2 hydroxyls at both ends) one group must not be in the main chain. For them we name it as **hydroxo-**. For example $HOCH_2CH_2CH(CH_2OH)CH_2OH$ is named as **2-hydroxomethyl-butanediol** and  is named as **2-hydroxo-1-cyclohexane carboxic acid**.

8 Ethers

Evaluate the two parts of the ether separated by the atom O, and pick the simpler one (usually alkanes), and name it as **Simpler Part Prefix - oxy Complex Part**. For example, compound $CH_3CH_2OCH = CH_2$ can be expressed as **ethoxy ethene**. and $CH_3O - Ph$ **methoxy benzene**.

When one of the parts is cyclic hydrocarbons, and that the ring has less than 5 carbon atoms, we can omit the 'yl' ending in the prefix.

Table 13: Ether Prefix Word

Chemical	Nomenclature
CH_3CH_2O-	ethoxy
	cyclobutoxy
	cyclohexyloxy

Cyclic ethers are named firstly the alkane chain without the ether's oxygen atom, and then specify the oxygen atom adding the **epoxy-** prefix.

Table 14: Cyclic Ethers

Chemical	Nomenclature
	1,2-epoxypropane
	1,3-epoxyp propane
	1,4-epoxybutane tetrahydrofuran

Note: Its index-marking rules are similar to alcohols.

9 Carboxylic Acids

By replacing the last letter e in the corresponding alkanes, alkenes, and alkynes that form the main chain, plus **-oic acid**. For acids that have more than one -COOHs change the -oic ending into -dioic, -trioic etc.

Another nomenclature for carboxylic acids are **Name of Hydrocarbons + [(di, tri, etc)]carboxylic acid**. And many other organic acids have their common names.

Table 15: Carboxylic Acids

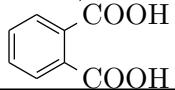
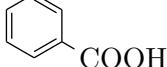
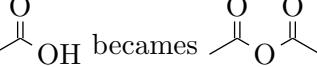
Chemical	Chain	Carboxylic Acids
$CH_3CH = CHCH_2COOH$	3-pentene	3-pentenoic acid
$CH_3CH_2CH(COOH)CH_2CH(COOH)CH_3$	hexane	2-ethyl-4-methyl-octanedioic acid
	benzene	1,2-benzene dicarboxylic acid

Table 16: Common Names

Chemical	Nomenclature
CH_3COOH	acetic acid
$HCOOH$	formic acid
	benzoic acid

Several generic types of organic compounds are seen as derivatives of carboxylic acids. And they are named by replacing part of the acid ending into their own suffixes. They include **Nitriles**, **Amides**, **Halocarbonyls** and **Anhydrides**. Nitriles are compounds that replace the -COOR group into -CN group, and is named by replacing **-ic acid** into **-nitrile**. *However, it seems that -anenitrile and -anonitrile are both acceptable.* Amides are nitrogen based groups connected directly to the carbonyl, and are named by replacing **-oic acid** into **-amide**. Halocarbonyls are halogens directly connected to carbonyl and named by replacing **-ic acid** into **-yl halide**. Anhydrides are two carboxylic acid eliminated by a water molecule, ( becomes ) named by replacing **acid** to **anhydride**. The example molecule is **Ethanoic Anhydride, Acetic Anhydride**.

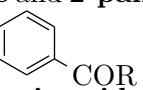
Note: Its index-marking rules are similar to alcohols.

10 Aldehydes and Ketones

Replacing the last letter e of the names of hydrocarbons with the same amount of carbon atoms with **-al** ending for aldehydes and **-one** for ketones. For more complexed aldehydes, use the name for the corresponding carboxylic acids and replace the **-ic acid** ending with **-aldehyde**.

Table 17: Naming Aldehydes and Ketones

Hydrocarbons	Name	Aldehydes or Ketones	Name
$CH_3CH(CH_3)CH_3$	2-methylpropane	$CH_3CH(CH_3)CHO$	2-methylpropanal
$CH_3(CH_2)_3CH_3$	pentane	$CH_3CO(CH_2)_2CH_3$	2-pantanone

There is also a way to name ketones with the R_1-CO-R_2 , for example, **propantone** can be called **dimethyl ketone** and **2-pantanone methyl propyl ketone**. For ketones directly connected to benzene,  you should find out the name of the carboxylic acid $RCOOH$ and replace the **-oic acid** ending with **-ophenone**

11 Esters

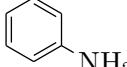
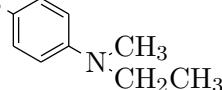
The alcoholic part of the ester is seen as a substituent and end with -yl hydrocarbonyl ending, and the acid part replace the **-ic acid** ending with **-ate**, indicating the acid part of a salt. For example,  is named as **Butyl benzoate**

12 Amines

For simple amines, consider using a hydrocarbonyl prefix and the -amine ending to name the substance. System nomenclature (1) evaluate the longest carbon chain that contains the specified nitrogen as main chain. (2) Mark the main carbon chain with smaller indices closer to the nitrogen. (3) Naming the branched chain using the carbon index and, if directly linked to the nitrogen, use capital letter N. (4) Replace the alkane ending -e with -amine.

If there are more than one nitrogen in the compounds, -amine becomes -diamine, -triamine, etc. For amides, see Carboxylic Acid section.

Table 18: Sample Amine Names, **System Names**

Chemical	Nomenclature
$(CH_3)_2NH$	dimethylamine or N-methylmethanamine
$(CH_3)_3N$	trimethylamine or N,N-dimethylmethanamine
$CH_3(CH_2)_3 - N(CH_3)_2$	N,N-dimethylbutanamine
	aniline or banzenamine
	N-ethyl-N,4-dimethylbenzenamine

13 Nitriles

$-CN$ as a maternal body is called **nitriles**, while as a substituent is called **cyano-**, **cyanide**. Firstly, regard the $-CN$ as $-COOH$ to name it as an carboxylic acid, then, replace the **-oic acid** ending with **-onitrile**. For example, **Benzonic Acid** becomes **Benzonitrile**.

14 Organometallic Compounds

Table 19: Place Organic Groups Before the Metal Atom

Chemical	Nomenclature
CH_3Li	Methylcopper
$(C_2H_5)_2Hg$	Diethylmercury

Table 20: Regard as Derivatives of Borane, Silane and Stannane

Chemical	Nomenclature
$(CH_3)_4Si$	Tetramethylsilane
$(CH_3)_3SnC_2H_5$	Ethyltrimethylstannane

For organic salt and positive metal ions, name them as a salt. For example, CH_3CH_2HgCl is named **ethylmercury chloride**

15 Heterocyclic Compounds

15.1 System Names for Single Heterocycle

(1) The suffix of the heterocyclic compounds is determined by the size of the cyclic ring,
(2) and the non-carbon atoms that form the heterocycle has special prefixes arranged in
a certain order (O, S, N). (3) Modify the name ending with the following rules

- If the ring contains **Nitrogen**, add an -e to the ending.
- If the ring doesn't contain **Nitrogen**, and is **saturated**, replace the last letter -e (if any) with -ane.
- If the ring contains **Nitrogen**, and is **saturated**, replace the last letter -e(or -ine for -irine, -epine, -ocene) (if any) with -idine.
- If the name contains two adjacent vowels, replace them to the last vowel.

Table 21: Cycle Size In Atoms and Corresponding Suffixes

Size	Suffix
3	-irine
4	-ete
5	-ole
6	-in(e)
7	-epin(e)
8	-ocin(e)

Table 22: Non-carbon Atom Prefix

Atom	Prefix
O	oxa-
S	thia-
N	aza-

Hydrogen Indication Mark out all the saturated carbon (with 2 hydrogen atom). These marked indices are called indicating hydrogen. It is expressed using **Index + H** before the name of the compound.

Table 23: Sample Names for Heterocyclic Compounds

Structure	Naming
	Naming Process: Thia-(1) + Ete Thiete
	Azete
	1,3-dioxole
	Naming Process: Aza-(1) + Ir(in) + (Nitrogen) (e) + (Saturated) Idine Azairidine
Multiple Heteroatoms	
	Naming Process Thia-(1,3) + Aza-(2) + -Ole(5) 1,3,2-Dithiazole

Table 24: Sample Names for Indicator Hydrogen

Structure	Naming
	1H-Pyrrole
	2H-Pyrrole
	3H-Pyrrole

Table 25: Common Names

Structure	Naming
	Furan
	Thiophene
	Pyrrole
	Thiazole
	Imidazole
	Pyridine
	Pyran
	Pyrimidine

15.2 Common Names for Heterocycles

15.3 Common Names for Condensed Heterocyclic Compounds

Nearly all of the condensed heterocyclic compounds have a common names, and the table demonstrates some of the most commonly used compounds.

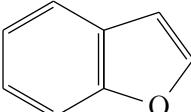
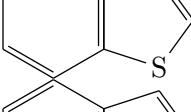
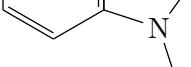
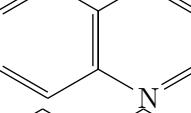
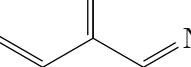
15.4 Condensed Heterocyclic Compounds Nomenclature

Step 1: Marking the Edge and Atoms in the Heterocycle Every condensed heterocycle can be splitted into many small unit cycles. The first step of expressing the whole is to express all of the subunits to mark the relative position in which they stack. The marking should follow these rules:

Rules to Determine Indices

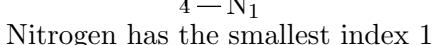
- Make the indices of all hetero-atoms the **smallest**.
- The carbon with no hydrogen should't be assigned with an index, assign them the previous instead with mark a,b,etc. instead. For example, 1-2-3-3a-3b-4.

Table 26: Common Names for Condensed Heterocyclic Compounds

Molecule	Name
	Benzofuran
	Benzothiophene
	Indole
	Quinoline
	Isoquinoline

- Among all the circumstances that match the first rule, try to make those carbons with no hydrogen's indices the **smallest**.
- Among all the circumstances that match the rule 1 and 3, try to make the indices of all the indication hydrogen the **smallest**.
- Priority: O, S, NH, N
- Assign the index (a, b, c, etc) of the line contours of the heterocycle according to the indices of atoms.

Table 27: Step 1: Rule 1

Correct	Wrong
 Nitrogen has the smallest index 1	

Step 2: Determine the Fundamental Ring Among all the subunits of the heterocycle, select the one which matched the following rules as the fundamental ring.

Table 28: Step 1: Rule 2 and Rule 3

Correct	Wrong
 4a is smaller than 8a	 or

Rules to Determine Fundamental Ring

- If the subunit rings contains both aromatic rings and heterotic rings, consider the **heterotic ring** as the fundamental ring. If there are more than one heterotic rings, choose the **larger one or with a special name**.
- If the subunit rings contains only heterotic rings, choose the **larger ring**.
- If the size of the rings are identical, choose the one with **most heterotic atom**.
- If the number of heterotic atoms are identical, choose the one with **maximum types of atoms**.
- If all of these are identical, choose the one with **smallest indices** of heterotic atoms.
- In the naming of each subunits, treat the shared heterotic atom as their own.

Step 3: Naming Now that we acquire all the subunit rings and their right sequences of indices and contours, we can name it using relative positioning, in a bracket, first sign the arrangement of the shared contour, than the line specified by a small letter. [3,2-b] is a legal notation. However, [3,2-b] and [2,3-b] is not the same. [3,2] specifies a contour of additional ring, and b specifies a contour of fundamental ring.

16 Common Functional Groups

The precedence of organic functional groups should be considered when there are multiple different groups in a compound. the topmost functional group should be regarded as the maternal body while the less precedent groups be substituents.

Table 29: The Naming Process of a Condensed Ring

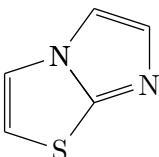
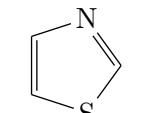
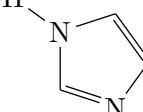
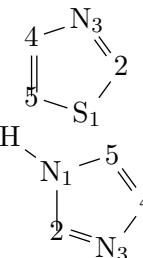
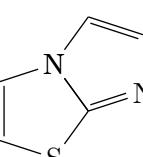
Target Molecule	
Naming Each Subunits	
	Thiazole (Fundamental Ring)
	1H-1,3-Diazole, Imidazole (Additional Ring)
Marking the Index Of Subunits	
	
Naming the Compound	
	Imidazo[2,1-b]thiazole

Table 30: List of Functional Groups

Chemical Structure	Prefixes	Suffixes
$-COOH$	carboxy	-carboxylic acid, oic acid
$-SO_3H$	sulfo	-sulfolic acid
$-COOR$	R-oxycarbonyl	R...carboxylate, R...oate
$-COX$	halocarbonyl	-carbonyl halide, -oyl halide
$-CONH_2$	carbamoyl	-carboxamide, -amide
$-CN$	cyano	-carbonitrile, -nitrile
$-CHO$	formyl	-carbaldehyde, -al
$-CO$	oxo	-one
$-OH$	hydroxy	-ol (phen)-ol
$-NH_2$	amino	-amine
$-OR$	R-oxy	-ether
$-R$	alkyl	
$-X$	halo	
$-NO_2$	nitro	
$-NO$	nitroso	

Cahn-Ingold-Prelog Sequence Rule Here we introduce a simplified version of the sequence rule to arrange the relative size of different functional groups.

Rule I The sequence of common atoms used in organic compounds is listed in descending order of size. **I, Br, Cl, S, P, F, O, N, C, D, H, Ø**.

Rule II Given that a functional group has only one atom that are directly connected. We start from that atom, and express all the atoms that are directly connected to it in descending size order. This forms a triary tree structure. For example, $-CH_3$ is expressed as C(H,H,H) and $-CHFCI$ is expressed as C(Cl,F,H). If the atom has double bond or triple bond to connect with an atom, if is regarded as two or three identical bond to the atom. For example, $-CHO$ is expressed as C(O,O,H). If the saturate bond is less than four(for non-carbon center atoms), we fill the tree with empty imagery atoms. $-OH$ is expressed as O(H,Ø,Ø).

Rule III If a single atom cannot get the sequential result of the groups, you should extnds to the atom that follows. however, the imagery atoms, and those atoms considered by equivalating double or triple bonds should be regarded as naked atoms without further branch (to avoid iteration hell). $-CN$ is regarded as C(N([C],[C],Ø,[N],[N]),  is regarded as C(C(H,C,[C]),[C],C(H,C,[C]))

Table 31: Precedence of Common Functional Groups

Chemical	Nomenclature
Higher Precedence	
$-COOH$	Carboxylic Acids
$-SO_3H$	Sulfuric Acids
$-COOR$	Esters
$-COX$	Carbonyl Halides
$-CONH_2$	Carboxamides
$-CN$	Nitriles
$-CHO$	Aldehydes
$O \begin{array}{c} / \\ \backslash \\ C \end{array}$	Ketones
$-OH$	Alcohols and Phenols
$-NH_2$	Amines
	Aromatic Rings
$-C\ C-$	Alkynes
$-C=C-$	Alkenes
$-O-$ R	Ethers Alkanes
$-X$	Halogens
$-NO_2$	Nitro
Lower Precedence	