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COMMISSION ON PHYSICAL ORGANIC CHEMISTRY*

**NOMENCLATURE FOR
STRAIGHTFORWARD
TRANSFORMATIONS**

Prepared for publication by

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Comments on these recommendations are welcome and should be sent within 8 months from January 1981 to the Secretary of the Commission

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Comments from the viewpoint of languages other than English are especially encouraged. These may have special significance regarding the publication in various countries of translations of the nomenclature eventually approved by IUPAC.

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NOMENCLATURE FOR STRAIGHTFORWARD TRANSFORMATIONS

Prepared for publication by J. F. Bunnett

PREAMBLE

These rules provide a general system of nomenclature for transformations whereby one organic compound is converted into another one. Except for substitution transformations, for which systematic names have been employed since 1954 (ref. 1), these processes have lacked systematic verbal representation. Some have been denominated either as "name reactions" (e.g., Michael reaction) or by various and sometimes inconsistent descriptive terms, but often they have been represented only by an equation or a relatively cumbersome multi-word description.

Three familiar classes of transformations are straightforward substitutions, additions and eliminations. Indeed, the first three groups of rules deal with just these classes.

Straightforward transformations are those that occur without molecular rearrangement. However, a straightforward transformation may involve configurational change. Transformations that involve molecular rearrangement (of skeleton or substituent positions) are intended to be treated later.

The naming of transformations is distinguished from the naming of reactions. The name of a reaction must state or imply all the reactants used and all the products formed. However, in naming a transformation one is ordinarily concerned only with changes in one particular species designated as the "substrate." Thus, 'nitration' refers to a process in which a hydrogen atom of a substrate is replaced by a nitro group, irrespective of whether the reagent is HNO_3 , N_2O_5 , $\text{NO}_2^+\text{BF}_4^-$ or EtONO_2 .

When two or more chemical species are involved in a reaction, it is often obvious which should be designated the "substrate." In other cases it is less obvious. Thus, in the reaction of aniline with benzoyl chloride to form *N*-phenylbenzamide, either reactant seems an equally probable choice as substrate. This single reaction comprises two distinct transformations: replacement of the chlorine atom of benzoyl chloride by an anilino group, and of a hydrogen atom of aniline by a benzoyl group. These rules provide separate names for the two transformations, and thus there is not a unique name for the *reaction* as a whole. The choice of which transformation to name, which is equivalent to choosing one reactant as the substrate, is made with reference to the context.

The naming of transformations is also distinguished from the designation of *reaction mechanisms*. Often two or more distinctly different mechanisms for the same transformation are indicated by experimental evidence, or are conceivable, and views as to what mechanism prevails may be in dispute or may change with time. The names for transformations provided by these rules do not include information about reaction mechanism. The chemist who wishes also to indicate the mechanism that obtains can do so by adding appropriate adjectives or phrases; e.g., "nitration via nitronium ions."

One type of mechanistic information should, however, be acknowledged in the naming of transformations. That is knowledge as to what bonds actually break or form during a reaction. For example, to name the hydration of benzonitrile to benzamide as though it involved replacement of the cyano group by a carboxamido group would be a travesty. The name given to a transformation should be in accord with knowledge as to the actual changes in connectivity that occur.

In some cases the same overall result may be achieved by quite different means. Thus, transformation of allyl benzoate to propyl benzoate can be performed either by dihydro-addition (of H_2) to the olefinic linkage, or by propoxy-de-allyloxylation (with propyl alcohol). To name these two processes identically would be more detrimental than helpful.

In other cases subtle variations in reaction conditions can alter the pattern of connectivity change. Thus, 1-methyl-2-butenyl hydrogen phthalate is hydrolyzed in weakly alkaline solution with cleavage of the alkyl-oxygen bond, and in concentrated alkali solutions with scission of the acyl-oxygen bond. In such a case one might wish to employ different names for the transformation to distinguish different routes, or one might justifiably use either name if distinguishing between them happened not to be important in a particular context, or not feasible.

1. J. F. Bunnett, "Systematic Names for Substitution Reactions," *Chem. Eng. News*, 32, 4019 (1954); *J. Chem. Soc.*, 4717 (1954).

Two rather different *purposes* are served by *systematic names* for transformations. One is indexing and the retrieval of information, and the other employment in speech and writing. Rather different criteria need to be met if names are to be satisfactory for the two purposes.

For indexing, names must be definitive. Although simplicity in a name is always a virtue, there is no requirement that indexing names be short, or that they avoid interposed letters or numbers, and they may utilize punctuation marks to specify certain types of information.

Names for use in speech need to be relatively short and euphonious, and they should contain features distinctive to the ear. They should be easily adapted into other major languages of science. Optimally names for specific transformations should be precise, but some sacrifice of precision can be tolerated if necessary to satisfy the criteria just mentioned. A name that is very difficult to pronounce or for the ear to comprehend is likely to be avoided in speech, and is therefore worthless for oral communication. Names for use in effective written discourse must meet similar criteria, for similar reasons.

For either purpose, there is need both for specific names that portray single transformations and for generic names that portray sets of closely related reactions. Thus, there is need for a name to represent the category of substitution reactions in which an alkoxy group replaces a halogen atom, but also for a name to represent the specific case in which an ethoxy group replaces a bromine atom. These rules provide for both generic and specific names.

Furthermore, these rules allow for the disclosure of varying amounts of information beyond identification of the groups that enter or depart. Thus, in the naming of addition to an olefinic linkage, one may name only the addends that attach to the two olefinic sites, or one may specify as well the stereochemistry of the transformation and/or the sites in a particular olefin to which particular addends attach. Further information about the conditions of a reaction, about reagents employed, about the presumed mechanism or of other sorts can be provided by use of additional words that precede or follow the name of the transformation. Example No. 14 following rule 1.1.4 and example No. 1 to the supplementary note (N.B.) following rule 2.1.7 indicate how additional information about the reaction conditions and about ideas of mechanism can be presented.

In the compilation of an index, one may wish to invert a name; thus, 'substitution, alkylthio-de-bromo-' instead of 'alkylthio-de-bromo-substitution,' for the purpose of grouping all substitutions together. Such an inversion is shown in example No. 3 to rule 2.1.2.5.

Attention is called to a difference in the endings between speech/writing and indexing names for substitutions. Justification for this difference stems in part from general considerations stated above, in part from the fact that speech/writing type names for substitution have been in use since 1954, and in part from the utility of indexing names in their inverted form as just mentioned. Indexing names may be employed in speech or writing if one wishes to do so.

Use of the '-ation' ending for speech/writing names for transformations of other types is avoided because the resulting names would so closely resemble those for substitutions that the eye or ear would have difficulty in distinguishing them. Thus, the approved 'hydro-de-bromination' for substitution is remarkably similar to the eschewed 'dehydrobromination' or 'de-hydro-de-bromination' for elimination, while the approved 'hydro-bromo-elimination' is distinctly different.

Some of the specific transformations falling within the scope of these rules involve chemical species of such complexity that even the so-called "speech/writing" names for them are of necessity too unwieldy for regular oral communication without additional visual aids (see example 6 under rule 2.1.3 or example 5 under rule 2.1.6.2). Such limitations are recognized and are inherent in the application of any rules of systematic chemical nomenclature to systems of some complexity.

The system of numbering of paragraphs in the following text anticipates the intercalation of extensions of these rules. "Rule xxx" represents a rule to be brought forth later.

RULES

1. Substitution Transformations

1.1 Univalent-univalent substitutions. These are transformations in which a univalent atom or group is replaced, at the same site but perhaps with change of configuration, by a univalent atom or group.

1.1.1 For speech/writing, the name comprises (a) the name of the entering group, followed by a hyphen, (b) the syllable 'de-', (c) the name of the leaving group, and (d) the suffix 'ation.' For euphony, slight changes in spelling may be made at the end of the name of the leaving group. Optionally, the hyphens may be omitted, but their omission is discouraged when the names of the groups are complicated.

1.1.2 For indexing, the name comprises (a) the name of the entering group, followed by a hyphen, (b) the syllable 'de-', (c) the name of the leaving group, followed by a hyphen, and (d) the suffix 'substitution.'

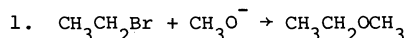
1.1.3 Introduction or replacement of hydrogen. Hydrogen of natural isotopic abundance is represented as 'hydro,' except that when a leaving group it is represented as 'hydrogen' in speech/writing names. (See examples 3, 4, 5, 6 and 8.) When a distinction is made between isotopes of hydrogen, ^1H is represented as 'protio,' ^2H as 'deuterio,' and ^3H as 'tritio.' (See example 7.)

For speech/writing, specific mention of hydrogen as an entering or leaving group may optionally be omitted. If hydrogen is the entering group, the name will then be composed of (a) the syllable 'de,' (b) the name of the leaving group, and (c) the suffix 'ation.' (See example 8.) If hydrogen is the leaving group, the name will be composed of (a) the name of the entering group and (b) the suffix 'ation.' (See examples 3, 4, 5, and 6.) In either case, for euphony slight changes in spelling may be made at the end of the name of the group mentioned.

1.1.4 Naming of groups. Leaving groups are named as they are in the substrate, and entering groups as they are in the product.

N.B. Other information. The site of substitution is not indicated in the name of the transformation, but can be indicated by additional words placed before or after. (See examples 10, 11 and 13.) The mechanism of substitution is also not indicated in the name, but can be indicated by additional words. (See example 14.) The stereochemistry of substitution may be mentioned. (See example 12.)

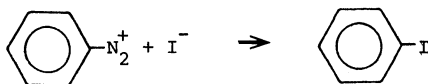
Examples.



Speech/writing: specific: methoxy-de-bromination
generic: alkoxy-de-halogenation

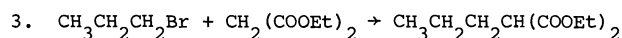
Indexing: specific: methoxy-de-bromo-substitution
generic: alkoxy-de-halo-substitution

2.



Speech/writing: specific: iodo-diazoni-ation
generic: halo-de-diazoni-ation

Indexing: specific: iodo-de-diazonio-substitution
generic: halo-de-diazonio-substitution



If propyl bromide is taken as the substrate:

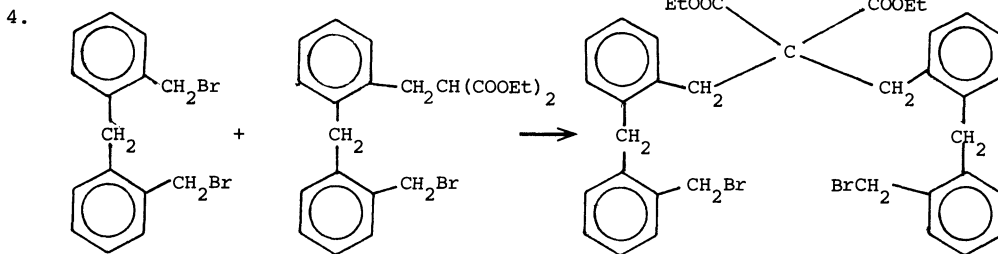
Speech/writing: bis(ethoxycarbonyl)methyl-de-bromination

Indexing: bis(ethoxycarbonyl)methyl-de-bromo-substitution

If diethyl malonate is taken as the substrate:

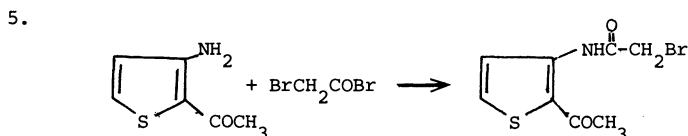
Speech/writing: specific: propyl-de-hydrogenation, *or* propylation
generic: alkyl-de-hydrogenation, *or* alkylation

Indexing: specific: propyl-de-hydro-substitution
generic: alkyl-de-hydro-substitution



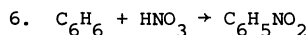
Speech/writing: generic: alkyl-de-hydrogenation *or* alkylation (if the ester is taken as substrate)

Indexing: specific: α -[α -(bromomethyl)benzyl]benzyl-de-hydro-substitution (if the ester is taken as substrate), *or* 1,1-bis(ethoxycarbonyl-2-(2'- α -bromomethylbenzyl)phenylethyl)-de-bromo-substitution (if the first component is taken as substrate).



Speech/writing: specific: bromoacetyl-de-hydrogenation, *or* bromoacetylation
generic: acyl-de-hydrogenation, *or* acylation

Indexing: specific: bromoacetyl-de-hydro-substitution
generic: acyl-de-hydro-substitution



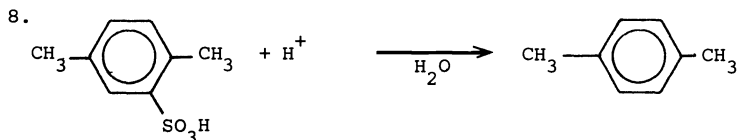
Speech/writing: nitro-de-hydrogenation, *or* nitration

Indexing: nitro-de-hydro-substitution

7. The same, with distinction between isotopes

Speech/writing: nitro-de-protiation
nitro-de-deuteration
nitro-de-tritiation

Indexing: nitro-de-protio-substitution, etc.



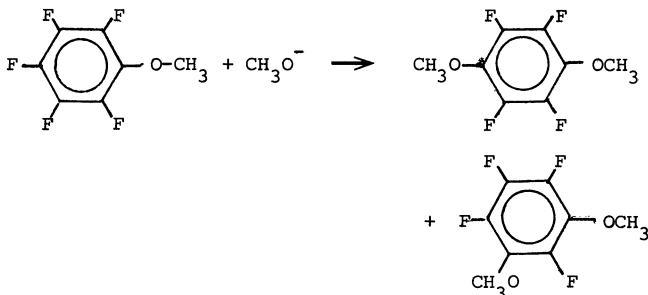
Speech/writing: hydro-de-sulfonation, *or* desulfonation

Indexing: hydro-de-sulfo-substitution

9. The same, with distinction between isotopes

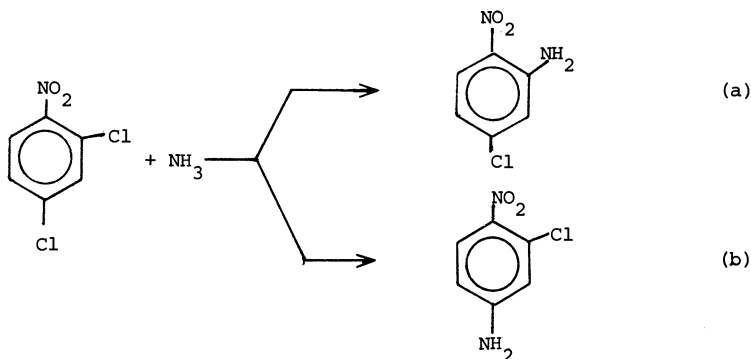
Speech/writing: protio-de-sulfonation
deuterio-de-sulfonation
tritio-de-sulfonation

10.



Either transformation is (speech/writing) methoxy-de-fluorination. Either might be called nucleophilic methoxy-de-fluorination. One might wish to distinguish *para* methoxy-de-fluorination from *meta* methoxy-de-fluorination in 2,3,4,5,6-pentafluoroanisole, or 3-methoxy-de-fluorination from 4-methoxy-de-fluorination; in such a case, the identity of the substrate should be mentioned unless obvious from the context.

11.



Specific names for both processes:

Speech/writing: amino-de-chlorination

Indexing: amino-de-chloro-substitution

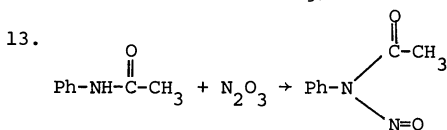
Speech/writing names referring to the sites of substitution in this particular substrate:

For 11a: 2-amino-de-chlorination in 2,4-dichloro-1-nitrobenzene

For 11b: 4-amino-de-chlorination in 2,4-dichloro-1-nitrobenzene

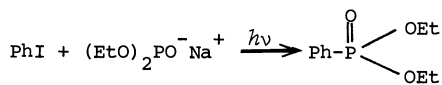
12. (*R*)-*sec*-butyl bromide + EtS⁻ → (*S*)-*sec*-butyl ethyl sulfide

The transformation is ethylthio-de-bromination (for speech/writing) or ethylthio-de-bromo-substitution (for indexing). Either may be followed by "with inversion of configuration."



The transformation is nitroso-de-hydrogenation (for speech/writing) or nitroso-de-hydro-substitution (for indexing). The site of substitution may be specified as *N*-nitroso-de-hydrogenation or *N*-nitrosation (for speech/writing), or as *N*-nitroso-de-*N*-hydro-substitution (for indexing).

14.



The transformation is diethoxyphosphinyl-de-iodination (for speech/writing) or diethoxyphosphinyl-de-iodo-substitution (for indexing). A chemist might wish to convey more information as well as an opinion about mechanism by stating that it is photo-induced diethoxyphosphinyl-de-iodination probably by the S_{RN}1 mechanism.

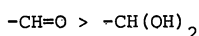
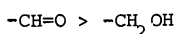
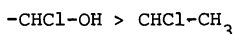
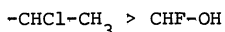
2. Addition Transformations

2.1 Addition of two univalent groups. These rules deal with transformations as a result of which two univalent atoms or groups (called addends) become attached to an unsaturated system. These transformations include addition to simple olefins, to carbonyl groups, to aldimines and ketimines, to dienes, to aromatic or heteroaromatic systems, to acetylenes, to carbenes, to 1,3-dipolar intermediates, and others of similar kind. The speech/writing and indexing names are identical.

2.1.1 Priority considerations. These are often relevant to the order in which addends are mentioned, and rarely to the order in which addition sites are mentioned.

2.1.1.1 The priority of addends named specifically is determined according to the Cahn-Ingold-Prelog rules (ref. 2) for the priority of ligands.

Examples of priority rankings: $-F > -COOH$



2.1.1.2 The priority of addends named generically is determined by the priority of the lowest priority member of the genre. Thus, the priority of the genre of halogens is determined by that of fluorine, and the priority of the genre of alkoxy groups is determined by that of the methoxy group.

2.1.1.3 The priority of addition sites is a secondary consideration, invoked only when there are two or more identical addends. When the addition sites are of the same element, a site with a lower number according to IUPAC nomenclature (see especially ref. 3) is mentioned earlier. When the addition sites are of different elements, a site with a higher atomic number is mentioned later.

2.1.2 Addition to a single olefinic or acetylenic linkage.

2.1.2.1 The fundamental name comprises (a) the name of the addend of lower priority, followed by a hyphen, (b) the name of the addend of higher priority, followed by a hyphen, and (c) the suffix 'addition.' Groups are named according to Rule 1.1.4. (See examples 2, 3, 6, 7 and 8.)

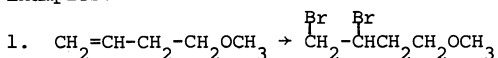
2.1.2.2 If the two addends are the same, the name comprises (a) the syllable 'di' or 'bis' (as appropriate; see ref. 4), (b) the name of the addend, followed by a hyphen, and (c) the suffix 'addition.' (See examples 1, 4 and 5.)

2.1.2.3 If it is desired to emphasize the category of addition to a single olefinic or acetylenic linkage, the Greek letters ' $\alpha\beta$ -' may be placed at the start of the name.

2.1.2.4 If it is desired to indicate the atoms in a particular olefin or acetylene to which addends attach, the number of the respective carbon atom in the alkene or alkyne may be given immediately before the name of each addend.

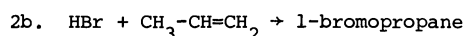
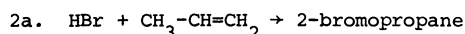
2.1.2.5 If it is desired to indicate the stereochemistry of addition, '*syn*-' or '*anti*-' may be placed at the very beginning of the name. '*syn*' and '*anti*' are used in the sense described by Bunnett (ref. 5), following Klyne and Prelog (ref. 6).

Examples:

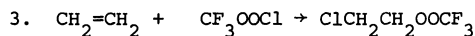


dibromo-addition, or $\alpha\beta$ -dibromo-addition, or 1,2-dibromo-addition to 4-methoxyl-1-butene, or 3,4-dibromo-addition to 3-butenyl methyl ether

-
2. R.S. Cahn, C. Ingold and V. Prelog, *Angew. Chem., Int. Ed., Engl.*, 5, 385 (1966); IUPAC Commission on Nomenclature of Organic Chemistry, *Pure Appl. Chem.*, 45, E 11 (1976).
 3. Rule A-3, "Nomenclature of Organic Chemistry," 1979 Edition, Pergamon Press, Oxford.
 4. Rule A-2.5, "Nomenclature of Organic Chemistry," 1979 Edition, Pergamon Press, Oxford.
 5. J. F. Bunnett, *Surv. Progr. Chem.* 5, 53 (1969).
 6. W. Klyne and V. Prelog, *Experientia*, 16, 521 (1960).



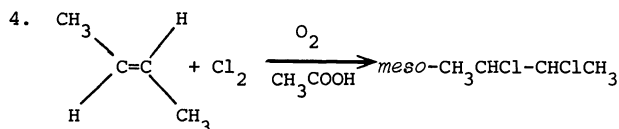
For 2a and 2b, hydro-bromo-addition, or $\alpha\beta$ -hydro-bromo-addition
 For 2a, 1-hydro-2-bromo-addition to propene



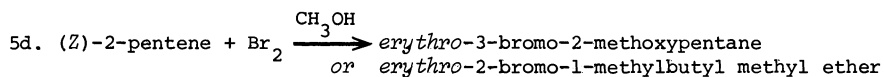
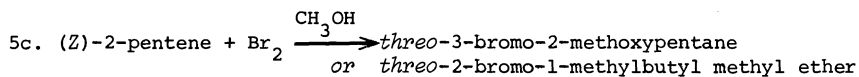
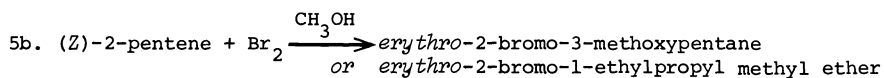
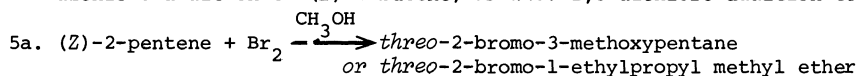
$\alpha\beta$ -(trifluoromethyl)peroxy-chloro-addition

In the compilation of an index, this transformation might be listed:

Addition, $\alpha\beta$ -(trifluoromethyl)peroxy-chloro-



dichloro-addition, or $\alpha\beta$ -dichloro-addition, or *anti*- $\alpha\beta$ -dichloro-addition, or 2,3-dichloro-addition to (*E*)-2-butene, or *anti*-2,3-dichloro-addition to (*E*)-2-butene



specific: For 5a-5d, incl. methoxy-bromo-addition, or $\alpha\beta$ -methoxy-bromo-addition

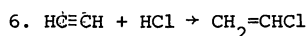
For 5a and 5c, *anti*- $\alpha\beta$ -methoxy-bromo-addition

For 5a and 5b, 3-methoxy-2-bromo-addition to (*Z*)-2-pentene

For 5a, *anti*-3-methoxy-2-bromo-addition to (*Z*)-2-pentene

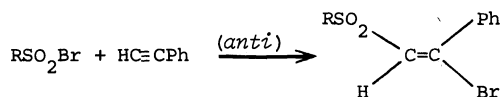
For 5d, *syn*-2-methoxy-3-bromo-addition to (*Z*)-2-pentene

generic: For 5a-5d, incl. alkoxy-halo-addition, or $\alpha\beta$ -alkoxy-halo-addition

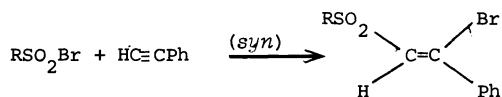


hydro-chloro-addition, or $\alpha\beta$ -hydro-chloro-addition

7a.

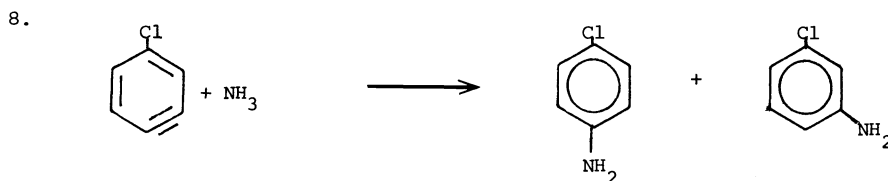


7b.



For 7a, *anti*-alkylsulfonyl-bromo-addition, or *anti*- $\alpha\beta$ -alkylsulfonyl-bromo-addition, or *anti*-2-alkylsulfonyl-1-bromo-addition to phenylacetylene

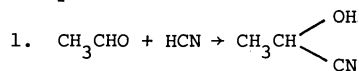
For 7b, *syn*-alkylsulfonyl-bromo-addition, etc.



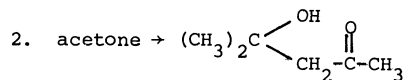
To form either adduct: hydro-amino-addition
 To form *p*-chloroaniline: 2-hydro-1-amino-addition to 4-chlorobenzene
 To form *m*-chloroaniline: 1-hydro-2-amino-addition to 4-chlorobenzene

2.1.3 Addition to a carbonyl group. Names are formulated as for addition to single olefinic linkages, except that the notation of positions of attachment is different. The addend attaching to oxygen is preceded by 'O-.' The addend attaching to carbon is preceded by 'C-.' In speech/writing, notation at the positions of attachment may be omitted if the context makes clear the character of the transformation.

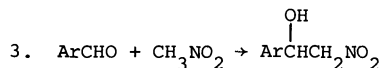
Examples:



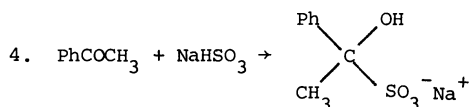
O-hydro-*C*-cyano-addition, or hydro-cyano-addition to acetaldehyde



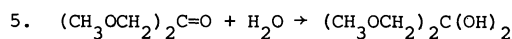
O-hydro-*C*-(2-oxopropyl)-addition, or *O*-hydro-*C*-acetyl-addition, or hydro-acetyl-addition to acetone



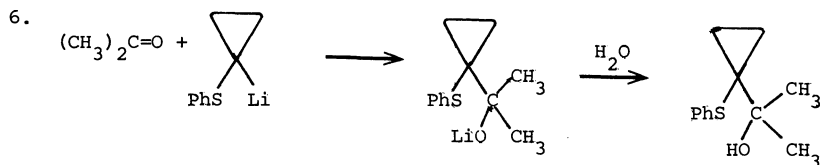
O-hydro-*C*-nitromethyl-addition



O-hydro-*C*-sulfonato-addition



O-hydro-*C*-hydroxy-addition



For transformation of acetone to intermediate:

generic: *O*-metallo-*C*-alkyl-addition

specific: *O*-lithio-*C*-[1-(phenylthio)cyclopropyl]-addition

For transformation of intermediate to final product:

Speech/writing: generic: hydro-de-metallation

specific: hydro-de-lithiation

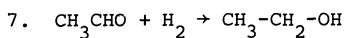
Indexing: generic: hydro-de-metallo-substitution

specific: hydro-de-lithio-substitution

For transformation of acetone to final product:

generic: *O*-hydro-*C*-alkyl-addition

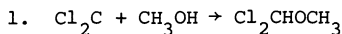
specific: *O*-hydro-*C*-[1-(phenylthio)cyclopropyl]-addition



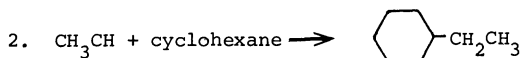
C,O-dihydro-addition

2.1.4 *Addition to a carbene or a nitrene.* The rules are mostly the same as for addition to a single olefinic linkage. For indexing it is requisite and for speech/writing usually desirable to emphasize the character of the transformation by specifying ' α ' or, for addition to a nitrene, '*NN*.'

Examples:

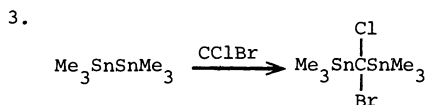


α -hydro-methoxy-addition



α -hydro-cyclohexyl-addition

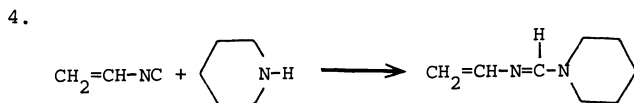
Note: To name this transformation as an insertion, see Rule xxx.



specific: α -bis(trimethylstannyl)-addition

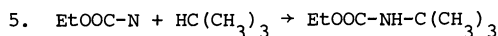
generic: α -distannyl-addition, or α -bis(trialkylstannyl)-addition

Note: To name this transformation as an insertion, see Rule xxx.



specific: α -hydro-piperidino-addition

generic: α -hydro-amino-addition

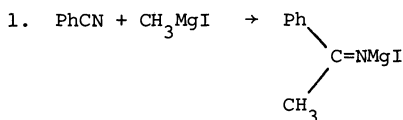


α -hydro-*tert*-butyl-addition, or *NN*-hydro-*tert*-butyl-addition

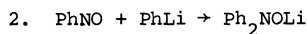
Note: To name this transformation as an insertion, see Rule xxx.

2.1.5 *Addition to imines, thiocarbonyl groups, cyano groups, etc.* The rules to be followed are analogous to those for addition to carbonyl groups.

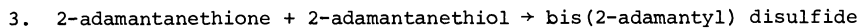
Examples:



C-methyl-*N*-iodomagnesian-addition



O-lithio-*N*-phenyl-addition



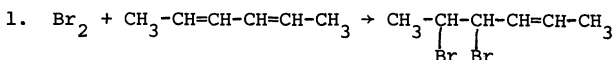
specific: *C*-hydro-*S*-(2-adamantylthio)-addition

generic: *C*-hydro-*S*-alkylthio-addition

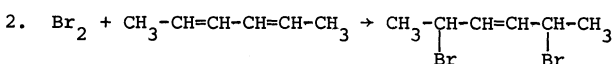
2.1.6 Addition to conjugated or cumulative unsaturated systems. Names are formulated as for addition to single olefinic or carbonyl linkages, except as now stated.

2.1.6.1 When the atoms doubly or triply bonded in the unsaturated system are all of carbon, they are lettered consecutively with Greek letters, atom α being at one end of the unsaturated system. When the atoms at the ends of the unsaturated system are of different elements, the atom of higher atomic number is lettered ' α .' For general representation of the transformation, the positions to which addends attach are indicated by the relevant Greek letters preceding the names of the addends, letters early in the alphabet being favored when a choice is possible. For representation of addition to a specific structure, the positions to which addends attach are indicated by the relevant numbers preceding the names of the addends.

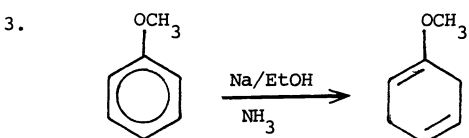
Examples:



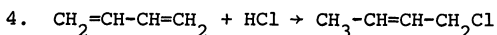
$\alpha\beta$ -dibromo-addition, or 2,3-dibromo-addition to 2,4-hexadiene



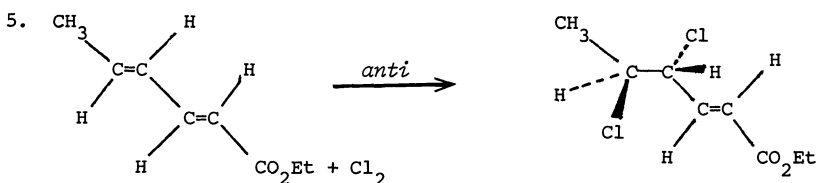
$\alpha\delta$ -dibromo-addition, or 2,5-dibromo-addition to 2,4-hexadiene



$\alpha\delta$ -dihydro-addition, or 2,5-dihydro-addition to anisole



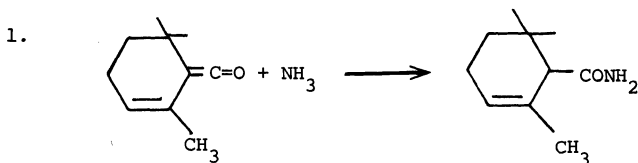
$\alpha\delta$ -hydro-chloro-addition, or 1-hydro-4-chloro-addition to 1,3-butadiene



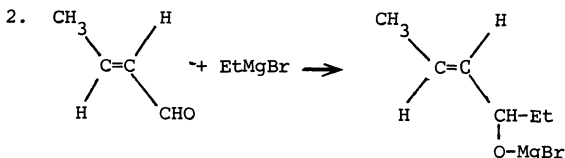
$\alpha\beta$ -dichloro-addition, or *anti*-4,5-dichloro-addition to ethyl(2*E*,4*E*)-hexadienoate

2.1.6.2 When one (or more) of the atoms of the unsaturated system is (are) an atom other than carbon, names are formulated as for addition to all-carbon unsaturated systems except that the identity of the heteroatom(s) is indicated in parentheses following the relevant Greek letter(s).

Examples:

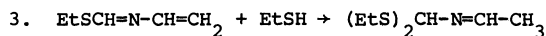


γ -hydro- β -amino-addition (to a ketene)



specific: β -ethyl- α (O)-bromomagnesium-addition, or 1-ethyl-O-bromomagnesium-addition to (*E*)-2-butenal

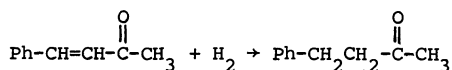
generic: β -alkyl- α (O)-halomagnesium-addition



specific: δ -hydro- α -ethylthio-addition, or 4-hydro-1-ethylthio-addition to 3-thia-5-azahepta-4,6-diene

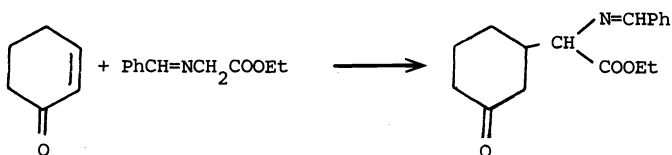
generic: δ -alkyl- α -alkylthio-addition

4.



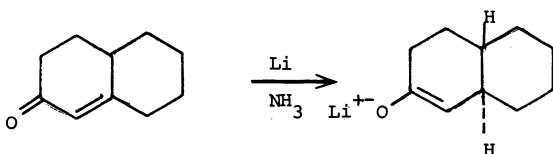
$\alpha\beta$ -dihydro-addition, or 3,4-dihydro-addition to 4-phenyl-3-buten-2-one

5.



$\alpha\beta$ -hydro-[(benzylideneamino)(ethoxycarbonyl)methyl]-addition, or 2-hydro-3-[(benzylideneamino)(ethoxycarbonyl)methyl]-addition to cyclohex-2-enone

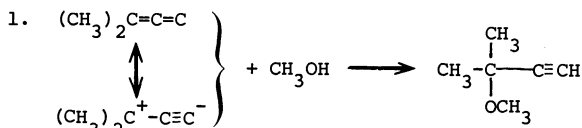
6.



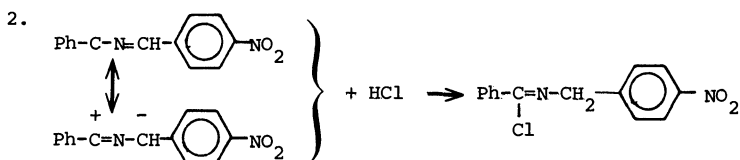
δ -hydro- α (O)-lithio-addition

2.1.7 Addition to a 1,3-dipolar intermediate. Names are formulated as for addition to other unsaturated systems treated above. Site designation depends on the type of name employed for the intermediate.

Examples:

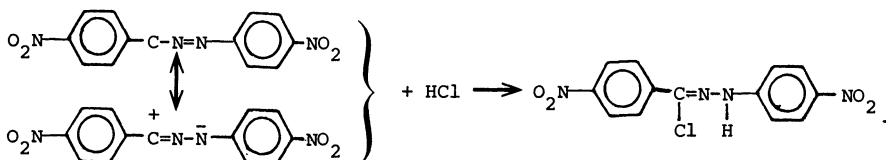


α -hydro- γ -alkoxy-addition to a vinylidenecarbene, or 1-hydro-3-methoxy-addition to 3-methylbuta-1,2-dienylidene



α -hydro- γ -chloro-addition to an azomethynlide, or 3-hydro-1-chloro-addition to α -(4-nitrobenzylideneamino)benzylidene

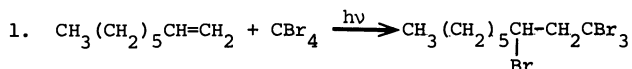
3.



N -hydro- C -chloro-addition to an azomethinimine, or 3-hydro-1-chloro-addition to 4-nitro- α -(4-nitrophenylazo)benzylidene

N.B. Other information. The mechanism of addition is not indicated in the name, nor are the reactants, by-products or conditions of a reaction, but these can be indicated by additional words.

Examples:



The transformation is $\alpha\beta$ -(tribromomethyl)-bromo-addition or 1-(tribromomethyl)-2-bromo-addition to 1-octene. Giving more information, one could describe it as photoinitiated $\alpha\beta$ -(tribromomethyl)-bromo-addition of CBr_4 by a radical mechanism.

3. Elimination Transformations

3.1 Elimination of two univalent groups. These rules deal with transformations in which two univalent atoms or groups (called eliminands) are detached geminally (to form a carbene, nitrene, etc.), vicinally (to form an olefin, a carbonyl group, an imine, etc.), from positions which are separated by one atom (to form certain reactive intermediates), or from positions separated by more than one atom (e.g., to form a conjugated diene). Elimination from two vicinal positions joined by a double bond (to form a triple bond between those positions) is embraced. Detachment of atoms or groups from positions separated by methylene groups, ether bridges and the like, accompanied by bonding of those positions to each other so as to form a ring structure of three or more ring members, is excluded. The speech/writing and indexing names are identical.

3.1.1 Priority considerations. These are often relevant to the order in which eliminands are mentioned, and rarely to the order in which elimination sites are mentioned.

3.1.1.1 The priority of eliminands named specifically is determined according to the Cahn-Ingold-Prelog rules (ref. 2) for the priority of ligands.

3.1.1.2 The priority of eliminands named generically is determined by the priority of the lowest priority member of the genre.

3.1.1.3 The priority of elimination sites is a secondary consideration, invoked only when there are two or more identical eliminands. When the elimination sites are of the same element, a site with a lower number according to IUPAC nomenclature is mentioned earlier. When the elimination sites are of different elements, a site with a higher atomic number is mentioned later.

3.1.2 Elimination to form a single olefinic or acetylenic linkage.

3.1.2.1 If eliminands are named specifically, the fundamental name comprises (a) the name of the eliminand of lower priority, followed by a hyphen, (b) the name of the eliminand of higher priority, followed by a hyphen, and (c) the suffix 'elimination.' Groups are named according to Rule 1.1.4.

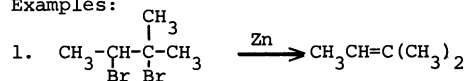
3.1.2.2 If the two eliminands are the same, the name comprises (a) the syllable 'di' or 'bis' (as appropriate; see ref. 4), (b) the name of the eliminand, followed by a hyphen, and (c) the suffix 'elimination.'

3.1.2.3 If it is desired to emphasize the category of elimination to form a single olefinic linkage, the Greek letters ' $\alpha\beta$ ' may be placed at the start of the name.

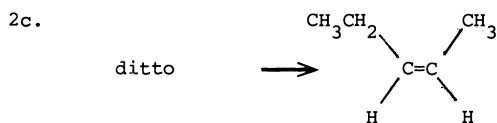
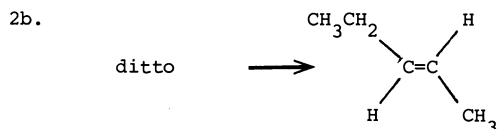
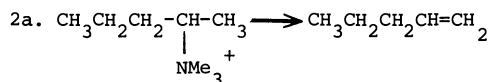
3.1.2.4 If it is desired to indicate the atoms in a particular substrate from which specific eliminands detach, the number of the respective carbon atom in the substrate may be given immediately before the name of each eliminand.

3.1.2.5 If it is desired to indicate the stereochemistry of elimination, '*syn*-' or '*anti*-' may be placed at the beginning of the name.

Examples:



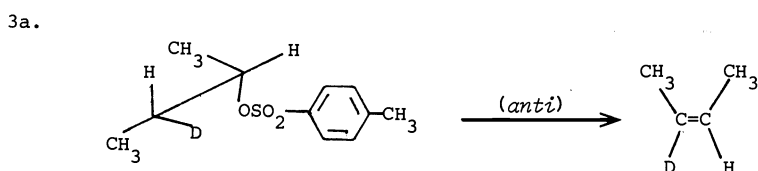
dibromo-elimination, or $\alpha\beta$ -dibromo-elimination, or 2,3-dibromo-elimination from 2,3-dibromo-2-methylbutane



For 2a, 2b, and 2c hydro-(trimethylammonio)-elimination, or $\alpha\beta$ -hydro-(trimethylammonio)-elimination

For 2a, 1-hydro-2-(trimethylammonio)-elimination from trimethyl(pent-2-yl)-ammonium ion

For 2b or 2c, 3-hydro-2-(trimethylammonio)-elimination from trimethyl(pent-2-yl)-ammonium ion

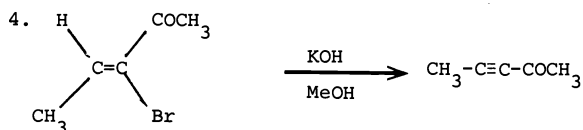


For 3a-3d, incl. hydro-(*p*-tolylsulfonyloxy)-elimination, or $\alpha\beta$ -hydro-(*p*-tolylsulfonyloxy)-elimination

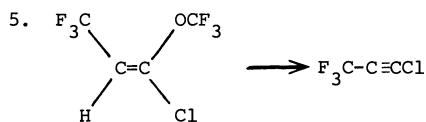
For 3a and 3c, protio-(*p*-tolylsulfonyloxy)-elimination

For 3b and 3d, $\alpha\beta$ -deuterio-(*p*-tolylsulfonyloxy)-elimination

For 3a, *anti*-protio-(*p*-tolylsulfonyloxy)-elimination, or *anti*-2-protio-1-(*p*-tolylsulfonyloxy)-elimination from *erythro*-[3-²H₁]but-2-yl *p*-toluenesulfonate



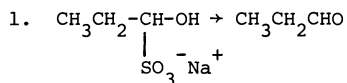
hydro-bromo-elimination, or *anti*-hydro-bromo-elimination, or 4-hydro-3-bromo-elimination from (*Z*)-3-bromo-3-penten-2-one



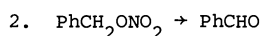
specific: hydro-trifluoromethoxy-elimination, or *anti*-2-hydro-1-trifluoromethoxy-elimination from (*E*)-1-chloro-3,3,3-trifluoro-1-trifluoromethoxypropene
 generic: hydro-alkoxy-elimination

3.1.3 Elimination to form a double bond between carbon and an atom of another element. Names are formulated as for elimination to form single olefinic linkages, except that the notation of positions of detachment is different. The eliminand detaching from the hetero-atom is preceded by its symbol. The eliminand detaching from carbon is preceded by 'C-.' In speech/writing, notation of the positions of detachment may be omitted if the context makes clear the character of the transformation.

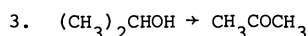
Examples:



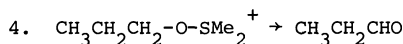
O-hydro-*C*-sulfonato-elimination



C-hydro-*O*-nitro-elimination

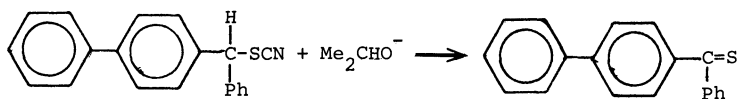


C,O-dihydro-elimination



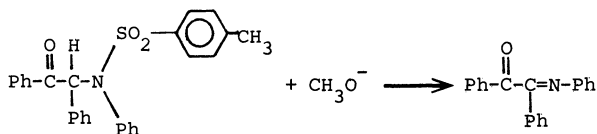
C-hydro-*O*-dimethylsulfonio-elimination

5.



C-hydro-*S*-cyano-elimination

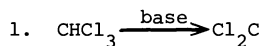
6.



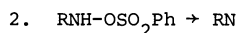
C-hydro-*N*-(*p*-toluenesulfonyl)-elimination

3.1.4 Elimination to form a carbene or a nitrene. The rules are mostly the same as for elimination to form a single olefinic linkage. For indexing it is requisite and for speech/writing usually desirable to emphasize the character of the transformation by specifying 'α' (unless the numbered positions from which the eliminands detach are given) or 'NN-' (for nitrene formation).

Examples:

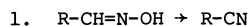


specific: αα-hydro-chloro-elimination
 generic: αα-hydro-halo-elimination

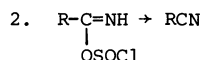


αα-hydro-phenylsulfonyloxy-elimination, or *NN*-hydro-phenylsulfonyloxy-elimination

3.1.5 Elimination to form a cyano group. The rules to be followed are analogous to those for eliminations to form carbonyl groups, imines, etc.



C-hydro-*N*-hydroxy-elimination

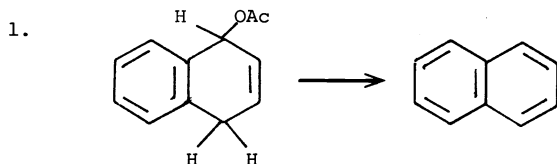


N-hydro-*C*-(chlorosulfinyloxy)-elimination

3.1.6 Elimination to form or extend a conjugated or cumulative unsaturated system. Names are formulated as for elimination to form single olefinic or carbonyl linkages except as now stated.

3.1.6.1 When the atoms doubly or triply bonded in the unsaturated system formed are all of carbon, they are lettered consecutively with Greek letters, atom α being at one end of the unsaturated system. For generic representation of the transformation, the positions from which eliminands detach are indicated by the relevant Greek letters preceding the names of the eliminands, letters early in the alphabet being favored when a choice is possible. For representation of elimination from a specific structure, the positions from which eliminands detach are indicated by the relevant numbers preceding the names of the eliminands.

Examples:

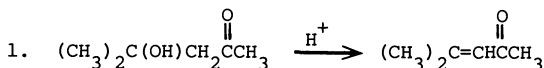


specific: α -hydro- δ -acetoxy-elimination, or 4-hydro-1-acetoxy-elimination from 1,4-dihydro-1-naphthyl acetate

generic: α -hydro- δ -acyloxy-elimination

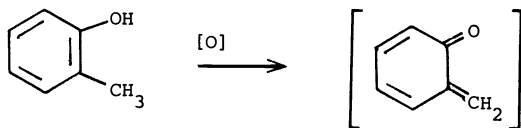
3.1.6.2 When one (or more) of the atoms of the unsaturated system formed is (are) an atom other than carbon, names are formulated as for elimination to form all-carbon unsaturated systems except that the identity of the heteroatom(s) is indicated in parentheses following the relevant Greek letter(s). For representation of elimination from a specific substrate, the positions from which eliminands detach are indicated by the numbers of the carbon atoms and by the symbols of heteroatoms.

Examples:



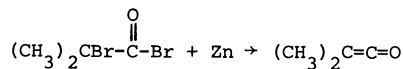
hydro-hydroxy-elimination, or $\alpha\beta$ -hydro-hydroxy-elimination, or 3-hydro-4-hydroxy-elimination from 4-hydroxy-4-methyl-2-pentanone

2.



$\alpha(O)\delta$ -dihydro-elimination, or O,α -dihydro-elimination from 2-methylphenol

3.

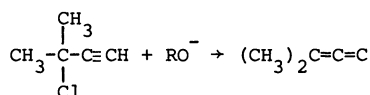


$\alpha\beta$ -dibromo-elimination, or 1,2-dibromo-elimination from 2-bromo-2-methylpropanoyl bromide

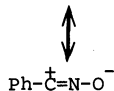
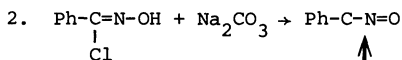
3.1.7 *Elimination to form a 1,3-dipolar intermediate.* Names are formulated as for elimination to form other unsaturated systems treated above.

Examples:

1.



α -hydro-chloro-elimination, or 1-hydro-3-chloro-elimination from 3-chloro-3-methyl-1-butyne



O-hydro-C-chloro-elimination from benzohydroximoyl chloride

N.B. Other information. If there are two identical but diastereotopic eliminands at one or both of the sites from which elimination occurs, such that different stereoisomers are formed depending on which are eliminated, it may be desirable to follow the name of the transformation with a phrase naming the product formed. The mechanism is not indicated in the name, nor are the reactants, by-products or conditions of a reaction, but these can be indicated by additional words.

Examples:

- The transformation in example 2c for rule 3.1.2.5 could be described as:
3-hydro-2-(trimethylammonio)-elimination from trimethyl(pent-2-yl)ammonium ion to form (Z)-2-pentene.