

Nomenclature of organic nitrogen compounds¹

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INTRODUCTION

As in the previous paper in this series (1), systematic nomenclature as used in the Geneva, the International Union of Chemists, International Union of Pure and Applied Chemists (IUPAC), or *Chemical Abstracts* (CA) systems is generally recommended where possible. It should be noted that this subject also is discussed in another source (2).

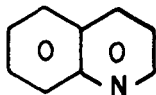
Use of trivial names generally is discouraged, except for widely used and well known common names.

In general, the rules given in the CA system (3) are followed. A number of the examples given in the CA paper are used here.

In this paper, aromatic 6-membered ring systems are indicated by the following types of structures:



benzene ring

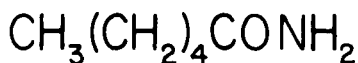


quinoline

AMIDES

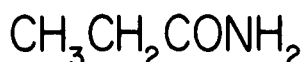
Amides are named using procedures similar to those for naming carboxylic acids. These procedures are discussed below.

Geneva names are formed from the hydrocarbon names by dropping the final "e" and adding "amide" or "diamide." The longest chain having the amide group in the terminal position is chosen. In unsaturated compounds, as many as possible of the double and triple bonds are included in the "longest" chain. For example:



hexanamide

Common names of acids are changed to amide names by dropping "ic acid" or "oic acid" and adding "amide." For example:

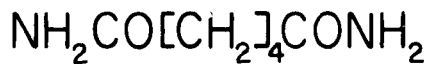


propionamide

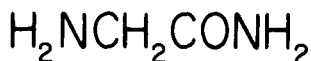
Amide names are formed from common names of polyacids when all acid groups have been replaced by amide groups. Amides names are

¹This paper is a part of the nomenclature program of the AOCs Nomenclature Subcommittee.

formed from common names of some unsubstituted amino acids. Examples are:

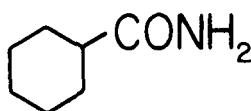


adipamide



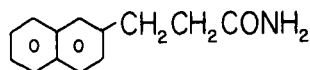
glycinamide

"Carboxylic" names of acids are changed to "carboxamide" as the suffix, as in the example below:



cyclohexanecarboxamide

Conjunctive names are formed as with carboxylic acids. An example is given:

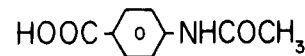


2-naphthaleneproplionamide

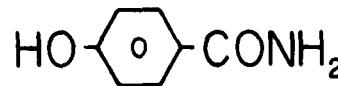
The amide function is preceded in the order of functions by functions, such as "onium" and acid. In compounds having several functional groups, the following list of precedence is used (3), where "onium" compounds have the highest order of precedence: "onium" compounds, peroxide, hydroperoxide, acid (carboxylic, carboximidic, carbohydroxamic, arsonic, arsonous, sulfonic, sulfinic, sulfenic, stibonic, stibonous, phosphonic, phosphonous, phosphinic, phosphinous, boronic, borinic, others), acid halide, *amide*, imide, amidine, aldehyde, nitrile, isocyanide, ketone, thione, alcohol, phenol, thiol, amine, oxyamine (RONH_2), imine organometallic compounds (with carbon-metal attached radicals), ether, sulfide, sulfoxide, sulfone.

In amides containing functional groups, the amide function is expressed as a prefix, or the compound is named using the suffix, according to the above mentioned list of precedence. The function group having the highest order or precedence should be used as the suffix.

The functional group is always on the end of the longest chain. For example:

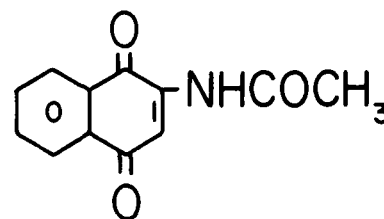


4-acetamidobenzoic acid



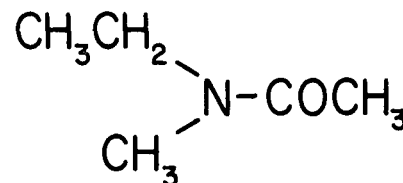
4-hydroxybenzamide

The order of precedence may be disregarded in a few cases where the amide function is acetamide or benzamide. An example follows:



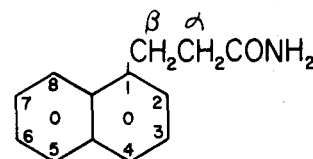
2-acetamido-1,4-naphthoquinone

Substituents are listed in alphabetical order. For example:



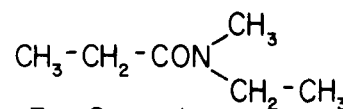
N-ethyl-N-methylacetamide

Greek letters may be used to indicate the position in side chains, α being next to the functional group, as in the example:



1-naphthaleneproplionamide

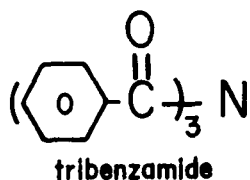
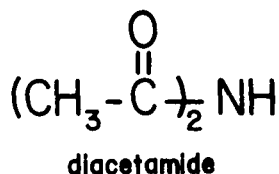
In cases where it is difficult to decide which is the side chain, the chains are numbered (1,2, etc.), starting with the carbon atom next to the functional group. Prime numbers are used for the other chain. For example:



N-ethyl-N-methylpropionamide

Polyacyl Derivatives

Diacyl and triacyl derivatives of ammonia are named as di- and tri- amides when the acyl groups are identical. Examples are:

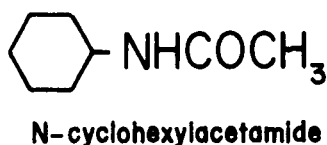
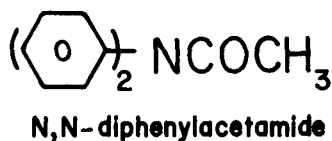
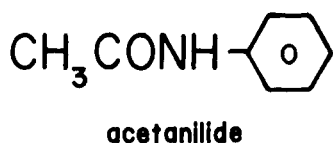


When the acyl groups are different, the amide is named on the basis of the largest acyl group present. For example:

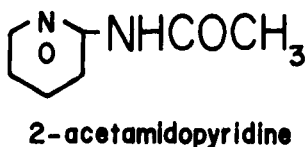


N-Substituted Derivatives

N-aryl derivatives of amides are named as anilides, anisidides, phenetidides, toluidides, xylidides, or N-aryl derivatives, when the N-aryl group is polycyclic. If two identical aryl groups are attached to the nitrogen, or the substituting group is alicyclic, the compound is named as an amide. Examples are as follows:



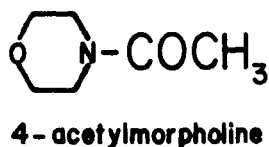
When N- substituents of acetamide or benzamide are heterocyclic, the compounds are named as acetamido or benzamido derivatives, as in the example below:



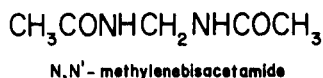
Other N- substituted amides are named as required by the order of precedence of functions. For example:



Amides in which the amide nitrogen is part of a heterocyclic ring and the acyl group is outside the ring are named as acyl derivatives of the cyclic compound. For example:

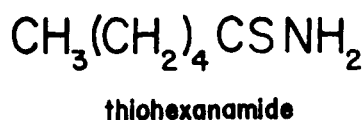


Where bivalent radicals occur, the "bis" nomenclature should be used in preference to "di" as in the example:

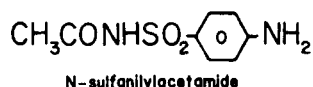


Sulfur Containing Amides

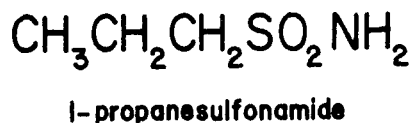
"Thio" is used as the prefix for sulfur. "Thiocarbamoyl" is used as the prefix for the $\overset{\text{S}}{\parallel}{\text{C}}-\text{NH}_2$ group. An example is given as follows:



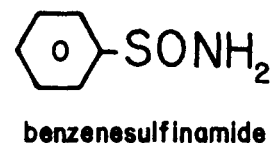
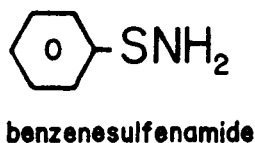
A mixed amide of a carboxylic acid and a sulfonic acid is named as a derivative of the carboxylic acid amide, as in the example:



Amides of sulfonic acids are sulfonamides. These are named by replacing the ending "ic acid" of the corresponding sulfonic acid with "amide." For example:

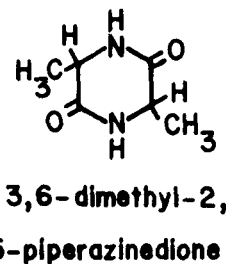


Amides of sulfenic acids are sulfenamides. Amides of sulfinic acids are sulfonamides. Examples are:

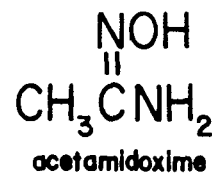


Others

Cyclic anhydrides of dipeptides are named as derivatives of 2,5-piperazinedione. An example is given:

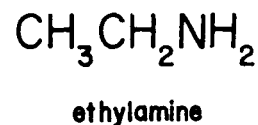


Compounds of structure $\overset{\text{NOH}}{\parallel}{\text{C}}-\text{NH}_2$ are amidoximes, not hydroxamamides. The corresponding radical $\overset{\text{NOH}}{\parallel}{\text{C}}-\text{NH}_2$, is hydroxyamidino. For example:

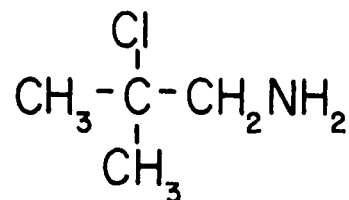


AMINES

Amines are named by adding the suffix "amine" to the hydrocarbon radical. For example:

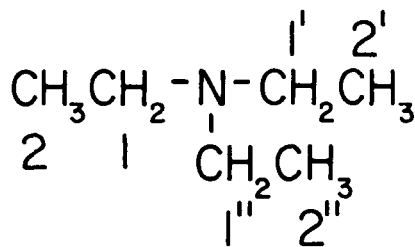


Substituted amines are named as derivatives of the largest straight chain amine, as in the example below:



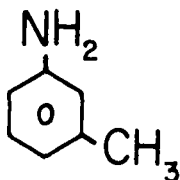
2-chloro-2-methylpropylamine

The aliphatic chains are numbered (1, 2, etc.) starting with the carbon atom next to the amino group. Prime and double prime numbers are used in secondary and tertiary amines. Substituents on the nitrogen are indicated by "N." An example is:

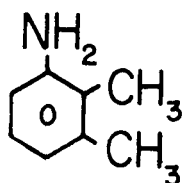


triethylamine

Trivial names are used for some aromatic amines, such as aniline, toluidine, and xylylidine. Examples are:

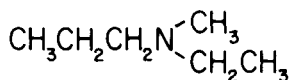


m-toluidine



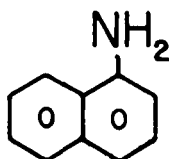
2,3-xylylidine

Mixed amines are named as derivatives of the largest radical. In cases of saturated and unsaturated radicals of the same carbon content, the unsaturated radical is favored. For example:

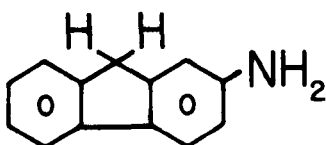


N-ethyl-N-methylpropylamine

Cyclic amino compounds where the ring does not contain nitrogen and where the amino group is attached directly to the ring are named by adding "amine" to (A) the radical name or (B) the parent compound name where "e" is elided before amine. The latter approach is preferred. Examples are:

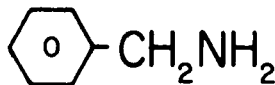


1-naphthylamine



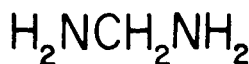
fluoren-2-amine

If the amino group is separated from the ring by an aliphatic chain: (A) the appropriate radical name if available or (B) a conjunctive name is used. An example is:

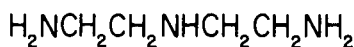


benzylamine

Polyamines are named by adding "diamine," "triamine," etc., to the name of the parent compound, provided it is not a nitrogen containing ring. The use of multivalent radicals for naming polyamines is usually a poor practice. Examples are:

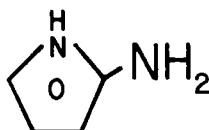


methanedi-amine



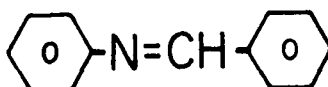
diethylenetriamine

Amino derivatives of heterocyclic compounds containing nitrogen in the ring always are named as amino substituents of the parent ring, as in the example below:



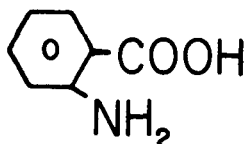
2-aminopyrrole

Azomethines, also known as anils or Schiff bases, should be named as amines. An example is given below:

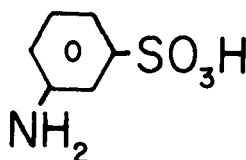


N-benzylideneaniline
or benzalaniline

Common names, such as anthranilic acid and metanilic acid, are acceptable. Examples are:



anthranilic acid

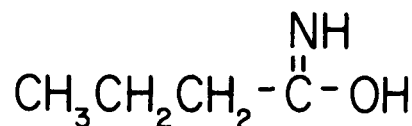


metanilic acid

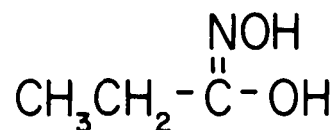
Common names are used for certain alkaloids containing amino groups. Examples of these include: atropine, morphine, papaverine, and quinine.

ACIDS CONTAINING NITROGEN

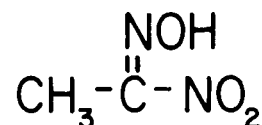
These include imidic, hydroxamic, nitrolic, nitrosolic, amic, anilic, and amino acids. Examples are as follows:



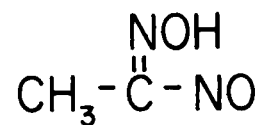
butyrimidic acid



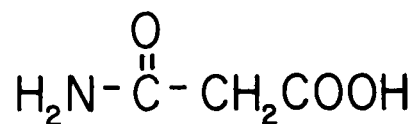
propionhydroxamic acid



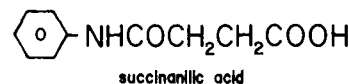
acetonitrolic acid



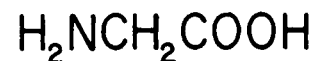
acetonitrosolic acid



malonic acid

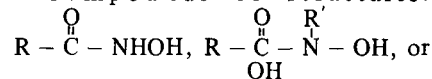


succinilic acid



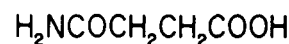
glycine

Compounds of structures:



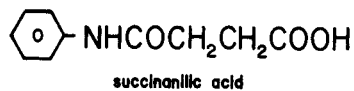
their tautomers, $\text{R}-\overset{\text{OH}}{\underset{\text{||}}{\text{C}}}=\text{NOH}$, should be named as hydroxamic acids rather than N-hydroxyamides.

When one carboxyl group of a dicarboxylic acid which has a trivial name has become a carboxamide group, the resulting acid should be named as an amic acid. For example:

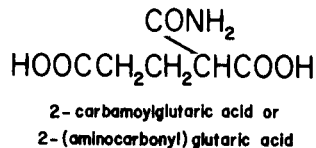


succinamic acid

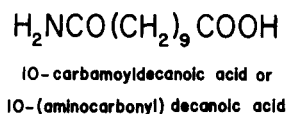
N-phenyl derivatives of these are named as anilic acids, as in the example.



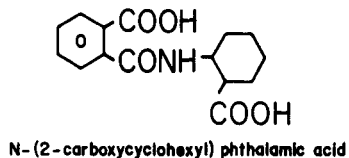
A mono- or diamide of a tricarboxylic acid is not named as an amic acid but as a carbamoyl derivative of the corresponding acid. An example is:



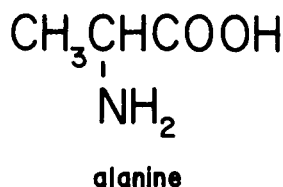
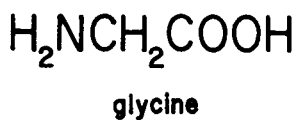
Amic and anilic acid names are not formed from Geneva names. For example:



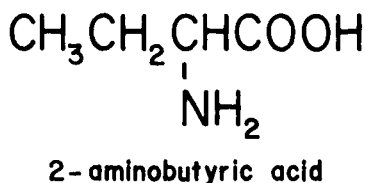
Precedence should be given to an amic or anilic acid over a simple monocarboxylic acid. An example is given:



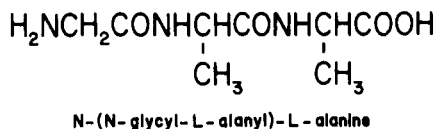
Amino acids should be named like hydroxy acids, except for those trivial names listed in IUPAC Rule AA-10 (4) and some others (3). Examples are:



Other amino acids should be named using the prefix "amino." For example:



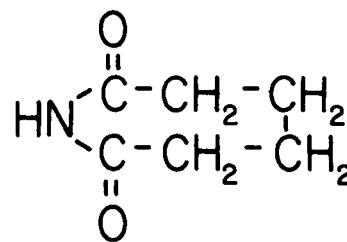
Peptides generally should be named as N-acyl derivatives of amino acids, as in the example.



IMIDES

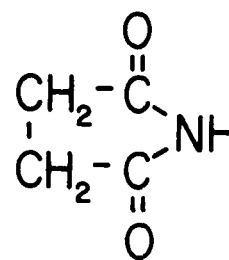
Imides, like acids, can be named using Geneva, common, or carboxy names.

Geneva names are formed by adding "imide" to the name of the corresponding hydrocarbon. A final "e" is elided from the hydrocarbon name, as in the example:



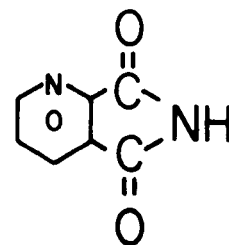
hexanimide
(adipimide)

Common names are formed using the lower aliphatic dicarboxylic acids. The final "ic" is dropped and "imide" added. For example:



succinimide
(or 2,5-pyrrolidinedione)

Carboximide names are formed by changing "dicarboxylic acid" to "dicarboximide." An example is:



2,3-pyridinedicarboximide

Imides follow amides in the order of precedence. The prefix "imido" is used where necessary, as in the example:

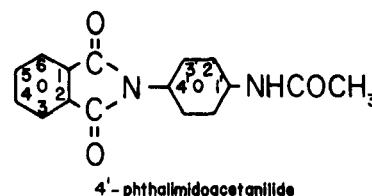


TABLE I
Heterocyclic Compounds

Name	Characteristic Function	From
lactam	$\begin{array}{c} -C-NH- \\ \\ O \end{array}$	amino carboxylic acids
lactim	$\begin{array}{c} -C=N- \\ \\ OH \end{array}$	enol of lactam
sulfam	$-SO_2NH-$	amino sulfonic acids
lactone	$\begin{array}{c} -C-O- \\ \\ O \end{array}$	hydroxy carboxylic acids
Example:		2-pyrrolidone

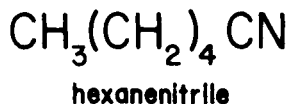
LACTAMS AND RELATED COMPOUNDS

Cyclic lactams, lactims, sultams, and lactones should be named as heterocyclic compounds, as in Table I.

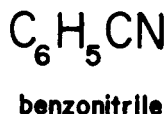
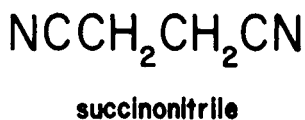
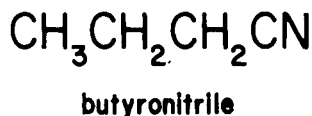
NITRILES

Nitriles should be named like the corresponding acids. Geneva, common, conjunctive, and carboxylic names may be used.

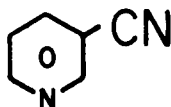
Geneva names are formed by adding "nitrile" to the hydrocarbon name. The nitrile group is in the terminal position, and the longest chain with the most unsaturation is chosen. Examples are:



Common names are formed from carboxylic acids by dropping "ic" and adding "nitrile" with a connective "o," whenever needed (exception: propionitrile instead of propionitrile). Examples are:

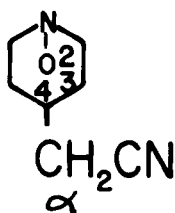


The carbonitrile names are formed by adding "carbonitrile" to the name of the hydrocarbon. An example is:



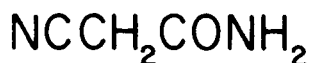
3-pyridinecarbonitrile

Conjunctive names are formed as with acids, as in the example:



4-pyridineacetone nitrile

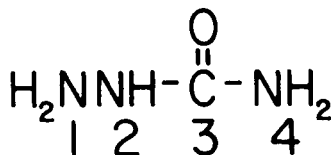
The nitrile function is expressed using the prefix "cyano" when groups of higher precedence are present. For example:



cyanoacetamide

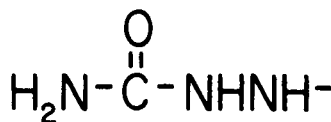
SEMICARBAZIDE DERIVATIVES

Semicarbazide of aminourea, such as:



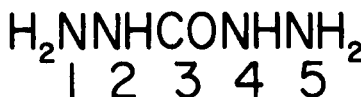
semicarbazide or aminourea

may be used as a parent compound and is numbered as shown above. In order of precedence, semicarbazide is classed with amides and may be expressed using the prefix "semicarbazido."

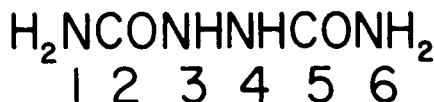


semicarbazido

The following semicarbazide analogues also may be used as parent compounds:

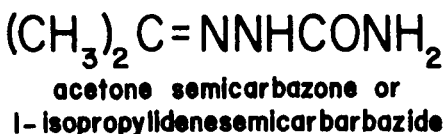


carbohydrazide



biurea

1,5-Dialkylidene derivatives of carbohydrazide may be named as carbohydrazones. Condensation products of semicarbazide with aldehydes and ketones are semicarbozones. Examples are:



1,5-diphenylcarbohydrazide



OTHER NITROGEN COMPOUNDS

The methods of naming and numbering heterocyclic systems are given in the IUPAC Rules (4) and in the Ring Index (5). Amidines should be named like the corresponding acids. Azides should be named like halogen compounds. Symmetrical azo compounds are named by adding the prefix "azo" to the name of the hydrocarbon. Betaines should be named as inner salts, rather than hydrated compounds. Organic cyanates, isocyanates, thiocyanates, and isothiocyanates should be named as esters. Imines are named by means of bivalent radicals using the appropriate alkylidene name. "Onium" compounds which are compounds containing organic cations are named in various ways as shown in the CA Rules, Section 392 (3).

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3. American Chemical Society, "The Naming and Indexing of Chemical Compounds from *Chemical Abstracts*," American Chemical Society, Easton, Pa., (1962).
4. International Union of Pure and Applied Chemistry, J. Amer. Chem. Soc. 82:5566 (1960).
5. Patterson, A.M., L.T. Capell, and D.F. Walker, "The Ring Index," Second Edition, American Chemical Society, Washington, D.C., 1960.

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