Pure Appl. Chem., Vol. 80, No. 2, pp. 277–410, 2008.
doi:10.1351/pac200880020277
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INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION*

GRAPHICAL REPRESENTATION STANDARDS FOR CHEMICAL STRUCTURE DIAGRAMS**

(IUPAC Recommendations 2008)

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Graphical representation standards for chemical structure diagrams

(IUPAC Recommendations 2008)

Abstract: The purpose of a chemical structure diagram is to convey information—typically the identity of a molecule—to another human reader or as input to a computer program. Any form of communication, however, requires that all participants understand each other. Recommendations are provided for the display of two-dimensional chemical structure diagrams in ways that avoid ambiguity and are likely to be understood correctly by all viewers. Examples are provided in many areas, ranging from issues of typography and color selection to the relative positioning of portions of a diagram and the rotational alignment of the diagram as a whole. Explanations describe which styles are preferred and which should be avoided. Principal recommendations include:

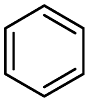
- Know your audience: Diagrams that have a wide audience should be drawn as simply as possible.
- Avoid ambiguous drawing styles.
- Avoid inconsistent drawing styles.

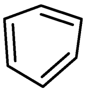
Keywords: graphical representation; recommendations, graphical; IUPAC Chemical Nomenclature and Structure Representation Division; chemical structures; chemical structure diagrams.

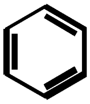
CONTENTS

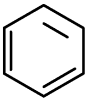
GR-0. INTRODUCTION

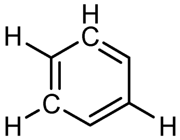
Although chemical structures have been called “the language of chemistry” [1], few documents have attempted to provide any sort of guidelines for the production of chemical structure diagrams [2–5]. The same task group that produced this document has recently published recommendations on the graphical representation of stereochemical configuration [6], but IUPAC commentary on the subject of overall graphical representation has been limited to small sections within larger documents, such as a discussion of the preferred orientation of the steroid ring system as part of the recommendations on the nomenclature of steroids [7]. In the 430-page *ACS Style Guide*, the chapter on “Chemical Structures” occupies only eight pages that include discussions of several topics in addition to simple representation [8]. And yet chemists have strong feelings for how chemical structure diagrams should look, even in the absence of formal guidelines. Show most chemists a series of diagrams of something as simple as benzene, and there will be near-unanimity about which ones are “good” diagrams and which ones are “bad”. As Robert Pirsig writes in *Zen and the Art of Motorcycle Maintenance*, “But even though Quality cannot be defined, *you know what Quality is*!” [9].

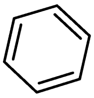












Production of good chemical structure depictions will likely always remain something of an art form. There are few cases where it can be said that a specific representation is “right” and that all others are “wrong”. These guidelines do not try to do that. Rather, they try to codify the sorts of general rules that most chemists understand intuitively but that have never been collected in a single printed document. Adherence to these guidelines should help produce drawings that are likely to be interpreted the same way by most chemists and, as importantly, that most chemists feel are “good-looking” diagrams.

The most important advice in any style guide is to *know your audience*. In the context of these recommendations, it follows that the more specific the audience for a structure, the less important it is for that structure to honor the guidelines discussed here. A structure drawn on the back of a table napkin will not be drawn with the same accuracy or precision as one that appears in a printed journal. There is nothing wrong with that. A napkin drawing has an audience of one—your colleague on the next stool—while a printed journal has a much broader audience. Similarly, the types of structures that are appropriate for the *Journal of Very Specific Chemistry* might not be appropriate to *Chemical & Engineering News* or *Science* or *Nature.*

The opposite, however, is not true. Structures drawn for a general audience can be understood without problems by a more specific one. Your colleague on the next stool can surely understand a nicely printed diagram if he or she can also understand your scribble-on-a-napkin.

Accordingly, these guidelines encourage those styles that are most likely to be understood by everyone and discourage the use of unusual, archaic, and ambiguous drawing styles.

Throughout these guidelines, you will see two recurring themes: reduction of ambiguity and proper use of context. With no context, the symbol VVVVVVVV might represent 4 tungsten atoms, 8 vanadium atoms, 17 connected carbon atoms, a wiggly bond, or a diagrammatic fracture. A simple line might represent a single bond, half of a double bond, a free valence, an iodine atom, or a negative charge. On occasion, it might even represent nothing more than a simple line itself. Context is critical. The end of one bond should not touch the end of another unless they truly are both bound to the same atom. Text should not be placed near the end of a bond unless it is intended to provide an atom label, or is so visually different from other labels (in font, size, style, color, or some combination of those) that it could not possibly be mistaken for an atom label. If you create diagrams that are difficult to interpret, you should not be surprised if people have problems interpreting them.

The same is true when creating diagrams that need to be interpreted by computer. In many ways, computers today are much more demanding than human chemists. Few programs will interpret a block of text as being an atom label, no matter how close it is to the end of a bond—unless the software is told, specifically, “That’s an atom label”. Fortunately, most software makes it easy to do so. On the other hand, software programs may let you assign specific meanings to objects that otherwise look identical, so that the symbol VVVVVVVV could be made to mean 17 connected carbon atoms without any ambiguity at all.

Whatever your audience, keep it in mind as you create your structural diagrams.

GR-0.1 Overview

The recommendations in this publication are presented approximately in the order that they should be considered by an author who is creating a chemical structure diagram. First, it is necessary to decide on basic drawing styles, including general issues such as colors and font types (GR-0). Drawing styles specific to chemical structure diagrams also need to be considered, primarily those related to the depiction of bonds (GR-1) and labeled atoms (GR-2). Once the basic styles have been chosen, the diagram itself can be produced, starting with the overall orientation of the diagram (GR-3) and continuing until all substituents have been positioned (GR-4). Other common features, including formal charges and unpaired electrons (GR-5) as well as delocalization (GR-6) have special needs that are considered separately, while the depiction of salts and related forms (GR-7) requires the relative positioning of several fragments that have been depicted individually. Various other issues are discussed in the remainder of the publication (GR-8 through the end).

Throughout this publication are numerous examples of chemical structures drawn in styles that are labeled as “preferred”, “acceptable”, “not acceptable”, or occasionally “wrong”. Due to space constraints in this document, only a few diagrams are shown for each case, with the intention that those examples are representative of the topic being discussed. The presence of one diagram labeled as “preferred” does not preclude the possibility of other “preferred” diagrams, including those with slight differences from the depicted structure in terms of bond length, line thickness, localization of double bonds in aromatic systems, or other minor details. Beyond that, it is worthwhile to clarify further the meaning of those terms as they are used here.

A chemical structure diagram is most commonly used simply as a means of identification, a way to answer the implied question, “What is the chemical structure of X?” The styles labeled as “preferred” show how the structure should best be depicted in such cases, where there are no other overriding concerns. These depiction styles are generally applicable across many classes of chemical structures.

Sometimes, however, overriding concerns are present. Even simple structures might contain several ring systems, substituents, and functional groups. The generation of an aesthetic diagram of the whole molecule might require that individual portions are depicted in ways that would not be ideal if that portion were viewed in isolation. The diagrams labeled as "acceptable" indicate additional depiction styles that could be considered if the preferred style is inappropriate for some well-considered reason.

Many of the structural depictions included in this document are provided as counterexamples, offering clarification of how structures should *not* be shown. Those depictions are labeled as "not acceptable", indicating that they should be strongly avoided in normal usage. Where possible, they have been accompanied by further description of why they are not acceptable, and why the alternative depictions are preferred or more acceptable.

Finally, a small number of examples are labeled as simply "wrong". Those show representations that should be avoided in all cases, generally because they depict something that is either self-contradictory or because they accurately represent a molecule other than the one intended.

For the sake of readability within this paper, angular measurements of diagrams are listed with exact numerical values, such as 180°. Unless otherwise specified, all such measurements should be considered to be approximate, and specifying a range within roughly 10° of the listed value. The same applies to textual descriptions of angles, so the term "collinear" should be interpreted as "forming an angle between 170° and 190°". In other words, two bonds that look nearly collinear should be treated as exactly collinear, even if that is not exactly true for their actual geometric relationship.

Similarly, any mention of bonds being "adjacent" or atoms being "connected to" refers to their appearance in the two-dimensional representation. Any of the four bonds of an atom with a physical (three-dimensional) tetrahedral configuration is physically adjacent to every other bond, but in a two-dimensional representation it is depicted as adjacent to only two others, and "opposite" to the third. In cyclohexane, each carbon atom is truly "connected to" four atoms: its two neighboring carbon atoms in the ring, and two external hydrogen atoms. In most diagrams, however, cyclohexane will be depicted as a regular hexagon with the hydrogen atoms implicit but not shown within the diagram. It is useful to describe those carbon atoms as being connected to only two other atoms, the two neighboring carbon atoms that are explicitly depicted. These conventions will be used throughout this publication.

The recommendations in this publication are intended for use in structural diagrams drawn in the "standard" two-dimensional format where single bonds are represented with one line segment connecting a pair of atoms, double bonds are represented with two parallel line segments connecting a pair of atoms, atoms are labeled with atomic symbols (or not shown at all in the case of carbon atoms and the hydrogen atoms bonded to them), and so on. There are other valid ways to represent structures including Newman projections, ball-and-stick models, and many others. These recommendations should not be over-generalized as applying to anything beyond the "standard" two-dimensional chemical structure diagrams.

GR-0.2 Presentation media

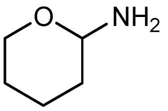
For the most part, these guidelines are written as in the context of a "perfect" presentation medium, where nothing will detract from the chemical structures themselves. Practical reality will rarely be that simple. Some styles that have been recommended for various printed publications are shown and contrasted in Table I, demonstrating the wide range of well-considered styles that are possible even within a single medium. When preparing diagrams for a low-resolution format such as the World Wide Web, on the other hand, it might be appropriate to make diagrams slightly larger or use a larger font than in printed journals, so that the diagrams can be read more easily on the computer screen. Presentations in printed journals have an absolute maximum width determined by the page size of that journal, and structures have to be sized and positioned accordingly. It is certainly reasonable (and altogether proper) to consider how the structures will eventually be presented and processed. There is no problem in deviating from these guidelines whenever necessary.

The prevalence of computers in chemical research provides some special problems. Compared to the number of human chemists, there are very few computer applications designed to process (display, store, search, analyze, etc.) chemical structure diagrams. Chemical structures that are likely to be interpreted by computer must be considered as having an *extremely* specific audience, and a fairly stupid one at that. Even the best computer programs available today are quite sensitive to the way that structures are drawn. These programs will surely become more intelligent over time, but they will not rival human intelligence in the near future. In addition to being easily interpretable by humans, structures drawn in the recommended styles are much more likely to be interpreted correctly by computers.

In some cases, no computer software currently available will be able to interpret a depiction that is otherwise completely reasonable, even preferred. We have tried to indicate those cases clearly, in sections of this document labeled with the phrase “SOFTWARE CAUTION:”, and we hope that software will evolve over time. If structures are required that must be interpreted by computers *now*—for example, for entry in a chemical registration system or for searching of an electronic chemical structure database—it is particularly important to understand the strengths and limitations of the software you are currently using. Again, structure drawings that follow these guidelines are more likely to be interpreted correctly than those that do not.

GR-0.3 Text

Any roman font is acceptable, but plainer fonts are preferred. Times, Times New Roman, Helvetica, and Arial are the most commonly seen serif and sans serif fonts, but that list is not exclusive. Normally, the fonts used in a chemical structure should match those used in any associated text, or be different from them in a clearly visible way (such as serif vs. sans serif).



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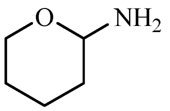

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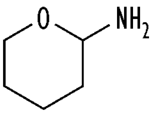

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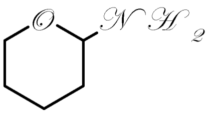
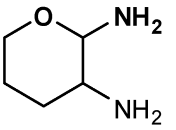


Not acceptable

Text should be scaled to a size that is comfortable for reading. In printed materials, that is usually in the range of 8–14 points. In other media, different sizes might be appropriate; in posters or projections, for example, a much larger size might be required. When increasing the size of text, it will usually also be necessary to increase the length of the bonds in the diagram (GR-1.1). Text that is smaller than five points in size is too small for most people to read comfortably, and is therefore not acceptable.

Formatting of text, including bold, italic, and underlined styles, should follow standard (nonchemical) style guidelines. For the most part, that means that the majority of text should be unformatted. Formatted text could be reasonably used to draw emphasis to a portion of a diagram; if emphasis is required, bold formatting is preferred over the use of italics or underlining because it provides a greater visual difference.



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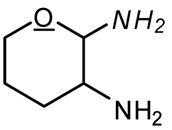
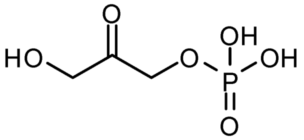


Not acceptable

Within the realm of biochemical structure diagrams only, the capital P symbol has different meanings depending on whether it is roman (a phosphorus atom) or italic (an abbreviation that represents a hydroxyphosphoryl or dihydroxyphosphoryl moiety in a phosphate group [10]). Due to the long history of usage, both the roman and italic forms of the capital P must remain acceptable; however, authors should consider that the italicized version may be unfamiliar to readers who are not familiar with biochemical nomenclature. For the broadest understanding, it is preferable to depict the phosphorus-containing fragments fully with explicit atoms and bonds. It is not acceptable to create new abbreviations (see GR-2.2) whose meaning is changed by the presence or absence of text formatting.



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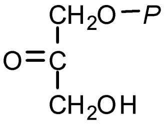
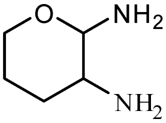


Acceptable
[for biochemical structure diagrams only]

The formatting for text should be used consistently throughout the diagram, whatever specific fonts, font sizes, and font styles are chosen. It is not acceptable to use multiple fonts and styles within a single diagram, again with intentional emphasis being an exception.

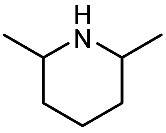


Not acceptable

Within those general guidelines, many publications have specific preferences regarding the use of text. When producing diagrams that are to be used by someone else, it is always recommended that authors check if there are any additional preferences that need to be followed.

GR-0.4 Lines

Lines are most commonly used in chemical diagrams to represent bonds, but may also be used in a strictly graphical sense, for example, to divide a larger space or as the shaft of an arrow. Most lines should be drawn at a width that is consistent with the remainder of the drawing, usually close to the width of the strokes of any accompanying text. Lines that are thinner than 0.5 points should be avoided. Thicker lines should be reserved for places where emphasis is required or (when drawn as bonds) to emphasize perspective.



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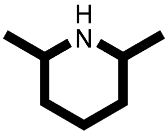

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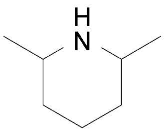


Not acceptable

Within those general guidelines, many publications have specific preferences regarding line widths just as they often do for text (GR-0.3). When producing diagrams that are to be used by someone else, it is always recommended that authors check if there are any additional preferences that need to be followed.

GR-0.5 Colors

Except when emphasis is desired, use of color should be avoided, and chemical structures should be displayed in the same color as any associated material. Most commonly, that means that the structures should be displayed in black on a white background, although some circumstances prefer alternative coloring schemes (projected transparencies are often displayed as white or yellow on a dark blue or black background).

When emphasis is desired, colors may be used to provide that emphasis. Any colors used in a document should be clear and visually distinct. Most commonly, red would be used as the primary color for emphasis. A dark blue or dark gray color would be a very poor choice for emphasis in a structure that is mostly black, and similar choices of low-contrast color combinations should be avoided.

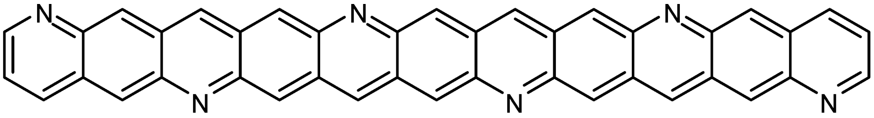
Authors are encouraged to remember that roughly 10 % of men are colorblind [11]. The combined use of red and green as contrasting colors in one diagram is strongly discouraged.

Authors of two-dimensional chemical diagrams should also keep in mind that there are traditional colors used for specific elements within the realm of three-dimensional modeling. Molecular models that display atoms as spheres will typically color the oxygen atoms as red, nitrogen atoms as blue, chlorine atoms as green, and so on, a coloring scheme that dates to an 1865 lecture by A. W. Hofmann where he used croquet balls in his demonstrations [12]. In current usage for molecular models, the specific shades of those colors may vary, as may the colors for less common elements. Since it is rarely necessary to color two-dimensional diagrams by element type, the traditional colors used in molecular modeling are simply not relevant in most cases. When it is desired to color two-dimensional diagrams by element type, it would be preferable to select a coloring scheme that is consistent with the traditional colors of three-dimensional modeling. It is not acceptable to color two-dimensional diagrams using color schemes that directly contradict those colors used for molecular modeling. That is, it is not acceptable to color all oxygen atoms yellow, all nitrogen atoms red, and all sulfur atoms blue within a single two-dimensional diagram.

GR-0.6 Size of diagrams

For the most part, the overall size of a structure diagram will be determined by the size chosen as the length of a standard bond and by the recommended angles between bonds in various circumstances as described in the remainder of this document. Although computers can store diagrams of any size, there are many other situations that impose restrictions on the space available for each structure diagram. In printed journals, for example, there is an absolute restriction that every structure must fit on the physical page, and the structures will often need to fit within specific column widths as well. Similarly, low-resolution media, such as the World Wide Web, may require a larger diagram overall in order to maintain legibility of fine details (see GR-0.2).

For very large, rigid molecules, there is little option but to shrink the diagram uniformly as much as necessary as to fit within the space available. When diagrams are resized, they should always be resized uniformly in both dimensions at the same time, and any associated text (such as atom labels) should be resized by the same amount.



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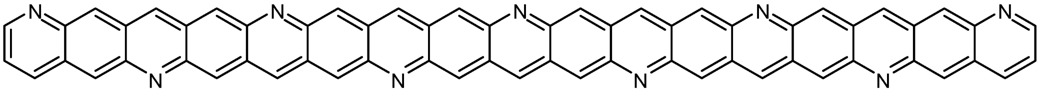
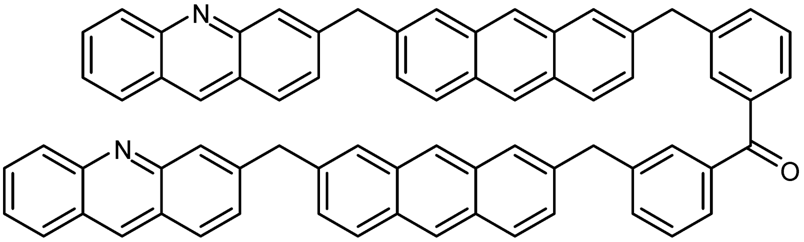


Preferred

When possible, it is preferable to rotate a portion of a structure diagram around a single bond, if doing so will allow the structure diagram to fit within the available space without needing to be resized. Rotation around single bonds connected to rings is best, followed by rotation around single bonds near the middle of chains, although rotation of any bond is acceptable as long as legibility is preserved.



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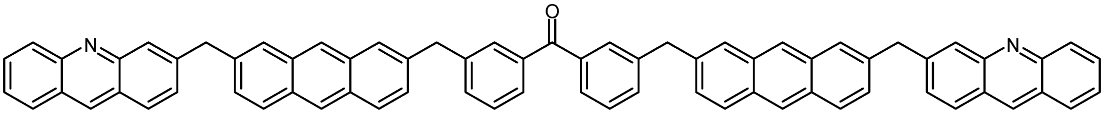

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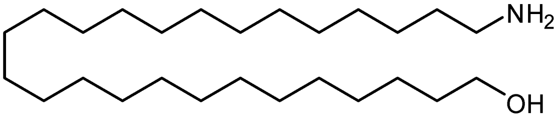

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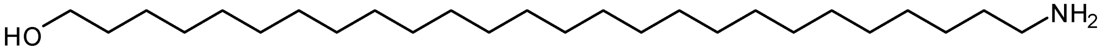

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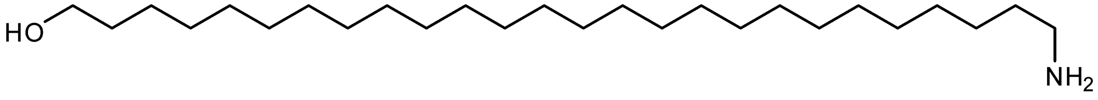
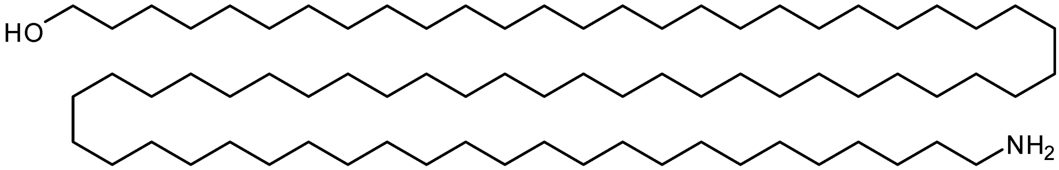


Acceptable

As discussed in GR-0.3, it is not acceptable to reduce the size of a diagram if doing so would produce atom labels that are illegibly small.



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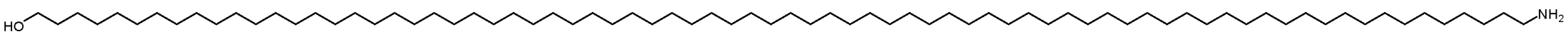
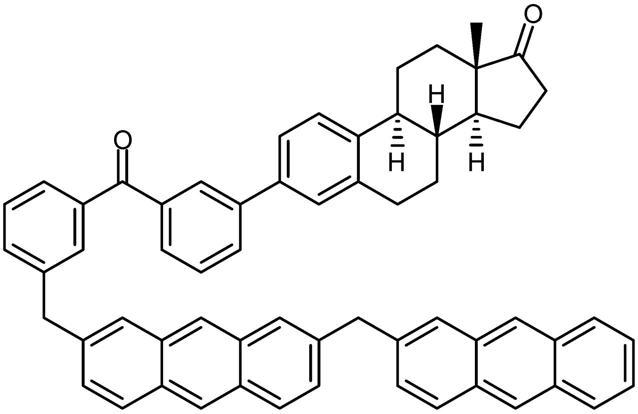


Not acceptable

If a portion of a structure diagram is normally depicted in a standard orientation (GR-3.6), that portion should remain fixed and only the other portion should be rotated.



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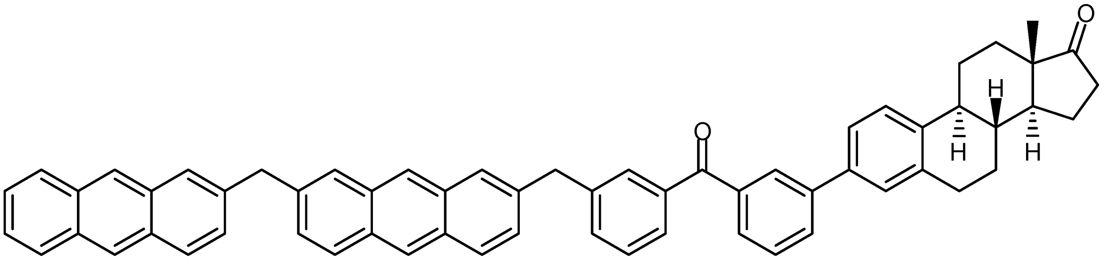
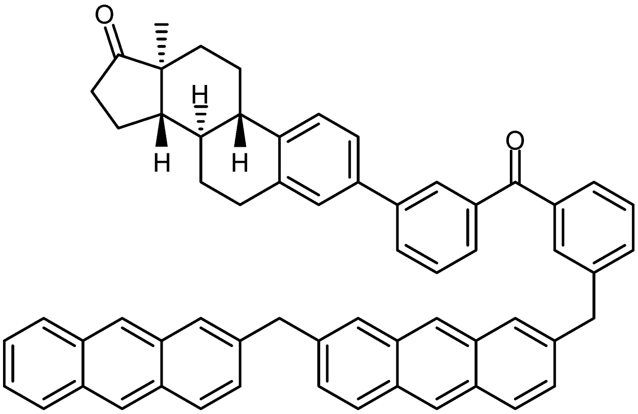


Acceptable



Not acceptable

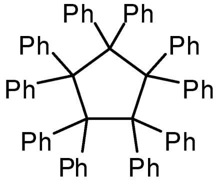
An alternative approach to reducing the size of large diagrams is to replace portions of the diagram with appropriate abbreviations as discussed in GR-2.2 and GR-2.3. Because abbreviations will often be much smaller than the portions of the diagram that they replace, their use can also help avoid overlap when no other options are available to make large diagrams legible.

$HO{-}[CH_2]_{26}{-}NH_2$

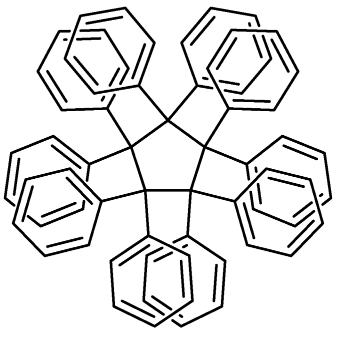
Preferred

$HO[CH_2]_{26}NH_2$

Acceptable



Preferred



Not acceptable

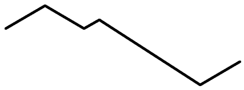
GR-1. BONDS

In most areas of chemistry, a bond represents an electronic association between two atoms. When drawing bonds, therefore, it is important to be unambiguous about (a) the nature of the electronic association—is the bond in question a single bond, double bond, or a bond of some other order—and (b) which two atoms it joins. Other types of bonding are also possible, including coordination bonds, which are discussed in GR-1.7. The use of bonds to represent configuration (e.g., using hashes and wedges) is discussed in a separate document [6].

GR-1.1 Bond lengths

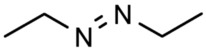
Within a given structure, most bonds should be drawn using a single consistent length. The length used for bonds should be long enough so that the bond is clearly visible between two atoms or atom labels; spacing between atoms that is less than twice as long as the height of an atom label should be avoided.

Preferred



Not acceptable

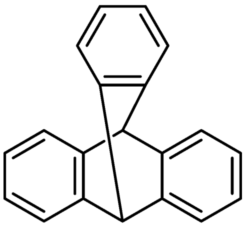
Not acceptable



Preferred

Not acceptable

Exceptions are certainly allowed, however, and are commonly seen in bridged polycyclic systems and sterically congested structures (including diagrams that depict atoms with high coordination numbers).



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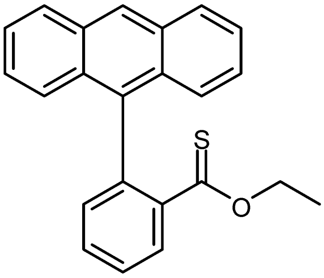
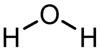


Preferred

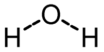
GR-1.2 Bond widths

Most bonds should be indicated with unbroken lines. The line should be approximately the same thickness as the stroke of the font used to depict atom labels in the structure (that is, the thickness of the vertical legs or the crossbar of a capital "H" in that font). Bonds that are more than four times as thick or less than one-quarter as thick as the atom label stroke width should be avoided.



Preferred

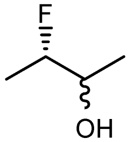
Not acceptable



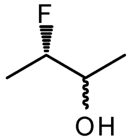
Not acceptable

GR-1.3 Bond patterns

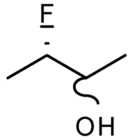
Hashed, dashed, and wavy bonds should have hashes, dashes, and waves that are clearly visible and unambiguous. Typically, that means that those portions of the bond should be separated from each other by two to four times the width of a single bond, and that each bond should have at least three separate hashes, dashes, or half-waves visible. The hashes, dashes, and waves should be consistent within each bond and throughout the structure diagram.



Preferred



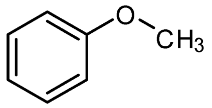
Not acceptable



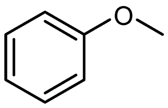
Not acceptable

GR-1.4 Terminal single bonds

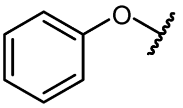
As discussed in GR-2.1.2, unlabeled atoms are assumed to be carbon atoms, and so terminal single bonds are assumed to represent methyl groups. Unlabeled bonds should not be used to represent unspecified or variable attachment points (see GR-9), as such diagrams are extremely prone to misinterpretation.



Preferred
(for methoxybenzene)

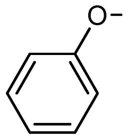


Acceptable
(for methoxybenzene)



Preferred
(for a phenoxy substituent)

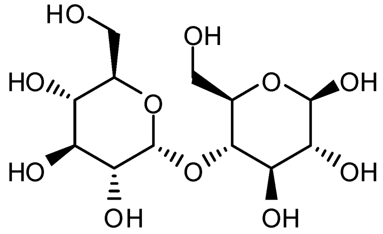
Shorter-than-usual terminal bonds are especially problematic, as they can be confused not only with methyl groups, but also with negative charges. Bonds of this type should be strongly avoided.



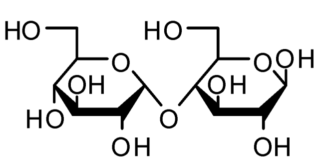
Not acceptable
(Would this represent methoxybenzene, a phenoxy substituent, or a phenolate anion?)

GR-1.5 Bonds with bends

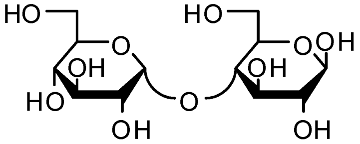
Bent bonds are used exclusively in two situations, both relating to the depiction of carbohydrates. They are used when representing the glycosidic linkage between two carbohydrates drawn as Haworth projections, where the individual carbohydrate rings must remain in the horizontal orientation required by the Haworth projections. Even in such cases, it is preferable to depict the glycosidic linkage using straight bonds, with the bonds angled slightly from the vertical orientation normally required by Haworth projections. It is acceptable to depict bent bonds in such cases, but they must be drawn as smooth curves. It is not acceptable to depict bent bonds with sharp corners, since such angular bends within bonds normally imply CH_2 groups, and will always present ambiguity between molecules with the normal glycosidic –O– linkage and similar analogs that truly do have a larger $–CH_2–O–CH_2–$ linkage instead.



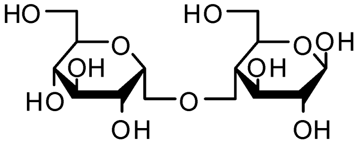
Preferred



Preferred

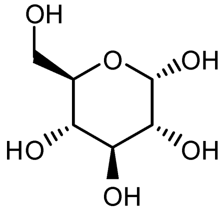


Acceptable



Not acceptable

Bent bonds are used also when depicting the cyclic form of carbohydrates in Fischer projections. As in Haworth projections, it is not acceptable to depict the connecting bond with sharp corners, since those corners could easily be interpreted as additional CH_2 groups.



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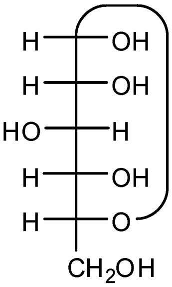
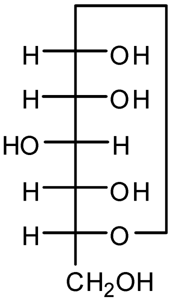
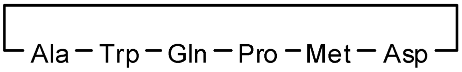


Preferred

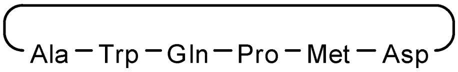


Not acceptable

Those concerns notwithstanding, bent bonds used to indicate closures in cyclic peptides and related molecules (GR-2.2.1) must be depicted with sharp corners, since the curved forms have rarely been used and will likely be confusing to a reader unfamiliar with them.



Preferred

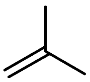


Not acceptable

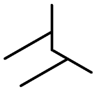
SOFTWARE CAUTION: At the time of writing of this document, the authors know of no computer software that is able to represent bonds with smooth curves. If chemical structure diagrams of polysaccharides are required for use within an electronic environment, the use of bent bonds may indeed be not acceptable in that case. However, since there are also few examples of computer software that can properly recognize Haworth projections in any circumstance, it is most preferred to use the flat Mills diagrams (as shown in the first Preferred carbohydrate examples above) in situations where polysaccharides must be interpreted by computer software.

GR-1.6 Multiple bonds

The individual segments comprising a double (or triple, quadruple, etc.) bond should be parallel and drawn in close proximity so that the segments are clearly associated with each other and do not form separate bonds or structural fragments. For practical purposes, separations greater than 33 % of the length of the bond should be avoided.



Preferred



Not acceptable

GR-1.7 Coordination bonds

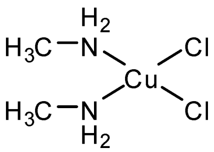
Historically, coordination bonds have been depicted in a variety of ways. Common usage now shows that such bonds are most often depicted as regular “plain” bonds. A dashed bond has also been seen, but less often.

With these recommendations, we suggest that coordination bonds be preferably represented as plain bonds. Dashed bonds are not acceptable because such bonds have been used to indicate stereochemical configurations rather than coordination.

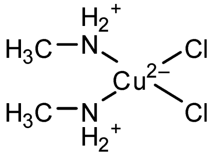
In chemical nomenclature, coordination bonds to single atoms are named using the kappa convention, while those to contiguous atoms are named using the eta convention [13].

GR-1.7.1 Coordination bonds to single atoms

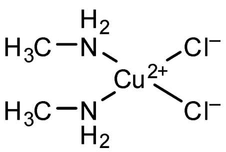
Bonds representing coordination from one atom to a single other atom should be represented as normal plain single bonds. Any hydrogen atoms bonded to the atoms at either end of such a coordination bond must be shown clearly, even if that produces a diagram where some atoms appear to have non-standard valences, such as a nitrogen atom with four attached bonds. It is not acceptable to add charges that depict formal zwitterions simply in an attempt to produce diagrams with standard valences, nor is it acceptable to depict coordination bonds by simple proximity between otherwise-unconnected fragments. The use of dative bonds to represent coordination is also not acceptable.



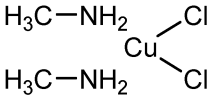
Preferred



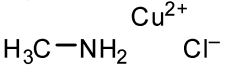
Not acceptable



Not acceptable



Not acceptable



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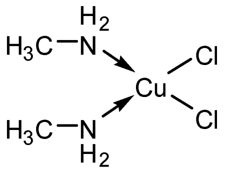
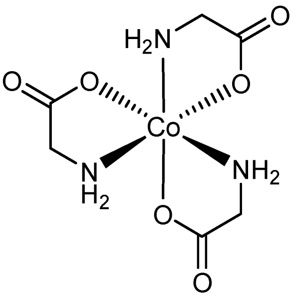


Not acceptable

SOFTWARE CAUTION: Some existing software may be unable to interpret properly coordination bonds drawn with single bonds and without charges, as recommended above. When creating chemical structure diagrams for use with such software, one of the otherwise "not acceptable" forms may in fact be the only way to produce a diagram that the software can understand. Authors who need to depict coordination bonds for use with chemical software programs should check the requirements of those programs before producing the diagrams.

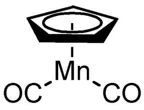
If a coordination bond is attached to an atom that does have a specified stereochemical configuration, then certainly a hashed or wedged bond depiction should be used instead, according to the other drawing conventions for representing configuration [6].



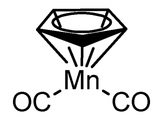
Preferred

GR-1.7.2 Coordination bonds to contiguous atoms

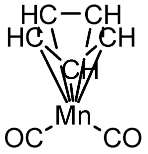
Coordination bonds to contiguous atoms (most commonly representing a form of π-bonding) should be drawn to indicate most clearly that special bonding pattern. Depictions that imply a regular covalent bond—and especially, depictions that show a regular covalent bond to *each* member of a delocalized system—are not acceptable.



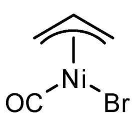
Preferred



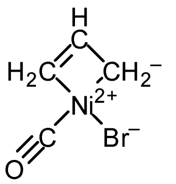
Not acceptable



Not acceptable

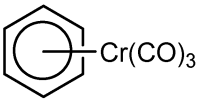


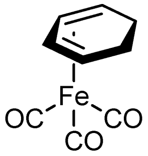
Preferred

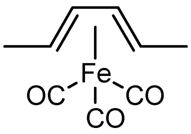


Not acceptable

When a coordination bond joins an atom to a contiguous system of three or more atoms, the contiguous system should be drawn using alternating single and double bonds only in those cases where it has only one such representation (as with buta-1,3-diene and related systems). Coordinated contiguous systems that can be represented by more than one pattern of single and double bonds should be depicted using curves to emphasize the coordination to the system, rather than with localized single and double bonds. This is true even if an uncoordinated analog of the same contiguous system normally would be represented with localized single and double bonds, as with the benzene system within tricarbonyl(η6-benzene)chromium. The use of curves in these molecules is consistent with the preference for using curves in systems that cannot be adequately represented by alternating single and double bonds (GR-6.5).


Preferred


Preferred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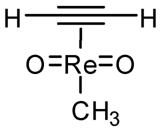
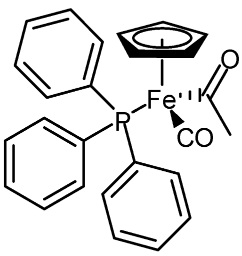
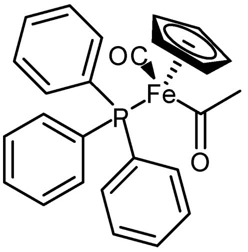
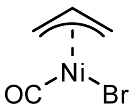

Preferred

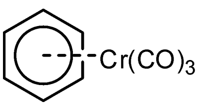
Bonds connecting to delocalized systems should most often be drawn as plain bonds. Solid wedged bonds and hashed wedged bonds might be appropriate when depicting the configuration of the atom on the non-contiguous end of the bond, although even in that case plain bonds would be preferred if it were possible to indicate the configuration using solid wedged bonds or hashed wedged bonds to other substituents.


Preferred


Acceptable

It is not acceptable to use dashed bonds to show bonding to a delocalized system.


Not acceptable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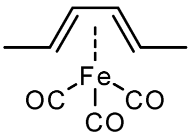
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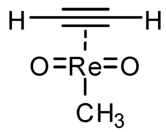
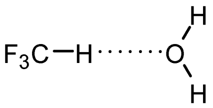

Not acceptable

SOFTWARE CAUTION: When working electronically, it is extremely important to specify a coordination bond appropriately, according to the capabilities of the software program you are using. If the coordination bond is specified inappropriately, the diagram may be interpreted as two disjoint fragments, with the coordination bond being interpreted as a normal bond to an unlabeled carbon atom. In addition to losing the intended delocalized character, this misinterpretation will also add an additional CH_3 to the structure's perceived formula for the "methyl group" at the center of the contiguous system.

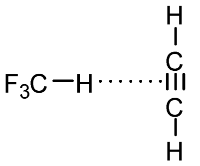
GR-1.8 Partial bonds

It is often useful to depict an association between atoms that is significantly weaker than a normal covalent, coordinating, or ionic bond. The most common type of "partial bond" is a hydrogen bond, which has been defined as "a form of association between an electronegative atom and a hydrogen atom attached to a second, relatively electronegative atom" [14]. The classical hydrogen bond is considered as an electrostatic interaction between polar groups $A^{\delta-}\text{–}H^{\delta+}$ and $B^{\delta-}$: $A^{\delta-}\text{–}H^{\delta+}\cdots B^{\delta-}$.

Partial bonds should be represented with dotted lines. As with all types of bonds, dotted bonds should be long enough to be clearly visible between two atom labels, and bonds that are less than twice as long as the height of an atom label should be avoided. Dotted bonds should always include at least three dots.



Preferred



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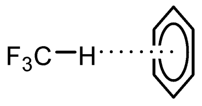
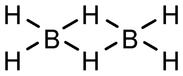


Preferred

SOFTWARE CAUTION: At the time of preparing this document, the authors are unaware of any computer software that can produce dotted bonds. In cases where it is not possible to produce true dotted bonds, it is acceptable to use dashed bonds instead.

GR-1.9 Multi-center bonds

From a molecular orbital perspective, it is possible to have bonding patterns where a pair of electrons is shared between more than two atoms. This sort of "multi-center" bonding is prevalent in the chemistry of boron compounds, for example, although it is seen in many other situations as well. As a matter of convention, any such multi-center character is ignored when producing chemical structure diagrams, and regular bonds connecting pairs of atoms are used instead.



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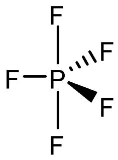
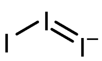


Preferred

In contrast with the depiction of coordination bonds (GR-1.7.2), curves should not be used when depicting multi-center bonds.

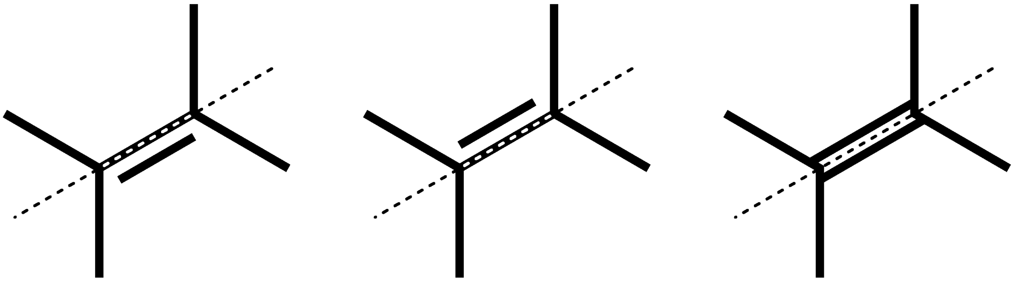


Preferred

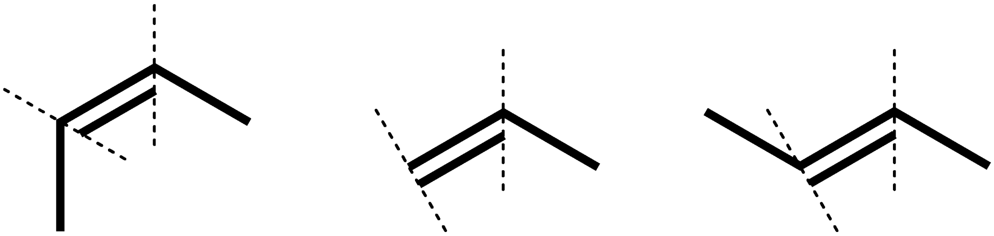
Not acceptable

GR-1.10 Sidedness of double bonds

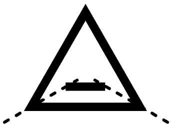
Double bonds traditionally appear in three orientations relative to the imaginary line connecting the centers of the atoms on either end of the bond. The double bond may be offset on either side of the center, or it may straddle the center exactly.

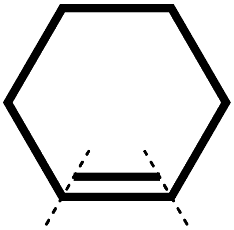


If the double bond is offset, one segment should be centered exactly, while the other one is offset. The segment of the double bond that is offset should usually be shortened at both ends. The amount of the shortening will depend on the spacing between the two segments and on the angles of the adjoining bonds. For best appearances, the endpoints of the second segment should be positioned so that they fall on the bisector of the angle between the double bond and its adjoining bond. If a bond is unsubstituted on one end, or if the only substitution on that end is *trans* relative to the second segment, then the segment should not be shortened on that end.

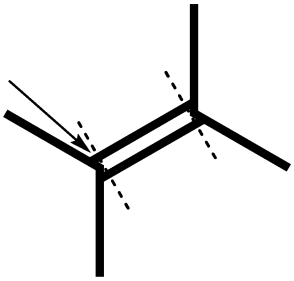


Because the amount of shortening is dependent on the adjacent angles, it is most pronounced in small rings.



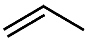


In contrast, centered double bonds should be extended to join seamlessly with the nearest adjacent bond on either end.



GR-1.10.1 Double bonds with asymmetric substitution

If a double bond has more substituents on one side than on the other, the double bond should be offset to that side.



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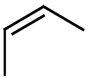

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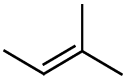
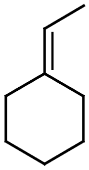


Preferred

In cases where the double bond has three substituents, and the two substituents on the same end of the double bond are identical or nearly so, it is reasonable for a double bond to be drawn in a centered configuration to emphasize the local symmetry. Since a centered double bond with a single substituent on an unlabeled carbon atom may look odd, this style should only be used when the side of the double bond with one substituent has an atom label.



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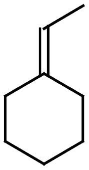
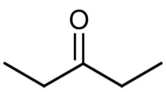


Preferred

GR-1.10.2 Double bonds with two substituents on one end, and no substituents on the other

Double bonds with two or more substituents on one end and no substituents on the other should be drawn with the two segments of the double bond centered relative to its atoms. Double bonds of this type are necessarily acyclic, and are most commonly found in carbonyl and acid functional groups.



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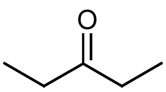
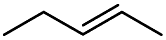


Preferred

GR-1.10.3 trans-*Double bonds with one substituent on each end*

Double bonds with one substituent on each end, and with those two substituents *trans* to each other, should be drawn with one segment offset. The directionality of the offset is not prescribed for chain bonds, and may be selected by the author according to the needs of the diagram. For *trans* bonds that are endocyclic, the double bond should be offset toward the center of the ring (bonds of this type are uncommon).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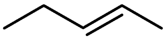
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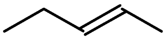
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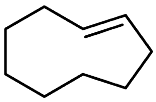
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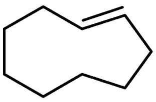
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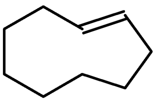
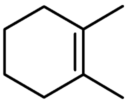

Not acceptable

GR-1.10.4 Double bonds with four substituents

Double bonds with two substituents on each end should normally be drawn with one segment offset. If one substituent on either end is a member of a ring, the double bond should be offset toward the center of that ring. If the double bond is a fusion bond between two rings, the bond should be offset in the direction of whichever ring has the greatest number of other double bonds. If both rings have the same number of double bonds, the double bond may be offset in either direction according to the preferences of the author.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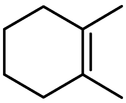
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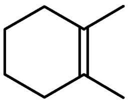
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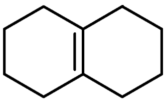
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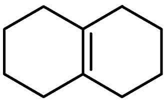
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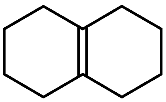
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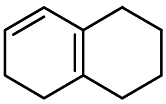
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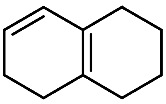
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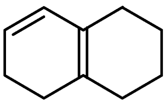
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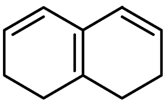
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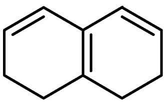
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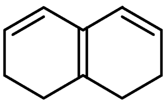
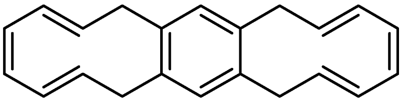

Not acceptable

In six-membered rings with alternating single and double bonds, it is especially preferred for the three double bonds to be offset so that they are all within the six-membered ring. That situation will usually follow as a direct consequence of offsetting the double bond toward the ring with the greatest number of other double bonds, but it would be preferable to offset the double bond toward the six-membered ring in all other cases as well.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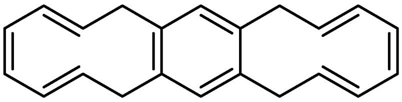
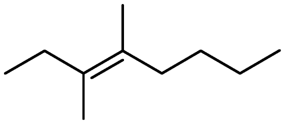

Not acceptable

Double bonds in acyclic systems may also be offset in either direction according to the needs of the author. It is also acceptable to draw a double bond with four substitutents in a centered configuration, but this style should be restricted to chain bonds where both substituents on one end are identical or nearly so.



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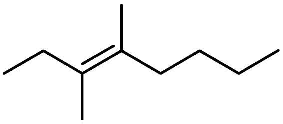

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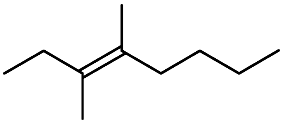

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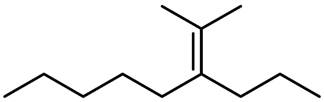

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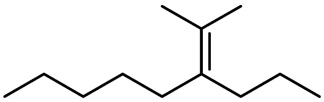

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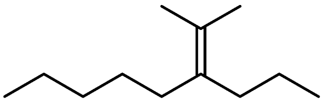


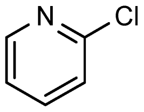
Acceptable

GR-2. ATOM LABELS AND OTHER CHEMICALLY SIGNIFICANT TEXT

Textual objects serve many roles in chemical structure diagrams, but are most frequently used to represent atoms via the atomic symbols of the elements or by abbreviations that imply one or more atoms in a specified bonding pattern.

GR-2.1 Elemental atom labels

Atom labels consisting of a single non-hydrogen element are the most universally understood type of chemical information after bonds themselves. Elements are indicated by their approved element symbols [13], using proper case (the first letter of a symbol is capitalized, and subsequent ones are lowercase).



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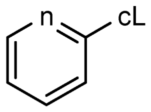
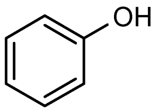


Not acceptable

GR-2.1.1 Hydrogen atoms

If hydrogen atoms are bound directly to a labeled atom, they may be indicated directly within the atom label. A single hydrogen atom is indicated by the letter "H" immediately after the other element symbol (or before the other element symbol, for atom labels attached to the left end of a bond). Multiple hydrogen atoms are further indicated by a subscripted number following the "H", indicating the total number of hydrogen atoms present. A labeled atom without "H" characters should be interpreted as having no hydrogen atoms attached. Such an atom might have been intended to represent a radical center or charged atom; however, it would be better to indicate the unpaired electron or charge explicitly in that case.



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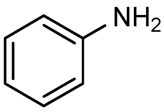

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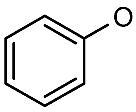
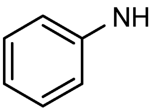
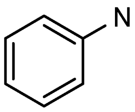


Wrong

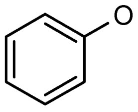


Wrong



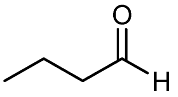
Wrong

Under no circumstances should a labeled atom without explicitly indicated hydrogen atoms be interpreted to indicate the presence of hydrogen atoms, even if those hydrogen atoms normally would be required to satisfy normal valence rules. Rather, such an atom may only represent an atypical valence state. On the other hand, wholly unlabeled atoms represent carbon atoms with the proper number of hydrogen atoms to satisfy a valence of four.

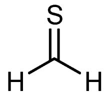


represents the PhO group
does not represent PhOH
does not represent PhO$^-$
does not represent PhO$^{\cdot}$

It is acceptable to depict hydrogen atoms separately, at the end of explicit bonds. This is especially common for aldehydes and related compounds. Explicit depiction of hydrogen atoms may also be necessary in situations where the bond to the hydrogen is of particular interest, including in some reaction mechanisms, but should be avoided in most cases.



Acceptable



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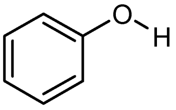

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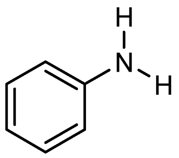
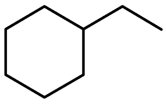


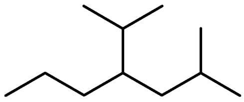
Acceptable

GR-2.1.2 Labeling of carbon atoms

Carbon atoms are traditionally left unlabeled when they are bonded to at least two other atoms: the presence of the carbon atom is implied by the “bend” in the bonds.



Preferred



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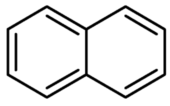
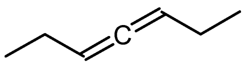


Preferred

On the other hand, any carbon atom with two identical collinear bonds should always be explicitly labeled, to remove the possibility of the two bonds being misinterpreted as one long bond.



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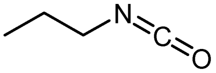
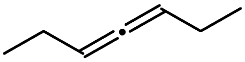


Preferred

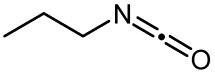
O=C=O

Preferred

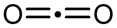
The use of a dot in place of an explicit carbon atom label is acceptable in allenes and related molecules with three consecutive carbon atoms. It is not acceptable to use a dot to represent a carbon atom when either of its adjacent atoms is other than a carbon atom.



Acceptable

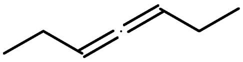


Not acceptable

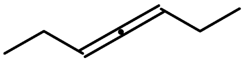


Not acceptable

When a dot is used to represent a carbon atom, it must be depicted clearly and unambiguously. The dot should be large enough to be clearly seen by the reader, and must be visibly separated from the adjacent bonds.



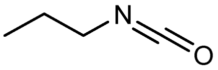
Not acceptable



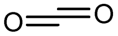
Not acceptable

It is not acceptable to indicate the presence of a carbon atom simply by depicting its two double bonds "on opposite sides".

Not acceptable



Not acceptable



Not acceptable

A carbon atom with no explicit bonds must always be labeled, lest it be overlooked as a stray ink smudge.

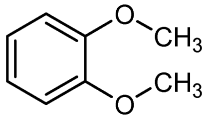
CH_4

Preferred

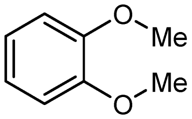
·

Not acceptable

Carbon atoms attached to exactly one bond to a non-carbon atom may or may not be labeled; the labels "CH_3" and "Me" may both be used, although it is not acceptable to use both "CH_3" and "Me" labels within the same diagram. As discussed in GR-2.1.1, it is wrong to label a terminal carbon atom with the letter "C" when a methyl group is intended.



Preferred



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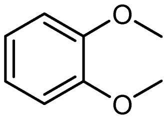
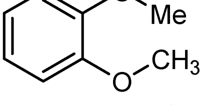
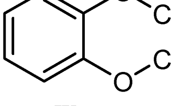


Acceptable

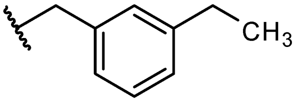


Not acceptable

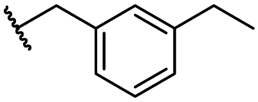


Wrong

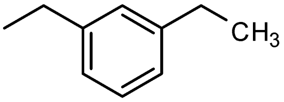
Terminal carbon atoms should preferably also be labeled in diagrams that represent a portion of a larger structure, to eliminate any possible misinterpretation that the diagram should be attached at the unlabeled terminal carbon atom rather than at its intended connection location.



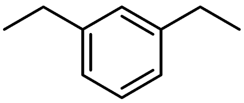
Preferred



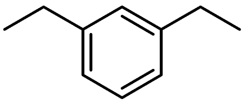
Acceptable



Not acceptable

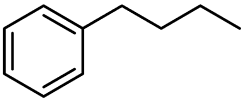


Preferred
[when representing
1,3-diethylbenzene]

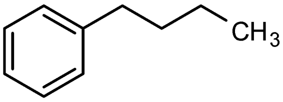


Wrong
[when representing
a 2-(3-ethylphenyl)ethyl substituent]

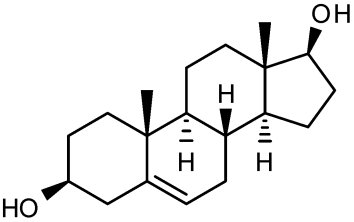
It is acceptable to add labels for terminal carbon atoms connected to unlabeled carbon atoms, but only when it is possible to do so without overlapping other portions of the diagram.



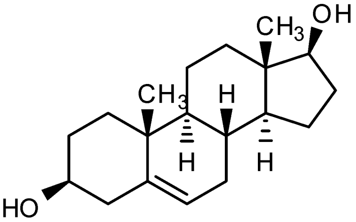
Preferred



Acceptable



Preferred



Not acceptable

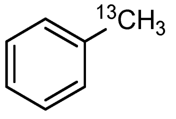
When ethane, ethene, ethyne, and related molecules are drawn with only one explicit bond, both terminal carbon atoms must be labeled explicitly to prevent the molecule from being interpreted as a stray line or set of lines.

H_3C-CH_3
Preferred

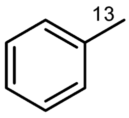
Not acceptable

GR-2.1.3 Isotopes

Isotopic substitution is indicated by a superscripted mass number appearing directly to the left of an element symbol (it is not possible to represent an isotope of an otherwise unlabeled carbon atom). The mass number should indicate the isotope's total mass, and should not indicate its deviation from the element's nominal mass at natural abundance.

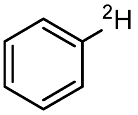


Preferred

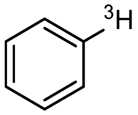


Not acceptable

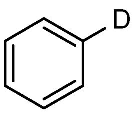
The hydrogen isotope of mass 2 may also be indicated by the symbol “D”. The hydrogen isotope of mass 3 may also be indicated by the symbol “T”. However, the symbols “D” and “T” should preferably not be used in diagrams that also include isotopes of elements other than hydrogen.



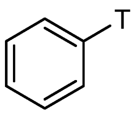
Preferred



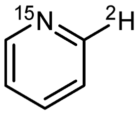
Preferred



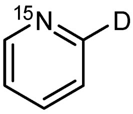
Acceptable



Acceptable

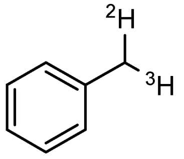


Preferred

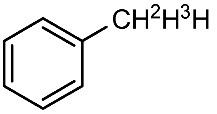


Not acceptable

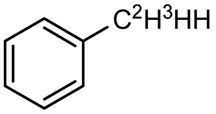
The creation of atom labels containing multiple isotopes of one element should preferably be avoided, but if such a label cannot be avoided, atoms in natural abundance should be listed first, followed by other atoms in increasing isotopic mass number. If an atom label contains both deuterium and tritium, the notation style for those isotopes should be used consistently.



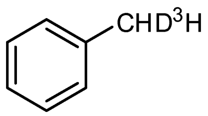
Preferred



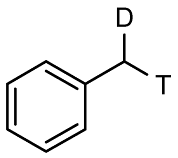
Acceptable



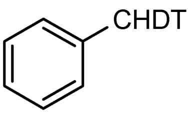
Not acceptable



Not acceptable



Acceptable



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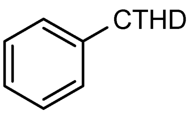
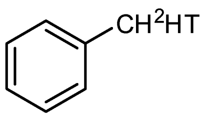
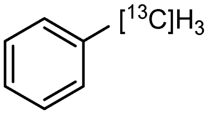


Not acceptable



Not acceptable

Isotopic labeling (partial rather than complete replacement of the atom by its isotope) is indicated similarly, but the isotopically labeled atom should additionally be enclosed in square brackets. Note that only the single element symbol should be so enclosed; if there are other elements (including hydrogen atoms) described in the atom label, they should be located outside the brackets.



Preferred

GR-2.1.4 Oxidation numbers

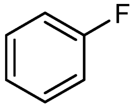
When required, oxidation numbers should be indicated by a superscripted roman numeral (or arabic zero) immediately following the atomic symbol. Oxidation numbers should preferably be omitted when the oxidation state is clearly indicated by the remainder of the structure, which is usually the case in diagrams that are fully specified with explicit bonds.

Pb	Pb^0	$O=Pb=O$	$O=Pb^{IV}=O$
Preferred	*Acceptable*	*Preferred*	*Acceptable*

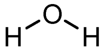
GR-2.1.5 Positioning of atom labels

Atom labels should be positioned so that all bonds connecting to the atom label point directly at the element symbol of the atom to which they are bonded. The bonds should approach the label closely, but should not impinge on the actual characters.

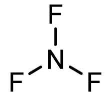
For single-character atom labels, the bonds should point to the center of the character.



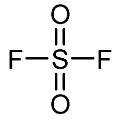
Preferred



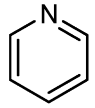
Preferred



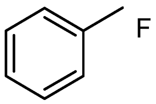
Preferred



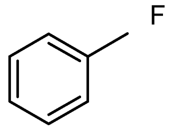
Preferred



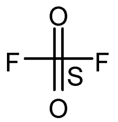
Preferred



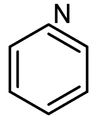
Not acceptable



Not acceptable

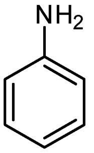


Not acceptable

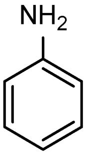


Not acceptable

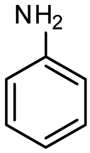
For multiple-character atom labels, the bonds should usually point to the center of the first letter (or to the center of the last letter for atom labels attached to the left end of a bond).



Preferred

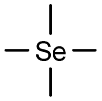


Not acceptable

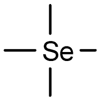


Not acceptable

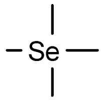
When the bonding pattern is highly symmetric, the bonds to multiple-character atom labels should instead point to the center of the entire symbol.



Preferred

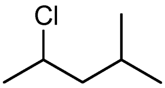


Acceptable

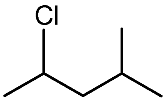


Not acceptable

In all cases, not only should the bonds point to the center of a letter or entire element symbol, but the label should be positioned with that center coincident with the location where the bond would have ended if the atom was not labeled. As a result, the visible portion of a bond to a labeled atom will be shorter in the diagram than the visible portion of a similar bond to an unlabeled atom.



Preferred



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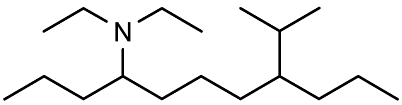
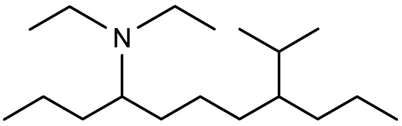


Preferred

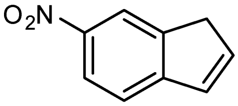


Not acceptable

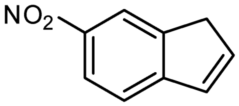
GR-2.1.6 Orientation of atom labels

Atom labels should be oriented so that they avoid congestion with other portions of the structure. When the atom label consists of only a single character, this is not an issue as there are no further issues of alignment to consider. When the atom label contains several characters and there are no bonds to the right of the label, the atom label should start with the symbol of the bonded atom located at the end of a bond and the rest of the label extending to the right as shown in several of the examples above. However, when the atom label contains several characters and there *are* bonds to the right, aesthetic positioning is more difficult. It is quite possible for an atom label to be longer than its associated bonds. Atom labels should never be positioned so that they obscure a bond completely.

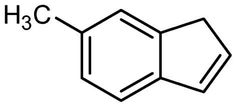
If an atom label with more than one element symbol or abbreviation has bonds to its right but does not have any bonds to its left, the atom label should be reversed.



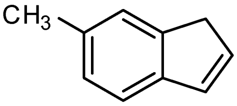
Preferred



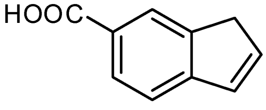
Not acceptable



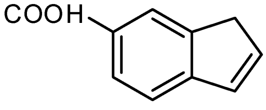
Preferred



Not acceptable

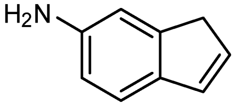


Preferred



Not acceptable

In reversed labels, the symbol representing the atom connected to the bond should still be positioned so that the bond points to its center; however, any subsequent symbols proceed to the left of the first element, rather than to its right. Repeat counts remain to the right of the symbol to which they apply, as do charges, and unpaired electrons (see GR-5).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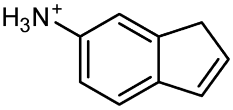
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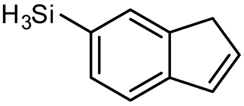
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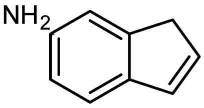
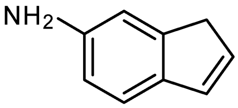
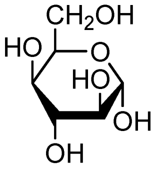
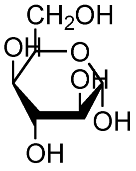

Not acceptable


Not acceptable

An atom label that does not have a bond to its right should preferably also be reversed if doing so will eliminate overlap with other portions of the diagram.


Preferred


Not acceptable

For structures drawn in the linear drawing style (GR-13), a bond on the right side of an atom label will always point to the rightmost character in that label, even if the physical bond is attached to an atom whose symbol appears earlier. This is acceptable when using that drawing style, although use of that style should be avoided in general as discussed elsewhere.

$$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$$

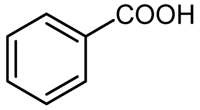
Acceptable (for linear drawings)

GR-2.1.7 Multi-line atom labels

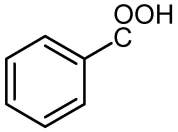
Atom labels with bonds both to the right and to the left may stack vertically. As above, the symbol of the bonded atom should remain positioned so that the bonds point to its center. The additional characters in the label may then be positioned on a second line either above or below the first symbol, according to whichever location has more room. Any charges, unpaired electrons, isotope mass numbers, subscripted repeat counts, etc., should remain on the same line as the associated element symbol.

The positioning and orientation of multiline atom labels is determined primarily by the orientation of bonds connected to that atom. The bond order of the bond(s) in question does not affect this determination.

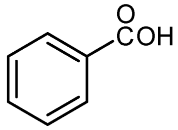
Multi-line labels on atoms with fewer than two attached bonds are not acceptable.



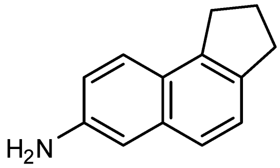
Preferred



Not acceptable



Not acceptable



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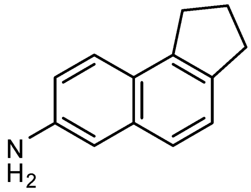
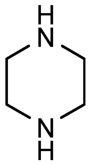


Not acceptable

On atoms with two attached bonds, an atom label should be oriented to minimize its overlap with any bonds in the structure. The label may be stacked vertically above or below, or may not be stacked at all depending on the orientation of the two bonds.



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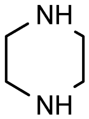
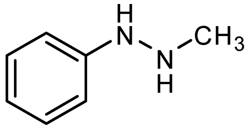
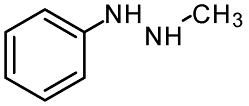


Not acceptable

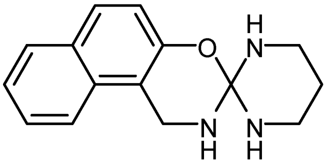


Preferred

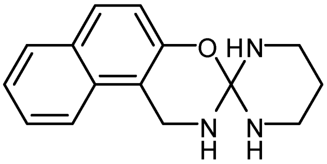


Not acceptable

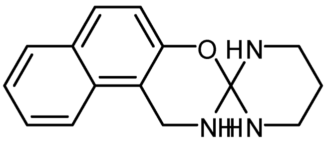
In some cases, the label of one atom might overlap with another atom or bond that is not directly connected to the first atom. Atom labels should be oriented to minimize overlap with all other objects (including atoms, bonds, charges, annotations, etc.), even those not connected directly.



Preferred

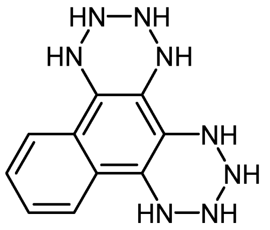


Acceptable

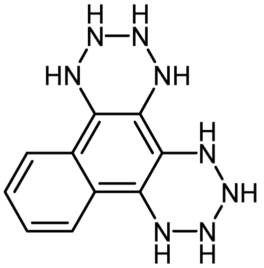


Not acceptable

When overlap can be equally avoided both by multi- and single-line atom labels, the single-line labels are preferred.

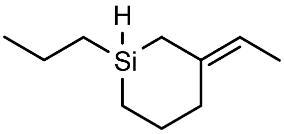


Preferred

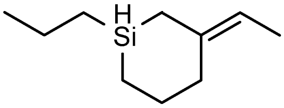


Acceptable

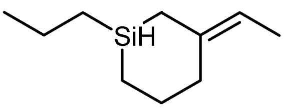
On atoms with three connected bonds where one of the connected bonds is oriented vertically, overlap can usually be minimized by positioning the atom label on two lines, stacked opposite to the orientation of the vertical bond. A single-line orientation is also acceptable as long as there is little resulting overlap.



Preferred

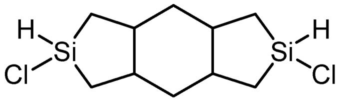


Acceptable



Acceptable

When an atom with three attached bonds has one of the attached bonds oriented horizontally, the smallest overlap is generally obtained by a single-line atom label oriented in the opposite horizontal direction.



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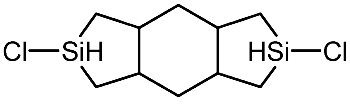
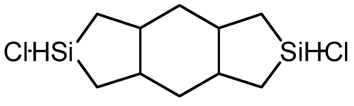
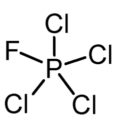


Acceptable

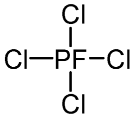


Not acceptable

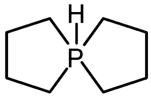
Atom labels containing more than one non-hydrogen element symbol are not acceptable when that atom has more than three other bonds. Atom labels containing a non-hydrogen symbol and one or more hydrogen symbols (or charges or unpaired electrons) may be positioned on multiple lines in any way that minimizes overlap.



Preferred



Not acceptable



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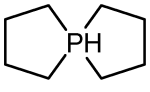
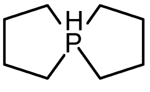


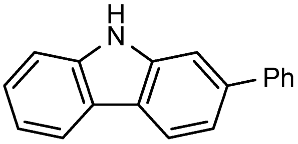
Acceptable



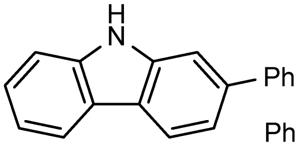
Acceptable

GR-2.2 Structural abbreviations

In addition to element symbols, atom labels may contain substituent abbreviations. The abbreviations shown in Table II may be used freely. Further definition is unnecessary.



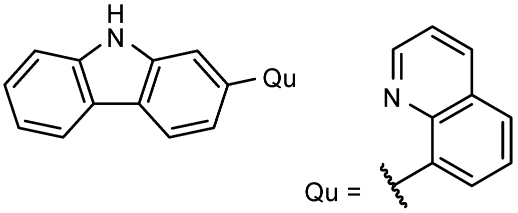
Preferred



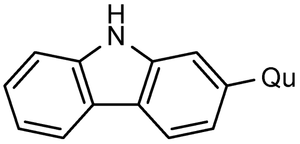
Ph = phenyl

Acceptable

Other abbreviations may be used if they are accompanied by a clear explanation of what structural fragment they are intended to represent.



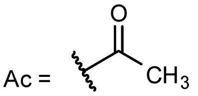
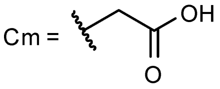
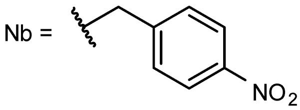
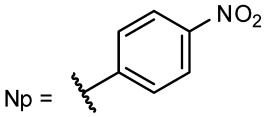
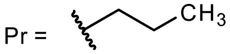
Acceptable



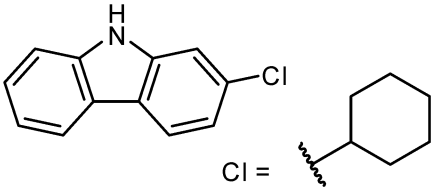
Not acceptable

Several structural abbreviations in current usage, as shown below, are identical to an element symbol. The use of these and any similar abbreviations should be restricted to situations where they are unlikely to be mistaken for the element symbols. Since these abbreviations conflict only with relatively uncommon metals, they are fairly safe to use in strictly organic contexts.

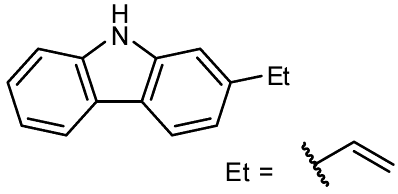
Table GR-2.2 Structural abbreviations that can be mistaken for elements.

Abbreviation	Element name	Abbreviation full name	Meaning as abbreviation
Ac	Actinium	**Ac**etyl	
Cm	Curium	**C**arboxy**m**ethyl	
Nb	Niobium	*p*-**N**itro**b**enzyl	
Np	Neptunium	*p*-**N**itro**p**henyl	
Pr	Praseodymium	**Pr**opyl	

Other than the abbreviations listed in Table GR-2.2, it is not acceptable to create new abbreviations with the same text as element symbols, even if those abbreviations are defined. Similarly, it is not acceptable to create new abbreviations with the same text (but different meaning) as other abbreviations in common use (see Table II).

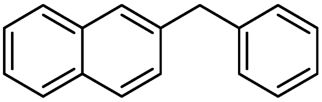


Not acceptable

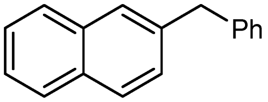


Not acceptable

The abbreviation Bz has historically been used for both benzyl and benzoyl moieties, and it has been the subject of contradictory definitions even in earlier IUPAC recommendations [13,15]. Because of that historical disagreement over the meaning of Bz, the use of alternative representations is preferred.



Preferred



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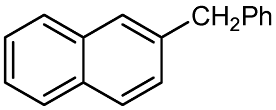

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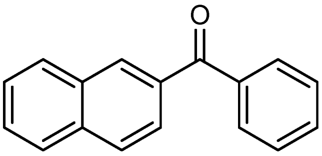

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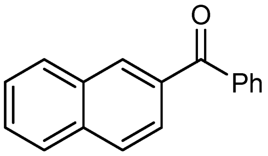
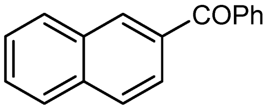


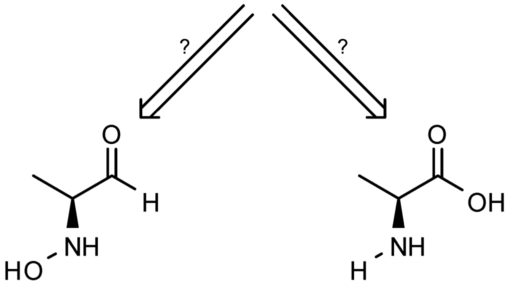
Preferred



Preferred

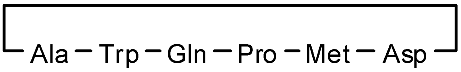
GR-2.2.1 Three-letter amino acid abbreviations

Three-letter amino acid abbreviations—and other abbreviations with two or more distinct points of attachment—should also be used with care, because the nickname itself gives no indication of the intended attachment order:

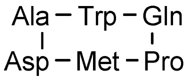


Abbreviations with two or more attachments will generally have a preferred orientation. In the case of individual amino acids as above, the N-terminus is always on the left by convention, and the C-terminus is always on the right [16]. Unfortunately, just because a convention exists does not guarantee that the reader—or the computer—will know and understand it.

Special care is needed when there might be a possibility of interpreting an abbreviation of this sort from the "wrong direction", such as in the depiction of cyclic peptides. If a cyclic peptide is written on two lines as in the diagram below and to the right, interpreting the cyclic peptide "clockwise" requires that the Pro-Met-Asp segment be interpreted from right to left. Similarly, interpreting the cyclic peptide "counterclockwise" requires that Gln-Trp-Ala segment be interpreted from right to left. If all of the abbreviations are rigorously interpreted with their N-termini on the left, the diagram could also be interpreted as intending an unusual head-to-head and tail-to-tail coupling of the two three-peptide segments that are individually depicted horizontally. Ambiguity is inevitable with diagrams of that sort, and therefore they should be avoided. When possible, cyclic peptides should preferably be depicted in a single line, with the cycle closed by plain bonds (GR-1.5). Such problems are general to any asymmetric abbreviation and not limited to amino acids. Other issues specific to amino acids and peptides are discussed in a separate document [16].



Preferred



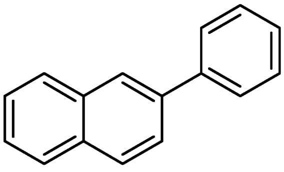
Not acceptable

SOFTWARE CAUTION: At the time of writing of this document, few software programs are able to interpret bent bonds at all, and the authors know of no computer software that is able to fully interpret complex cyclic peptides as depicted above. If chemical structure diagrams of cyclic peptides are required for use within an electronic environment, the use of bent bonds may indeed be not acceptable in that case, and an alternative diagram may be required that avoids the use of abbreviations with two or more attachments.

GR-2.2.2 Single-letter abbreviations

There are many other sets of abbreviations that are used with specific molecule classes. In particular, the use of single-character abbreviations can be extremely confusing. Surely, nobody would interpret BENZENE as anything other than C_6H_6, but it *could* be Asx-Glu-Asn-Glx-Glu-Asn-Glu according to the one-letter system of amino acid nomenclature [16]. The use of single-character abbreviations should be limited to contexts where their intended meaning is clear.

It is acceptable to use the Greek lowercase letter phi (ϕ) to represent a phenyl group. That abbreviation has a long history, and ambiguity is unlikely since that letter is rarely used for other purposes in chemical structure diagrams.



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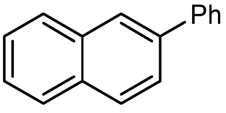

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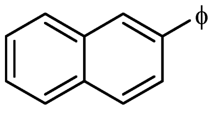
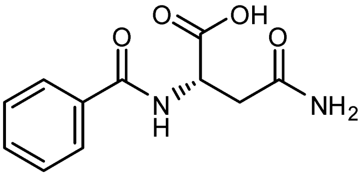
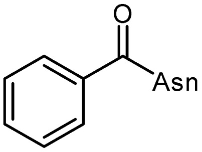


Acceptable

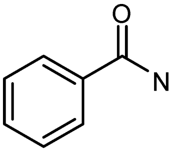
The use of Latin alphabet single-character abbreviations in conjunction with other structural features (atoms and bonds) is not acceptable; abbreviations of this type are best restricted to running text. If it is absolutely necessary to mix abbreviations with other structural features, abbreviations with more than one letter should be used instead. The use of the italic letter P is an exception that should not be used outside the scope of biochemical structure diagrams (see GR-0.3).



Preferred



Acceptable



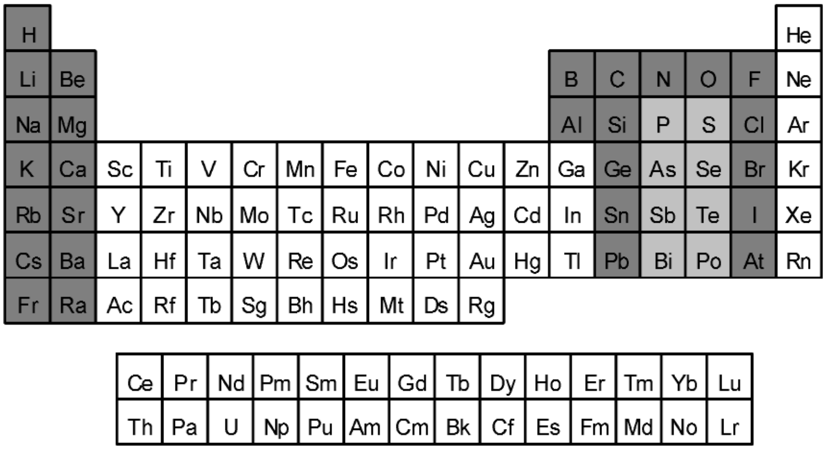
Not acceptable
[N is the single-letter abbreviation for Asn]

GR-2.3 Atom labels representing more than one non-hydrogen atom

When clarity is critical and space is not a concern, fully expanded structures (showing an explicit bond between every pair of non-hydrogen atoms) are always preferable to structures showing more complex atom labels. However, space often *is* a concern, particularly when preparing structures for publication. The following recommendations should provide some guidelines for producing complex atom labels that are likely to be understood correctly in most circumstances.

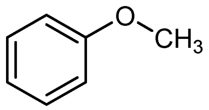
GR-2.3.1 General guidelines

Atom labels representing more than one non-hydrogen atom—also sometimes known as “contracted” labels—rely on the fact that many elements have consistent and well-understood bonding patterns. The elements shown with a dark gray background below are fairly safe to use in contracted labels, with a few exceptions as will be discussed. The elements shown with a light gray background are less safe, as they all have common forms with several different valence states. The remaining uncolored elements have highly variable bonding patterns and should not be used in contracted labels, but always drawn with explicit bonds.



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Tb	Sg	Bh	Hs	Mt	Ds	Rg							

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr



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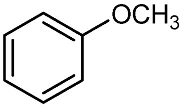

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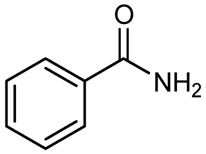

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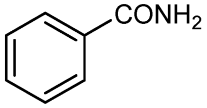

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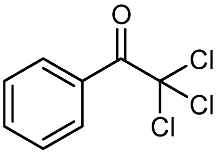

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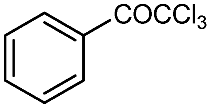

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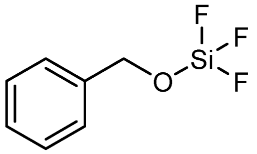

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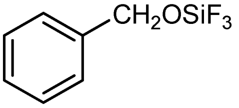
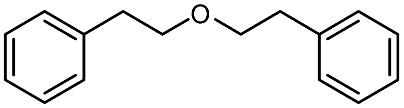


Preferred

GR-2.3.2 Contracted labels with more than one explicit bond

Contracted atom labels may have at most two bonds, one extending horizontally from each of the first and last characters in the label. Such labels should be read from left to right, with the first element connected to the leftmost bond and the last element connected to the rightmost bond.



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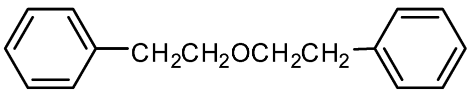
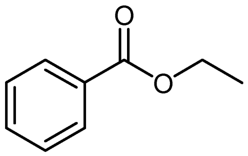


Acceptable

It is not acceptable to create contracted labels with more than one bond attached to the first (or last) element within the label, or to create contracted labels with bonds connected to an interior element within the label.



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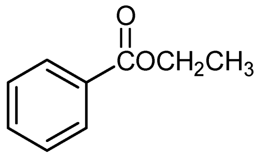
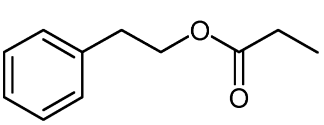
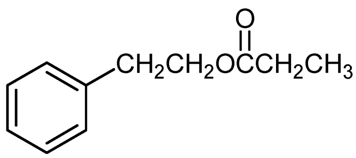


Not acceptable



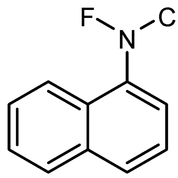
Preferred



Not acceptable

GR-2.3.3 Orientation of symbols within contracted labels

Contracted atom labels attached to only one bond should be read outwards from that bond, usually from left to right if the bond is on the left of the label. If the bond is instead attached to the right of the label, the label will normally be read from right to left, but ambiguities can result. Accordingly, contracted labels with a bond on the right should be avoided except for simple cases, usually limited to relatively small labels containing four or fewer combined element symbols and abbreviations. Contracted labels with a single bond attached to an interior atom or with multiple connecting bonds should always be read from left to right, but these also are prone to ambiguity and should similarly be avoided except for simple cases.



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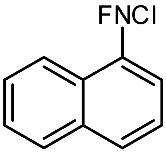

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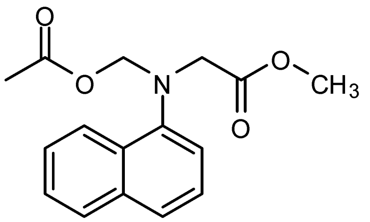

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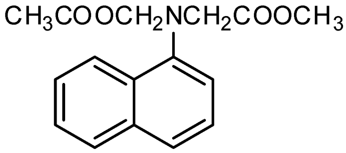
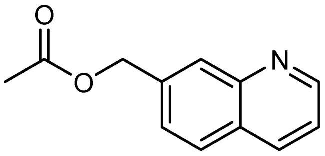


Not acceptable

Relatively long labels with bonds to the rightmost character should be avoided, since their interpretation can be extremely difficult. The following two cases demonstrate this problem. Although the labels appear superficially very similar, the first must be interpreted from left to right, and would represent an acetoxymethyl substituent, while the second must be interpreted from right to left, and would represent a methyl ester of a carboxylic acid. (The use of parentheses to indicate branching explicitly, as discussed in GR-2.3.5, can be used to reduce some of the potential for ambiguity.)



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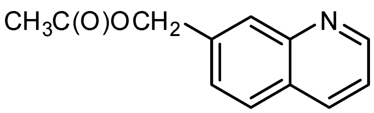

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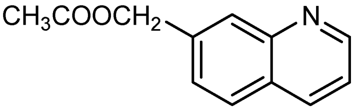
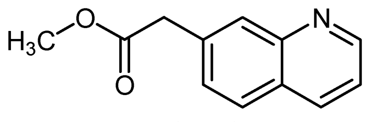


Not acceptable



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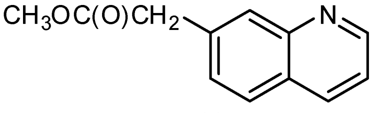

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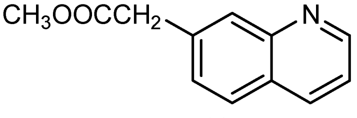
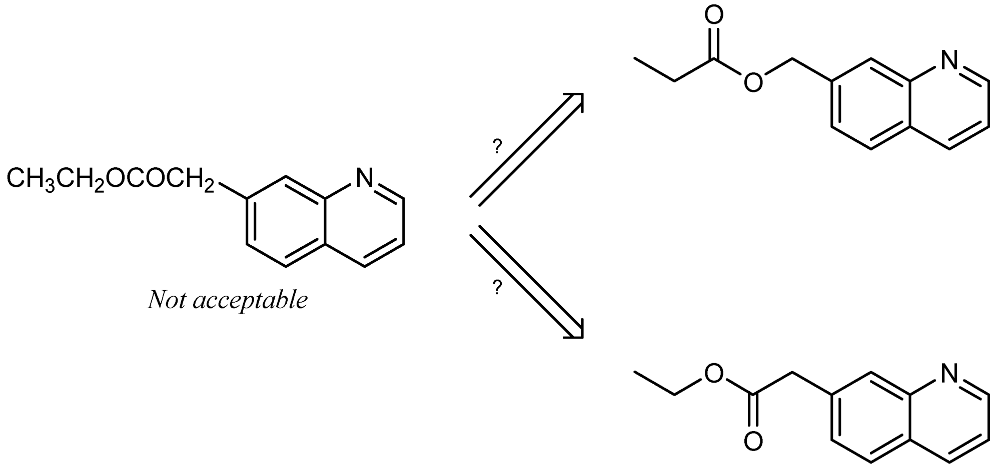
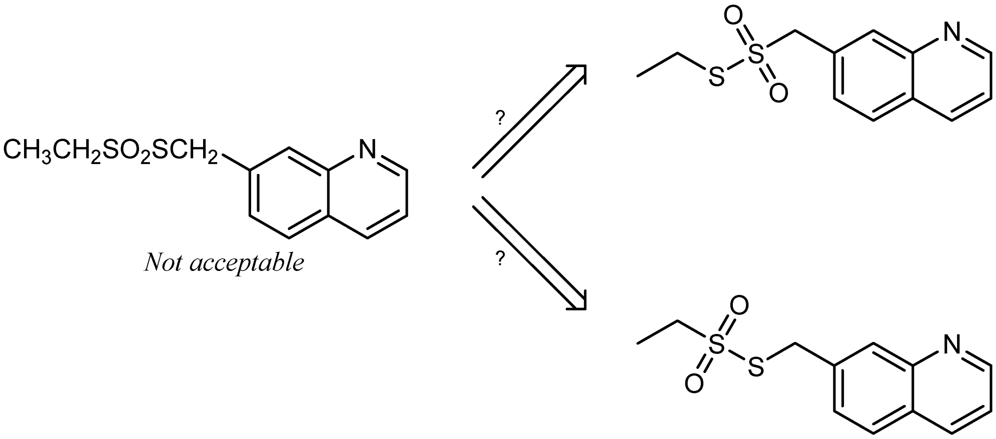


Not acceptable

In extreme cases, a single label could represent different structural fragments depending on whether it was interpreted from right to left or from left to right.



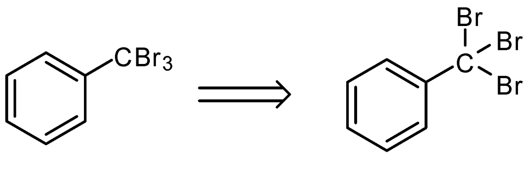
Not acceptable



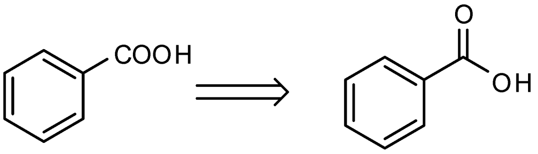
Not acceptable

GR-2.3.4 Interpretation of contracted labels

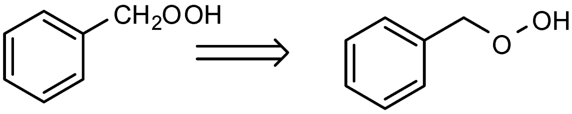
In general, contracted labels are interpreted to fill as many valences as possible, as quickly as possible. Consider a simple case such as shown. A carbon atom is the first atom in the label, and it is connected to a single bond, so it has three remaining open valences. The next atom in the label is bromine, and is repeated three times. Bromine has one open valence, so together the three bromine atoms fill the three open valences on the carbon atom. There are no more atoms, and no open valences, so this label has been interpreted completely. This is a very simple case.



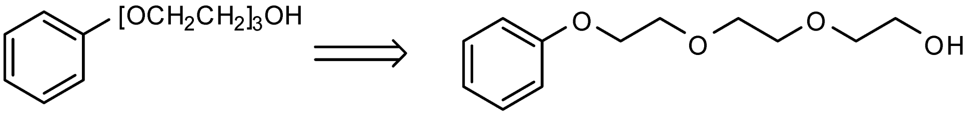
The common carboxylic acid group provides a more complex example. Again, the first carbon atom has three remaining valences. In this case, the next atom is oxygen, which has two available valences, and both of those are used to form a double bond with the carbon atom, leaving the carbon atom with one remaining valence. The third element is another oxygen, but this time only one of its valences is used to create a single bond to the carbon atom. That fills all of the available valences for the carbon atom, but leaves one remaining valence on the oxygen atom, which is in turn filled by the fourth atom, a hydrogen atom.



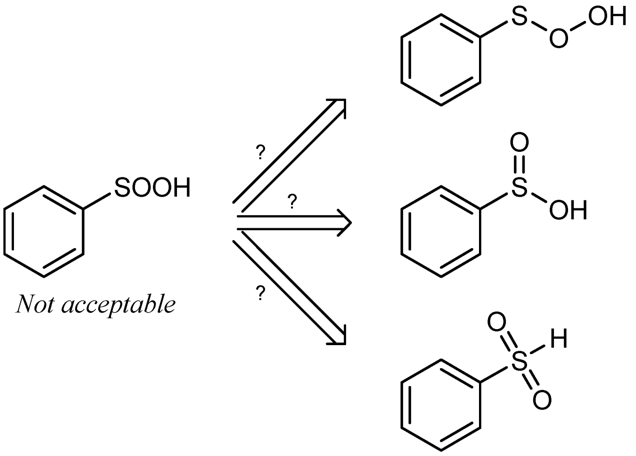
In the similar case of a peroxide, two valences on the first carbon atom are filled immediately by two hydrogen atoms. With only one valence remaining on the carbon atom, the first oxygen atom has no option but to chain with the second, forming a very different bonding pattern from that of the carboxylic acid.



Divalent structural fragments may be enclosed in brackets and followed by a repeat count to represent repeating fragments concisely.

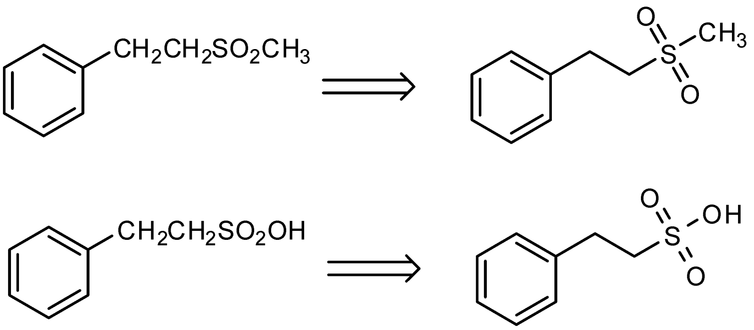


As discussed above, a valence-based interpretation of atom labels will be successful only for elements with predictable bonding patterns. Some elements, including sulfur, commonly exist in a variety of valences. Contracted labels containing these elements should be avoided, particularly when those element symbols are immediately followed by multiple chalcogen or halogen symbols.

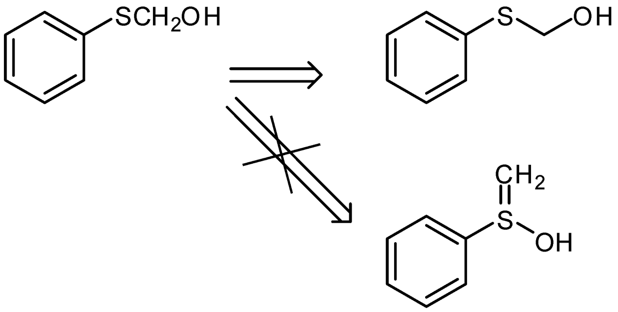


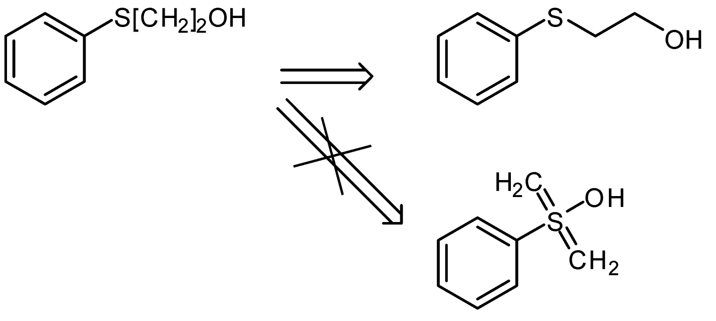
Not acceptable

When used as part of a larger label, the textual fragments SO_2, SeO_2, and TeO_2 should be used only to represent sulfones, selenones, and tellurones, respectively, and should never be used to represent the linear isomers or any other branching form.

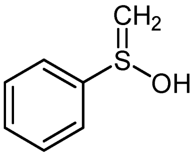


Even in the presence of other atoms with variable valence, the CH_2 fragment should always be interpreted as a chaining moiety, even when followed by a repeat count. Structures containing branching methylidene fragments should be drawn with explicit atoms and bonds.





CH_2 fragments intended to represent branches should always be indicated with a leading equals sign and enclosed in parentheses as discussed in GR-2.3.5.



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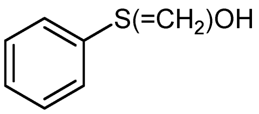
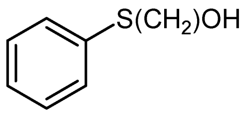
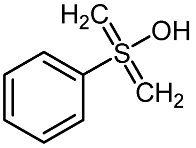


Acceptable



Not acceptable



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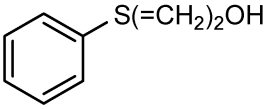
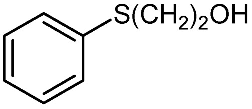
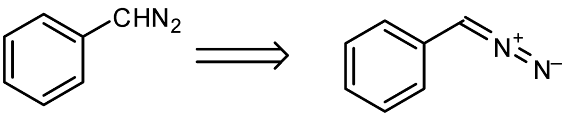


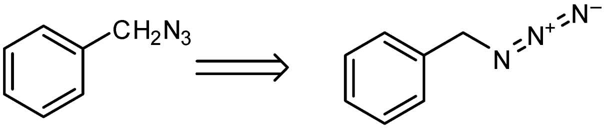
Acceptable

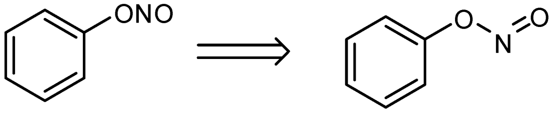


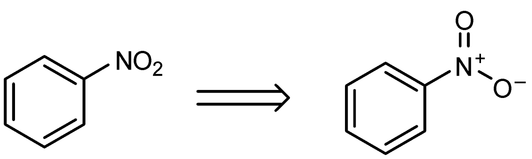
Not acceptable

Some very common contracted labels cannot be interpreted with a simple application of valence rules, but also need some implicit charges to be added. A larger list of these labels is shown in Table III.



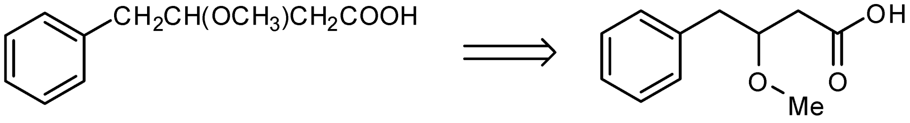




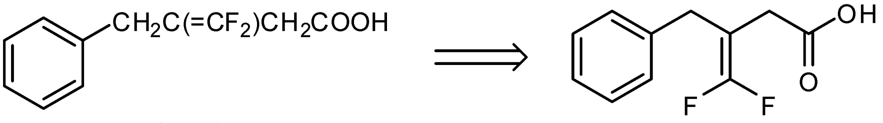


GR-2.3.5 Branching

Simple branching patterns may be implied by the basic valence rules described above, and do not require special notation. More complex branching may be clarified by placing parentheses around all elements within a branch. One valence for the first element within the parentheses is used for connecting the previous atom outside the parentheses; subsequent atoms within the parenthesized section are then bound to the first or subsequent atoms, even if an atom outside the parentheses has remaining open valences.



Branching chains where the branch is connected to the main chain by a double bond should be indicated by placing an equals sign immediately within the opening parenthesis. If desired, such labels can often be rewritten to avoid the necessity for the equals sign by swapping the text within the parentheses with the text after.



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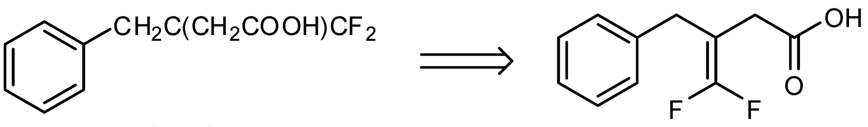
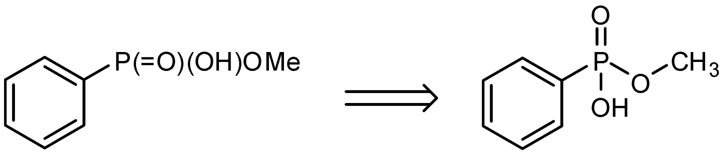


Preferred

When the only element within the parentheses is a single oxygen, sulfur, selenium, or tellurium symbol, the equals sign may be omitted



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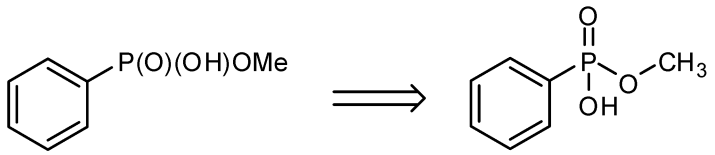
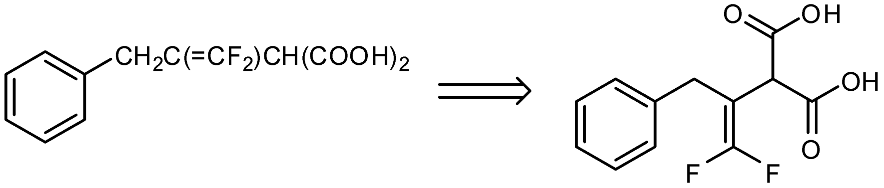


Preferred

Parentheses may be nested, but highly complex labels of this type can be extremely difficult to understand, and should be avoided.



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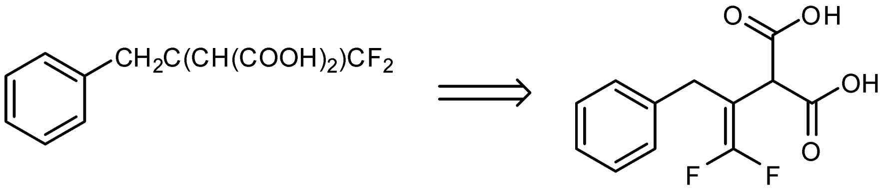


Not acceptable

GR-2.3.6 Explicit single bonds

Explicit single bonds are generally not necessary within atom labels and should be avoided. They should be strongly avoided in contexts where they might be mistaken for negative charges. In cases where explicit single bonds are desired for clarity, it would likely be even clearer to draw the structure out fully, rather than trying to denote the single bonds inline using text.

$—CH_2CH_2CH_3$
Preferred

$—CH_2—CH_2—CH_3$
Acceptable

$—CH_2CH_2COO^-$
Preferred

$—CH_2—CH_2—COO^-$
Acceptable

GR-2.3.7 Structural abbreviations

Abbreviations that contain a single attachment point may be freely used in contracted atom labels. To avoid any possible misinterpretation about whether such abbreviations truly do contain only a single attachment point, they should always appear furthest from the explicit bond within a label or within a parenthesized portion of a label.

$—CPh_3$
Preferred

$Ph_3C—$
Preferred

$—CH_2CH_2CHClPh$
Preferred

$—CH_2CH_2CH(Ph)CH_2CH_3$
Preferred

$—CH_2CH_2CHPhCH_2CH_3$
Not acceptable

GR-2.3.8 Ordering of multiple symbols attached to the same atom

If a single atom is bound to both hydrogen atoms and non-hydrogen atoms, any hydrogen atoms should be presented adjacent to the first atom, followed by the others, reading outward from the bond.

$—\mathrm{CHPh_2}$	$—\mathrm{CPh_2H}$	$\mathrm{Cl_2HC}—$	$\mathrm{HCl_2C}—$
Preferred	*Not acceptable*	*Preferred*	*Not acceptable*

If more than one single-element symbol or abbreviation is attached to the same non-hydrogen atom, the element symbols should be presented first in alphabetical order (after any hydrogen symbols), followed by the abbreviations in alphabetical order, reading outward from the bond.

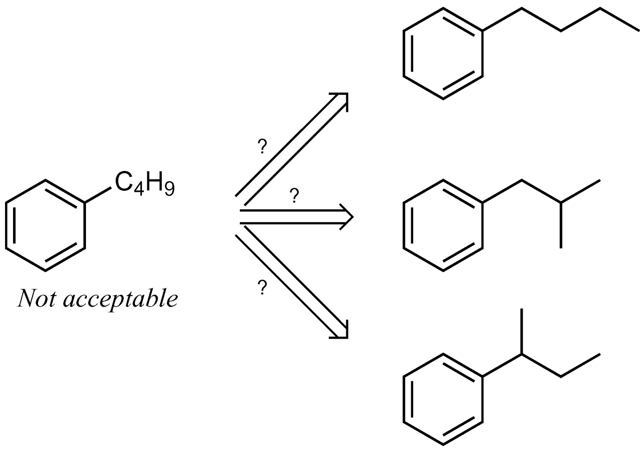
$—\mathrm{CBrClF}$	$—\mathrm{CHBrCl}$	$—\mathrm{CFBu_2}$	$\mathrm{FCl_2C}—$	$\mathrm{Ac_2HC}—$
Preferred	*Preferred*	*Preferred*	*Preferred*	*Preferred*

Fragments containing multiple symbols should appear only after all hydrogen symbols, single-element symbols, and abbreviations, since that arrangement will often avoid the use of parentheses.

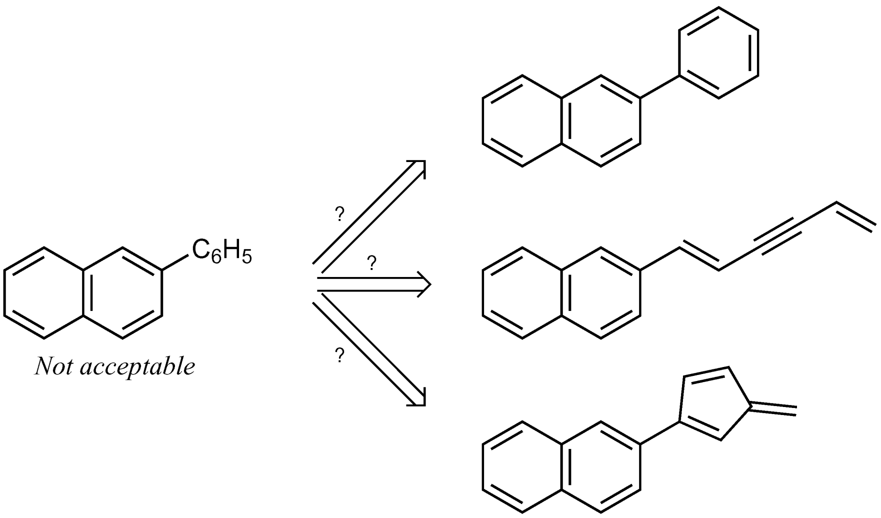
$—\mathrm{CHClCH_2CH_3}$	$—\mathrm{CH(CH_2CH_3)Cl}$
Preferred	*Not acceptable*

GR-2.3.9 Atom labels without explicit connectivity

Atom labels are inherently ambiguous when written as simple counts of elements. The reader cannot know whether one specific isomer was intended, or whether the diagram indicates that the exact isomer truly was not known. Such labels are not acceptable; either the atoms and bonds should be drawn explicitly, or one of the alternative atom label styles discussed above should be used instead.



Not acceptable



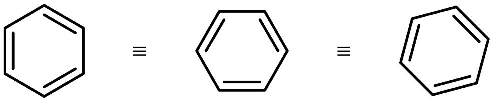
Not acceptable

GR-2.4 Formulas

Formulas may be considered as atom labels not connected to any bonds. They may be preferred to structural diagrams for simple molecules such as NaCl and MeOH. Formulas should always be interpreted from left to right, but otherwise observe restrictions similar to other kinds of atom labels. For organic molecules with more than one carbon atom, structure diagrams with explicit atoms and bonds are preferred over formulas. Guidelines for producing and using formulas of inorganic molecules are presented in ref. [13].

GR-3. ORIENTATION OF STRUCTURES

When considering the guidelines to follow for the orientation of chemical structures, perhaps the most important thing to keep in mind is that, as far as chemical meaning is concerned, *they do not matter*. With a single exception in the case of Fischer projections [17,18], simple rotation of a chemical structure within the plane of the diagram will never affect its chemical meaning. Flipping a portion of a structure requires a corresponding adjustment of stereobonds (solid wedged bonds must be changed to hashed wedged bonds, etc.), but changes nothing otherwise. In terms of chemical meaning, the orientation of structures is irrelevant.



On the other hand, practicing chemists generally have an idea of the orientations they expect. This is especially true for various classes of biological molecules, and particularly for those with multiple stereogenic centers, but it is an issue for all structures to some extent. Although benzene could be drawn in any orientation (as shown at right, above), most chemists would expect to see it with “points up and down” or possibly with “points left and right” (left and center structures above, respectively). So, selecting a reasonable orientation for chemical structures serves only to present chemical information in a way that is most convenient and least surprising to other chemists. That is still important, for sure, but nowhere near as important as making sure that the chemical structure itself is as accurate as possible, whatever its orientation.

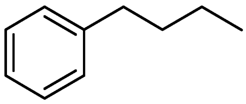
Selection of a reasonable orientation is an art form even more so than other aspects of structure representation. It is therefore worth emphasizing, again, that these guidelines are only *guidelines*. They are provided so that an author who wants to "follow the rules" has some rules to follow. They are not expected to be comprehensive for all possible chemical structures, and they are certainly not intended to be definitive. If you have a structure that you think looks better if these guidelines are not followed, then by all means draw it in the way that looks best to you. There is absolutely no problem with that.

It should also be considered that the recommendations that follow are for the depiction of chemical structure diagrams *in isolation*. That is, as discussed in GR-0.1, they are for use when answering the question, "What is the chemical structure of X?" When depicting relationships between molecules, it is entirely appropriate to modify the orientation of the individual diagrams so that they accurately describe whatever relationships are being depicted. In an extreme example, ligands participating within an inorganic complex must certainly be oriented to demonstrate their role within that complex, regardless of their preferred orientation in unbound form. Similarly, reaction diagrams will often be arranged to emphasize the movement of electrons during the reaction [19]. To accomplish that, the individual reaction components may be depicted in orientations that are far from what would be preferred in isolation. When chemical structure diagrams are used in larger contexts, the diagrams may need to be modified appropriately.

GR-3.1 General guidelines for orientation of structures

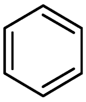
GR-3.1.1 Structures should be oriented horizontally

In general, structures should be oriented so that their main axis is horizontal.



Preferred

However, this guideline is intended for structures whose longest axis is significantly longer than their shortest axis. In cases where the longest and shortest axes of a structure are more nearly the same size, it is common for the structure to have a preferred vertical orientation. These cases will be discussed further in subsequent sections.



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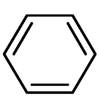

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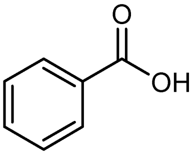

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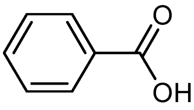

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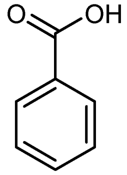
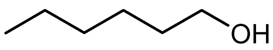


Acceptable

GR-3.1.2 Principal groups should be toward the right

Chemical structure diagrams should be oriented so that any principal groups, if present, are positioned toward the right side of the structure. In a perfect application of this guideline, principal groups would be identified using the comprehensive hierarchical guidelines provided in other IUPAC recommendations [20]. For most practical purposes, it is sufficient to treat "principal groups" and "acyclic heteroatoms" as synonymous. Thus, this rule could be oversimplified to say that any acyclic heteroatoms should be oriented toward the right side of the structure.

Since systematic numbering starts nearest the principal group(s), this guideline also implies that structures should be oriented so that systematic numbering increases from right to left within the structure.



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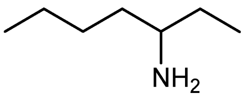

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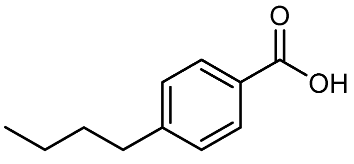
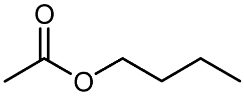


Preferred

However, organic esters should be oriented so that the parent acid points toward the right, even if the ester principal group is positioned toward the overall left of the diagram.



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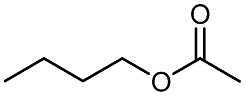

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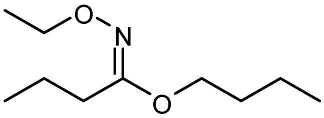

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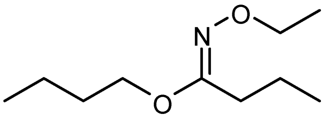
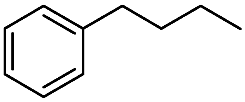


Acceptable

GR-3.1.3 Rings should be toward the bottom-left

In the absence of a different overriding concern, the principal ring system (see GR-4.2.1) within a structure should be oriented toward the bottom-left of the structure.



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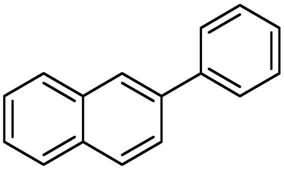


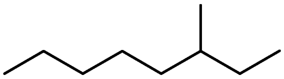
Preferred

GR-3.2 Orientation of chains

There are two main styles for depicting acyclic structures and fragments, the “chain” (or “zigzag”) form, and the “linear” form. Since it is possible to use the linear form only for relatively simple structures, the chain form is more generally useful. The linear form, however, remains acceptable for any structure to which it is suited. Most issues that apply to the chain form would also apply to the linear form. Other issues specific to the linear form are discussed in GR-13.

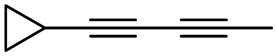
GR-3.2.1 Structures should be oriented horizontally

As stated in the general overview, all structures should be oriented horizontally when possible. This is always possible for the main chain in an acyclic structure.



Preferred

When orienting a chain horizontally, care should be taken to consider the chain as a whole. In many cases, a horizontal chain implies that the chain's first bond be oriented 30° from horizontal, but the recommendation is for the chain itself to be horizontal, even if that means that the individual bonds within the chain are not aligned at multiples of 30°.



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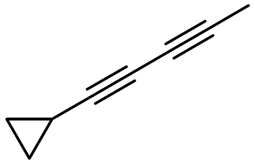

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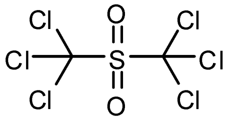

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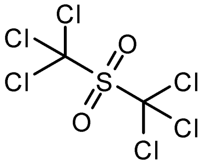

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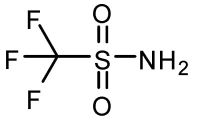

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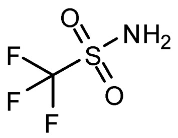
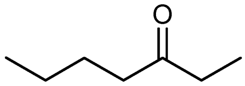


Acceptable

GR-3.2.2 Branching double bonds should be upwards

A doubly bonded substituent that branches from a horizontal chain should preferentially be positioned above the chain rather than below it, even if that requires a change in the "zigzag direction" of the chain. This is most commonly seen in ketones, carboxylic acids, and related molecules.



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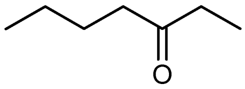

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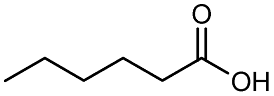

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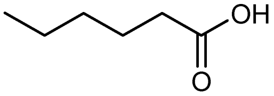


Acceptable

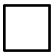
GR-3.3 Depiction of rings

Unlike chains, which typically have two possible conformations at every non-terminal atom, rings have fewer degrees of freedom. It is especially important to depict rings correctly, since readers will often have firm expectations of how a ring should appear.

GR-3.3.1 Simple rings with eight or fewer ring atoms

Isolated rings that do not share any atoms with other rings should be depicted as regular polygons if they contain eight or fewer atoms within the ring.


Preferred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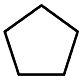
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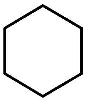
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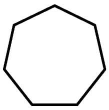
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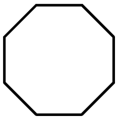
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Not acceptable


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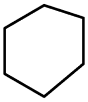
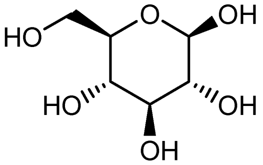

Not acceptable

As discussed in the recommendations for graphical representation of stereochemical configuration [6], Haworth projections are also preferred, although only for the depiction of carbohydrates and structurally related molecules. Similarly, other sorts of perspective diagrams are preferred when discussing conformation (since there is no other reasonable way to depict boat and chair forms, etc.) and acceptable when it is desired to emphasize configuration.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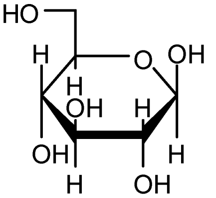
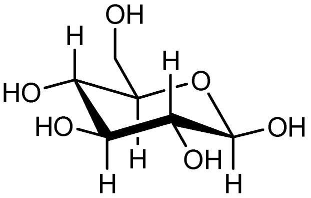

Preferred
(in Haworth diagrams)


Preferred
(when discussing conformation)

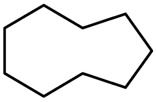
GR-3.3.2 Simple rings with nine or more ring atoms

Isolated rings with at least nine atoms within the ring should be drawn with reentrant bond angles ("puckered"), as tracing the boundary of a properly depicted fused ring system (see GR-3.3.3).

One goal of depiction of these large rings is to preserve standard bond lengths and angles as much as possible. Ideally, every pair of standard-length bonds should be separated by 120°, but that is not even theoretically possible for rings with an odd number of atoms. If it is not possible to preserve 120° angles, it is acceptable to use other angles that are present in regular pentagons (108°), heptagons (approximately 129°), and octagons (135°).

Some examples are shown, for rings with 9 through 14 atoms. Note that there will often be more than one reasonable conformation as the rings get larger. For each ring size, the first diagram shows the preferred conformation for rings without any restrictions, such as the unsubstituted C_nH_{2n} cycloalkanes. In the presence of substituents or double bonds within the ring, it may be necessary to select one of the other conformations to avoid overlap or to preserve double-bond configuration.

9 atoms: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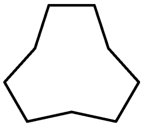
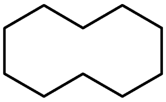

Acceptable

10 atoms: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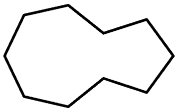
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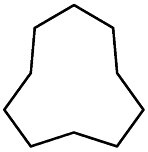
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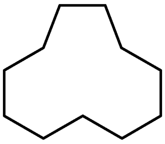
11 atoms: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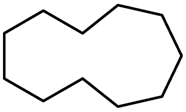
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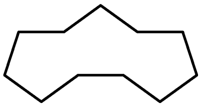
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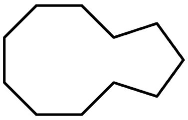
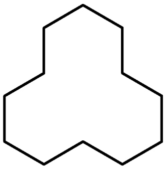

Acceptable

12 atoms: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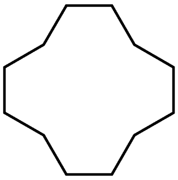
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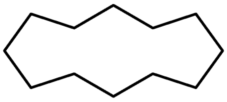
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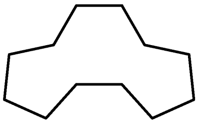
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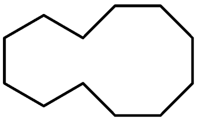
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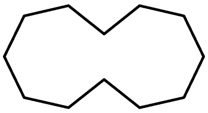
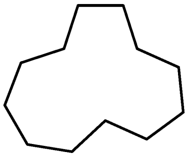
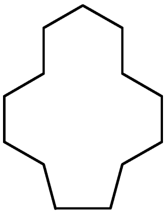
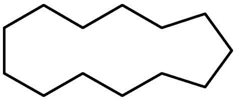

Acceptable


Acceptable

13 atoms:


Preferred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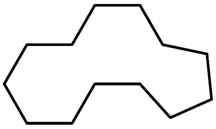
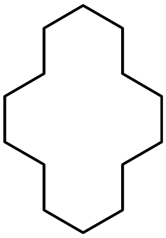

Acceptable

14 atoms:



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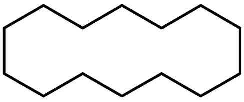

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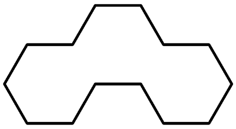

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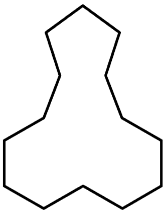
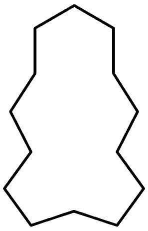


Acceptable



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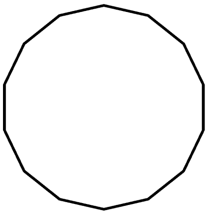
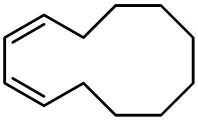


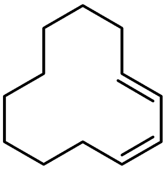
Not acceptable

Many factors need to be considered and balanced when choosing which conformation to use when depicting any given large ring. The conformations described as preferred in the Table immediately above are not necessarily preferred for molecules other than the specific unadorned cycloalkanes depicted.

The single most important factor to consider when selecting a conformation is the configuration of any double bonds within the ring. Each double bond must be depicted in the correct stereochemical configuration without exception.

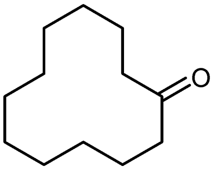


Preferred
[representing (1Z,3Z)-cyclododecadiene]



Wrong
[representing (1Z,3Z)-cyclododecadiene]

The positioning of substituents on a large ring should also be considered, although the positioning of substituents is less important than the preservation of double-bond stereochemistry and the positioning of fused rings. While it is preferable to have as many substituent atoms outside the ring as possible, it is acceptable to have some substituents inside the ring if they can be positioned without distortion or overlap.



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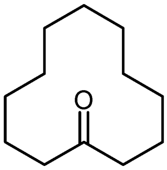

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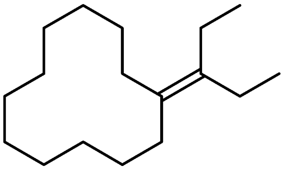

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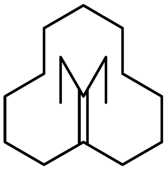

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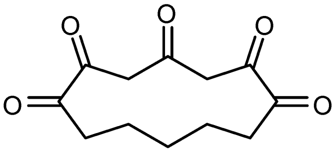

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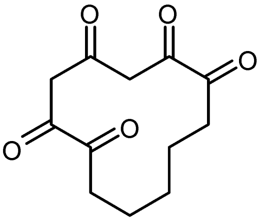

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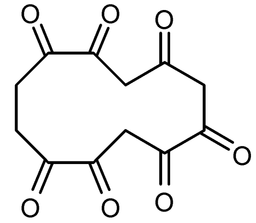

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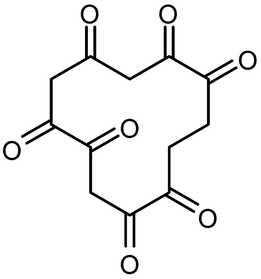
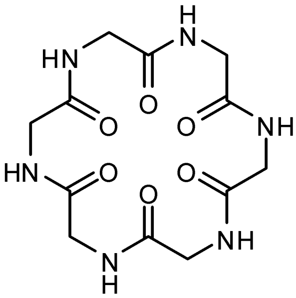


Acceptable

It is entirely possible to have more than one reasonable conformation of a large ring, one with more substituents inside and one with fewer. The pair of diagrams shown might be used to illustrate different modes where the macrocycle might form a complex with an ion via the nitrogen atoms in the ring or via the oxygen atoms.



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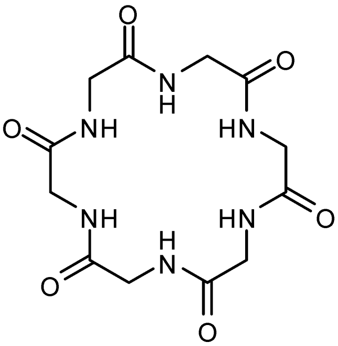
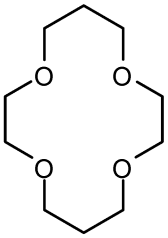


Preferred

Finally, in the absence of other constraints, large rings that contain unsubstituted heteroatoms should be depicted with those heteroatoms at the "inward-facing" locations. In addition to producing diagrams of large rings in conformations that are appropriate when describing inorganic complexes, this approach often will also emphasize the overall symmetry of the ring system.



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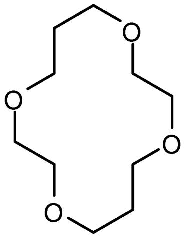

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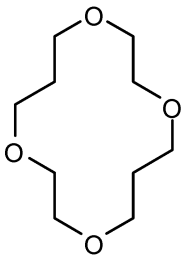
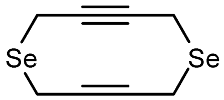


Acceptable

Large rings that contain triple bonds should depict the triple bonds in a linear fashion, just as they would be depicted in an acyclic diagram.



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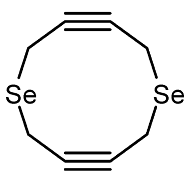

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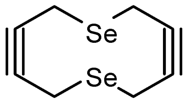

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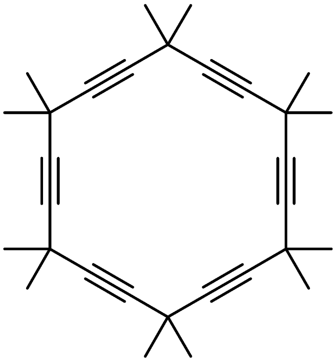

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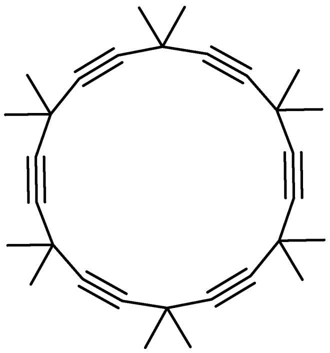
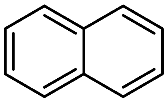


Not acceptable

GR-3.3.3 Fused rings

Simple fused ring systems where no atom is a member of more than two individual rings (*ortho*-fused but not *peri*-fused) should be depicted as a series of rings that are each depicted as described in GR-3.3.1 and GR-3.3.2, with the various rings abutting each other at a shared bond. All of the atoms of one ring should be placed outside of the other ring.

For aesthetic reasons, these guidelines occasionally differ from the guidelines provided in the "Nomenclature of fused and bridged fused ring systems" [21]. The orientation instructions within that document are intended for use only while determining the numbering of atoms within a fused or bridged fused ring system. The guidelines presented here should be used when depicting that ring system after its atoms have been numbered.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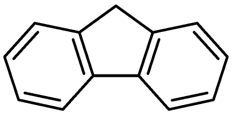
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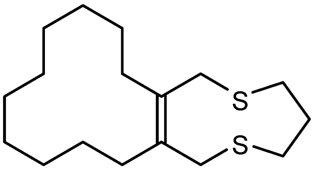

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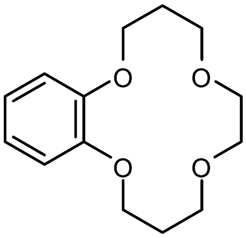

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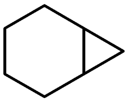
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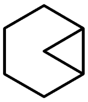
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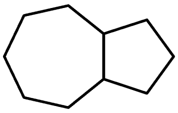
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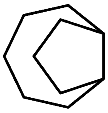
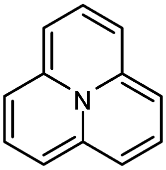

Not acceptable

When three six-membered rings are fused so that each pair shares a bond and they all share one common atom, it is also possible to abut the rings without distortion.



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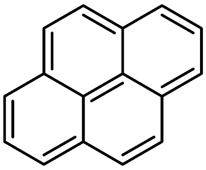
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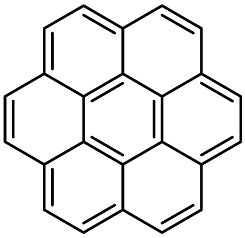
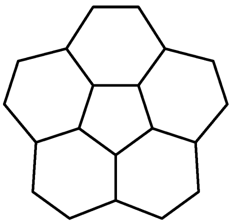

Preferred

Three-way fusions involving rings of other than six atoms will generally require distortion of one or more of the ring systems. When the ring system is symmetric, distortions that preserve the symmetry are preferred to those that break it. Otherwise, it is preferable to leave as many six-membered rings undistorted as possible.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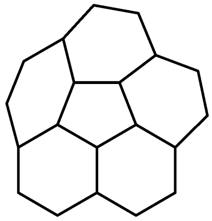
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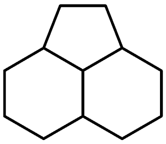
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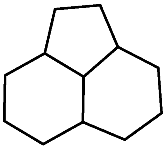
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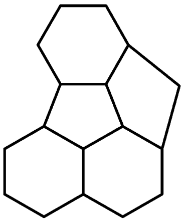
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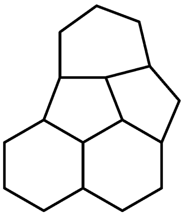
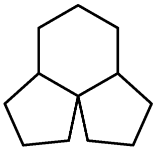

Not acceptable

Particular care should be taken when depicting molecules that have atoms with exactly two fusion bonds. When several of the associated rings have five or fewer atoms, it is generally possible to produce a legible structure while using regular polygons for each ring.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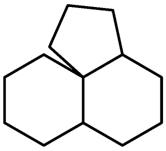
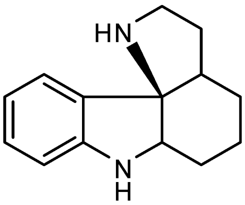

Preferred

In some cases, particularly in the presence of heteroatoms or other substituents on adjacent atoms, the use of regular hexagons will lead to unavoidable overlap. One or more of the rings must be distorted in order to remove the overlap. Five-membered rings offer a particularly facile distorted form where they may be drawn as a "truncated hexagon" with three 120° angles, two 90° angles, and one very long bond. However, even that style will not always succeed in removing overlap. When all three rings have six members, significant distortion will always be necessary to produce a passably legible structure diagram.



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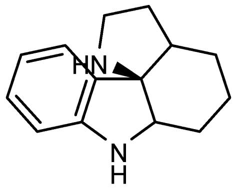

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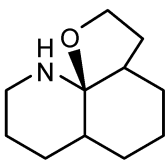

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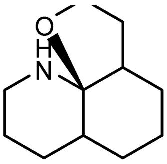

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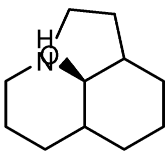
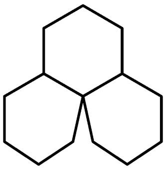


Not acceptable



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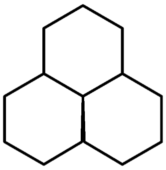
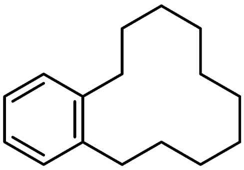


Not acceptable
[when representing the molecule at left]

The shape of a large ring that is part of a fused ring system may be influenced by other components of that system, requiring a shape or orientation for the larger ring that would not be preferred if it was not fused (see GR-3.3.2). Rings that share a single fusion bond should preferably be arranged so that the fusion bond is in a "*cis*-like" configuration relative to the larger ring. This is especially important in situations where the combination of ring sizes involved in the fusion would result in bonds that exactly overlap if the larger ring were in a "*trans*-like" configuration.



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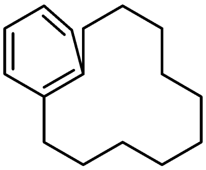

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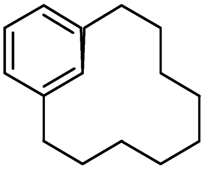
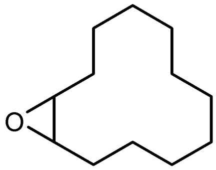


Not acceptable
[representing the molecule at left]



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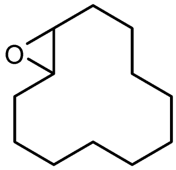
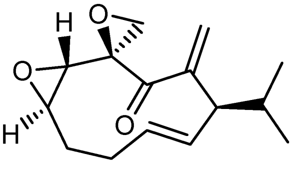


Not acceptable

In some cases, the most legible depiction of a fused ring system may even require the positioning of some substituents within the larger ring.

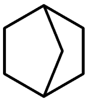


Preferred

GR-3.3.4 Bridged rings

The depictions of bridged ring systems may be viewed as being composed of two parts: a simple ring or fused ring system, and one or more bridges that connect atoms in that simple ring or fused ring system. Viewed in this fashion, the simple ring or fused ring system should be drawn according to the recommendations for those systems, with the bridges then positioned so that they best avoid overlap and preserve legibility. For any bridged ring system, there is always more than one way to select the single/fused rings and the remaining bridges. When possible, it is preferred to select the simpler systems so as to maximize the number of undistorted six-membered rings.

As discussed in GR-3.3.3, the guidelines discussed here should be followed when producing aesthetic depictions and are not necessarily the same as those that must be followed when determining systematic names [22].



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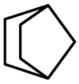

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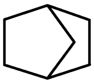

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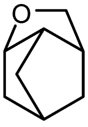

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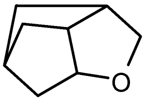

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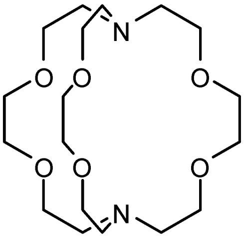

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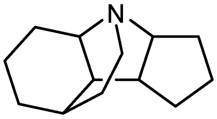

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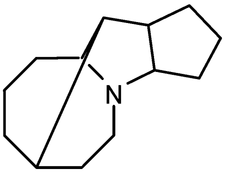

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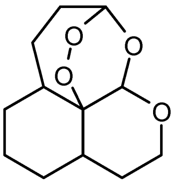
If maximizing the number of undistorted six-membered rings results in unavoidable overlap of atoms or bonds, a different bridge or set of bridges should be selected.



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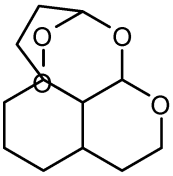

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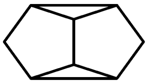

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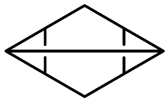
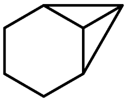


Not acceptable

Authors should be especially mindful of diagrams that produce three collinear atoms with an additional bond between the first and last atoms of the three. Molecules of this sort are thankfully rare, but typically require extensive distortion in order to produce an understandable diagram.



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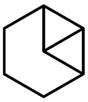

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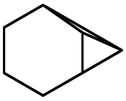

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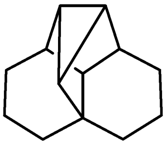
[when representing
the molecule at left]



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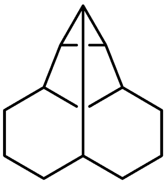

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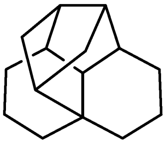
the molecule at left]



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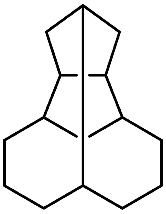

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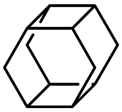
the molecule at left]

In extreme cases, a perspective-based depiction may be the only reasonable way to produce an understandable diagram. Molecules that approximate regular polyhedra are especially well suited to a perspective-based depiction.



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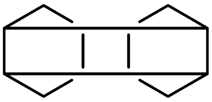

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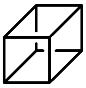

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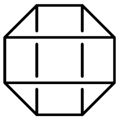
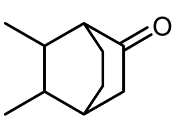


Not acceptable

It is preferable to minimize the number of substituents on bridges, although generally not at the expense of maintaining undistorted six-membered rings.



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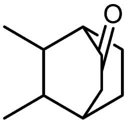

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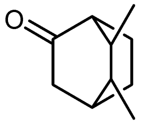

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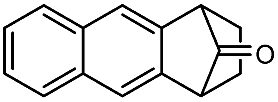

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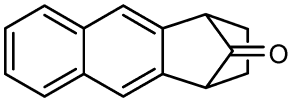

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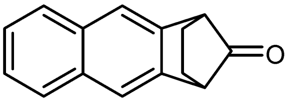
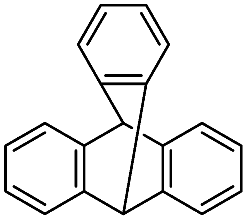


Not acceptable

In extreme cases, significant distortion of a bridge may be necessary to reduce overlap enough to produce an understandable diagram



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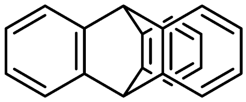
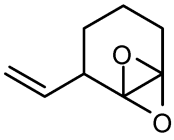


Not acceptable

When three or more simple rings share one bond, it is critically important that all three rings remain visible without obscuring each other. Occasionally, it may be possible to "nest" rings of different sizes inside each other without distortion. However, some sort of distortion will always be necessary if at least three of the rings are of the same size.

SOFTWARE CAUTION: Although one hopes that no human would create diagrams with rings that exactly overlap in this manner, such overlap is regrettably common in diagrams produced by computer software. Authors are always encouraged to review the output of computer programs carefully, lest any atoms or bonds be completely obscured and the apparent meaning of a diagram be other than was intended.



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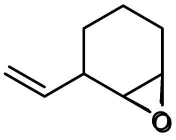

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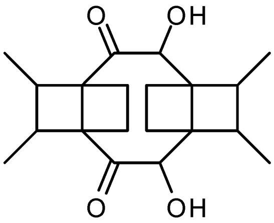

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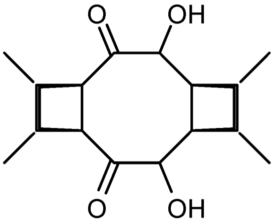
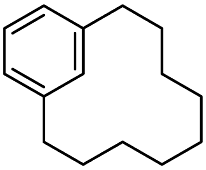


Not acceptable
[when representing the molecule at left]

In bridged ring systems that contain large rings (GR-3.3.2) and additional fused rings (GR-3.3.3), the various requirements of those systems must all be balanced to produce the best overall depiction. The shape of a large ring that is part of a bridged ring system will often be influenced by other components of that system, often requiring a shape for the larger ring that would not be preferred if it was not bridged (see GR-3.3.2).

Rings that share two bonds should preferably be arranged to minimize the distortion of both rings. Typically, that will result in both shared bonds being *trans*-like relative to the larger ring.



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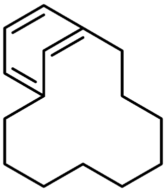

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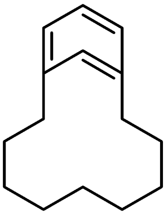
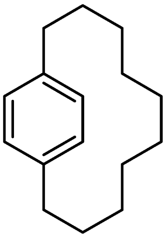


Not acceptable

Rings that share three fusion bonds should be arranged so that the outer two shared bonds are *trans*-like relative to the larger ring while the central shared bond is *cis*-like relative to both.



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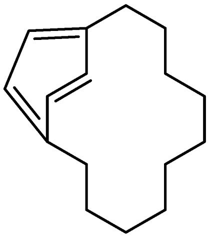

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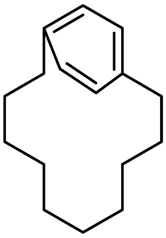

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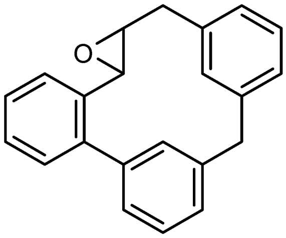
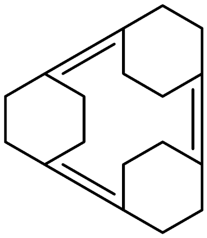
It may be necessary to depict fused rings on a "*trans*-like" fusion bond as long as the combination of the bond angles in the two rings allows such positioning without overlap.



Preferred

Phane compounds can be especially difficult to display aesthetically. For molecules of this type, it is preferable to preserve the regular appearance of the smaller, embedded rings, even if doing so requires significant distortions to both the bond lengths and the bond angles of the larger rings.



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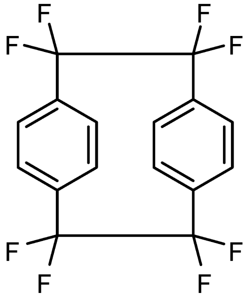
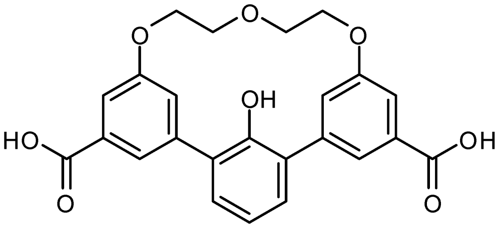


Preferred

In some cases, the positioning of substituents within the larger ring is unavoidable.



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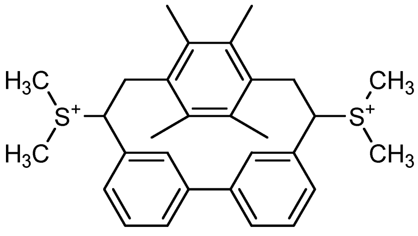

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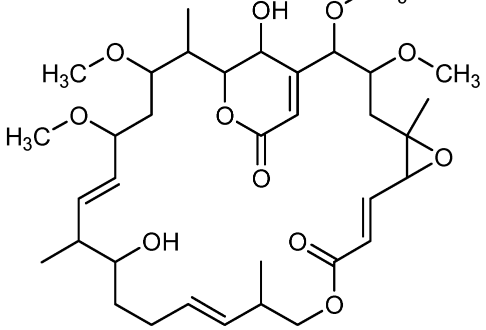


Preferred

GR-3.4 Orientation of rings

When present, ring systems generally serve as the focal point of a chemical structure. Although there are exceptions, the "principal" ring system is normally positioned in a preferred orientation, and only then are all other substituents positioned accordingly.

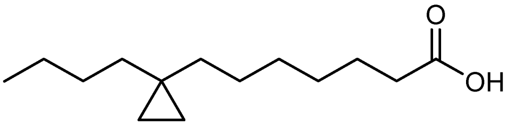
GR-3.4.1 Selection of the principal ring system

In many cases—and particularly when there is only one ring system in the entire structure—selection of the principal ring system is obvious. In more complicated cases, there is substantial flexibility. Although it is always acceptable to select the principal ring system according to the hierarchy described in the "Nomenclature of fused and bridged fused ring systems" guidelines [21], rigorous application of that hierarchy is unnecessary if the main intention is simply to produce an aesthetic diagram. For most practical purposes, it is sufficient to select the principal ring system as

- the one that has the largest number of fused rings;
- if there is more than one such system, the one with the largest individual rings (eight-membered, seven-membered, etc.);
- if there is still more than one system, the one with the greatest unsaturation; or
- if there is still more than one system, the one with the greatest number of heteroatoms

Those four guidelines are a tremendous oversimplification of the full Fused Ring Systems guidelines, but they will serve most purposes. Phrased differently, the principal ring system may be considered to be "the ring system that seems most important". Those guidelines will usually produce the ring system that most chemists would consider to be "most important" in a structure, but they need not be followed rigorously, either. In a discussion of several related molecules, for example, it would be reasonable to select a single ring system to be considered as "most important" across the collection. So the single-ring benzoic acid might well be considered "more important" than a two-ring naphthyl group in a collection of structures that consist of 2-fluorobenzoic acid, 2-chlorobenzoic acid, 2-bromobenzoic acid, 2-hydroxybenzoic acid, 2-cyclohexylbenzoic acid, 2-(2-naphthyl)benzoic acid, etc.

Nor should the simple presence of a ring be an absolute determining factor for the orientation of a structure! In a structure with a chain that is large compared to the size of the largest ring system, it is often reasonable to treat the chain as the principal system for orienting the structure, and allow the ring(s) to be drawn as simple substitutents once the main chain is positioned.



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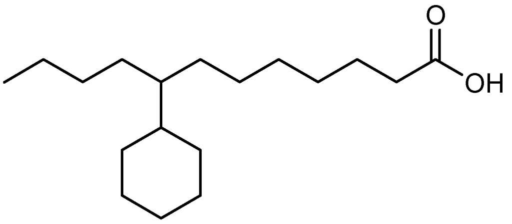

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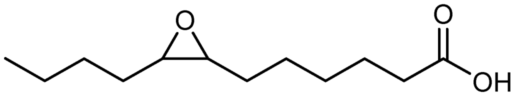


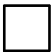
Preferred

GR-3.4.2 Orientation of principal ring system

If the structure features a ring system that may be reasonably treated as a principal ring, that ring should be presented in its preferred orientation. Isolated, non-fused rings of 3, 4, 5, 7, or 8 atoms should preferentially be drawn with a horizontal bond at the bottom of the ring or the top of the ring. Isolated, non-fused six-membered rings should preferentially be drawn with a vertical bond at the left of the ring.


Preferred


Preferred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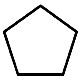
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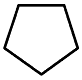
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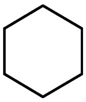
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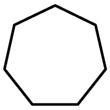
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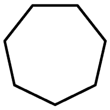
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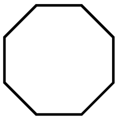
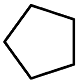

Preferred

If an alternative orientation is required for some specific purpose (e.g., to emphasize symmetry, or to maximize the number of horizontal substituents), it is acceptable to orient rings of eight or fewer atoms so that an atom is located at the extreme left or right of the horizontal centerline of the ring.


Acceptable


Acceptable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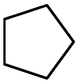
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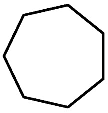
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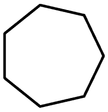
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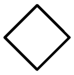
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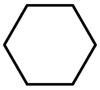
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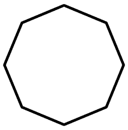
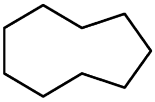

Acceptable

Rings with nine or more members should be treated analogously to the corresponding fused ring system for selection of preferred orientation.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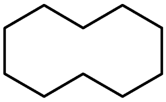
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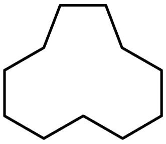
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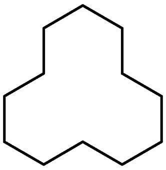
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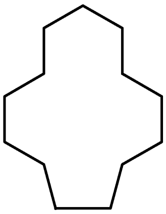
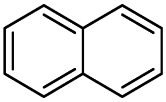

Preferred

For ring systems containing at least two fused rings, that system should be presented in its preferred orientation. For most practical purposes, it is sufficient to orient the ring system so that:

- The fused ring system is oriented more or less horizontally. A symmetry axis (or plane) should be vertical or horizontal.
- If the system contains multiple "rows" of rings, any "extra" rings should be positioned so that they are toward the right and the top of the ring system.
- Larger rings should be toward the left and smaller rings toward the right.
- Heteroatoms should be toward the right and, with slight preference, toward the bottom.

As discussed in GR-3.3.3, the guidelines discussed here should be followed when producing aesthetic depictions and should not necessarily be followed when determining systematic names.



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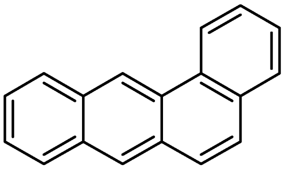

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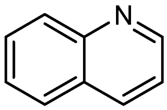

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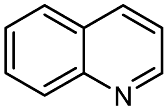
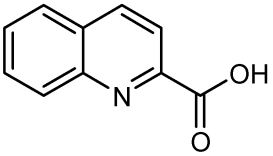


Preferred

It should also be noted that several classes of molecules, including steroids [7] and many other natural products [23], have preferred orientations that are specific to those classes. In some cases (including most steroids), the preferred orientation of the class is very similar to the recommendations for fused rings in general. In other cases, the preferred orientation of the class may be very different. When working with one of these molecules, the class-based orientation is preferred. Some molecules may contain elements of more than one class, for example, a steroidal glycoside. In such a molecule, either class may be chosen as the principal one, depending on which features the author wishes to emphasize.

As discussed in GR-4.2.1, these guidelines need not be followed slavishly. According to these guidelines, a quinoline system should be drawn horizontally, with the nitrogen toward the right and, most commonly, toward the bottom. Any further substituents would be positioned with respect to that ring system, as shown below, left. In some cases, however, it is useful to emphasize some other portion of the structure. In a context where the acid group is the most interesting feature, it might be reasonable to invert the ring system to position the acid group more prominently toward the top right. Those portions of these guidelines that make sense should still be followed, however—the quinoline system should still be oriented horizontally, and not at an angle.



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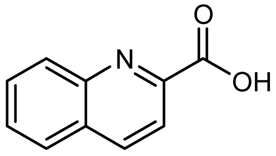
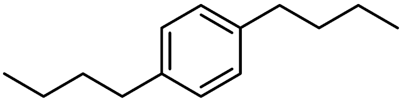


Preferred

GR-3.4.3 Substituents on ring systems

In the absence of a different overriding concern, the largest ring system within a structure should be oriented toward the bottom-left of the structure and substituents should be arranged to spread horizontally rather than vertically. Other orientations are acceptable as long as they remain legible, but those horizontal orientations tend to produce more compact diagrams that additionally are easier to interpret when included in a document with associated text that also reads horizontally.



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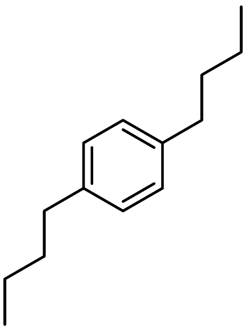

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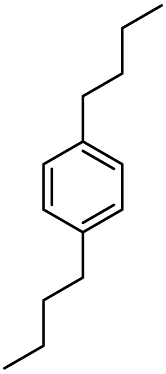

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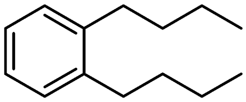

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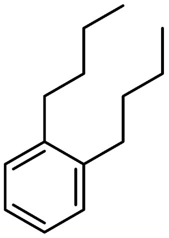

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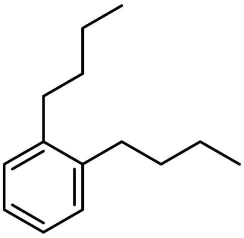

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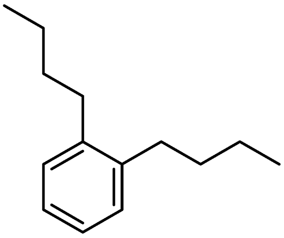


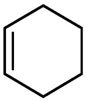
Acceptable

GR-3.5 Positioning of double bonds in rings

In the general context of structure-orientation issues, the positioning of double bonds in rings is a minor issue, far less important than the positioning of the rings themselves in relation to other portions of the structure. Still, there can be a question of positioning of double bonds in rings with highly symmetric substituents (or with no substituents at all). Also, there is always a question of the cyclic positioning of double bonds within ring systems with the maximum number of non-cumulative double bonds ("mancude" ring systems), including aromatic systems. The placement of the two lines composing a double bond relative to each other is discussed in GR-1.10.4.

GR-3.5.1 Positioning of isolated double bonds

Double bonds should be positioned toward the left (and secondarily toward the top) of a ring.



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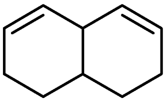
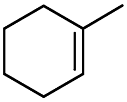


Preferred

However, the positioning of double bonds is of less concern than the positioning of fused ring systems and of substituents. For example, a fused ring system should be oriented horizontally even if doing so will position a double bond further rightward than would otherwise be possible.



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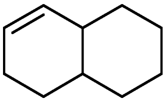
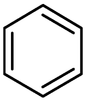


Preferred

GR-3.5.2 Alternating double bonds may be in either resonance form

In delocalized single-ring systems containing alternating single and double bonds, the bonds may be drawn in either of two resonance forms, both of which are equally preferred.



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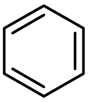
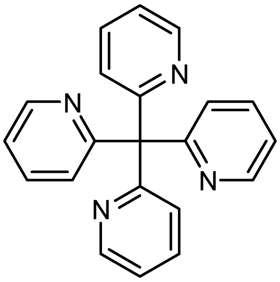


Preferred

In highly symmetrical structures, it is preferable for the double bonds within aromatic systems to be drawn in a symmetrical fashion as well.



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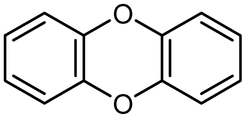


Preferred

GR-3.6 Structural classes with standard orientations

Several classes of molecules—and especially several classes of biochemical molecules—are traditionally drawn using styles that are specific to those classes. Drawing styles for those classes are illustrated within the documentation for each of those classes:

- amino acids [16]
- carbohydrates [15]
- steroids [7]
- tetrapyrroles [24]
- carotenoids [25]
- other natural products [23]
- polymers [26,27]

GR-4. POSITIONING OF SUBSTITUENTS

Beyond the overall orientation of structure diagrams, the relative positioning of substituents within a diagram also influences how that diagram is understood by the reader. Preservation of legibility and reduction of ambiguity continue to be of critical importance here, as in other areas of graphical representation.

GR-4.1 Bond angles at chain atoms

When chemical structures are depicted in two dimensions, they should be drawn in a way that accurately represents the true three-dimensional structures. The key word in the previous sentence is "represents". A two-dimensional structure still remains a schematic representation, and some liberties should be taken with bond lengths, angles, etc., to produce a drawing that is most easily recognized.

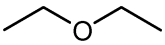
Collinear bonds are of particular concern when producing two-dimensional diagrams. Two bonds should be drawn collinearly in two dimensions if and only if they connect collinearly in three dimensions, and they should be drawn at an angle in two dimensions if and only if they connect at an angle in three dimensions.

It is worth noting that the linear drawing style (GR-13) has very different rules for drawing bonds, and is considered separately.

GR-4.1.1 Atoms with two bonds drawn

Most atoms with two single bonds (or one single bond and one double bond) should be depicted with the bonds separated by a 120° angle. For a series of single bonds, a *trans*-like depiction is strongly preferred and arbitrary "bends" in the chain should be avoided without specific reason.

Preferred



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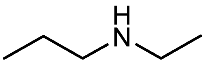
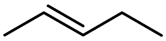


Preferred

The relative orientation of adjacent bonds around a double bond should preserve the *cis/trans* configuration of that double bond



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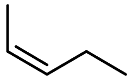

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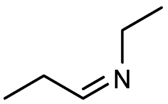
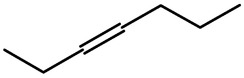


Preferred

A single bond connected to a double bond by a 180° angle indicates that the *cis/trans* configuration is unknown in the corresponding structure. This depiction style should only be used when the double bond has exactly two substituents, one on each end, and both substituents should be drawn collinearly [6].



Acceptable

Not acceptable

When an atom has two single bonds that are truly collinear in the real three-dimensional molecule, the bonds should be separated by a 180° angle in two dimensions as well. Such cases are common for AX_2 derivatives of noble gases and metals.

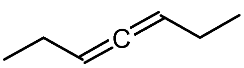
$F{-}Xe{-}F$

Preferred

$N{\equiv}{-}Hg{-}{\equiv}N$

Preferred

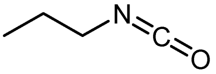
Atoms that are isoelectronic with carbon and bearing two double bonds (or one single bond and one triple bond) should be drawn with the bonds separated by a 180° angle. As discussed in GR-2.1.2, any carbon atom with two double bonds should always be explicitly labeled, to remove the possibility of the two bonds being misinterpreted as one long bond.



Preferred

$O{=}C{=}O$

Preferred



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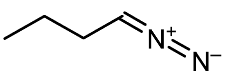

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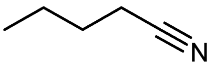

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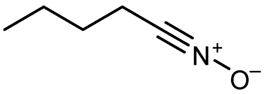

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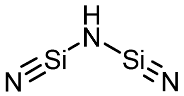

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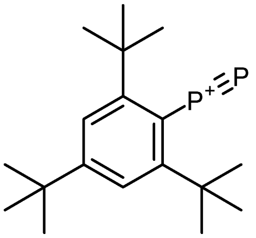
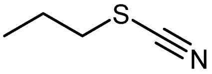


Preferred

Carbon atoms connected to two heteroatoms by one single bond and one triple bond are equally preferred with or without explicit labeling of the central carbon atom.



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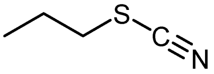

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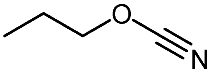

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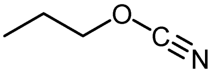
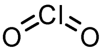


Preferred

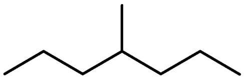
Again, some rare cases exist where an atom with two double bonds should not have those bonds arranged collinearly, but that is limited to atoms with electronic structures other than that of carbon.



Preferred

GR-4.1.2 Atoms with three bonds drawn

Atoms with three bonds drawn should almost always be depicted with three equal 120° angles separating the bonds. In this context, a double bond is considered as one "bond", not two, and similarly for a triple bond.



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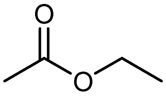

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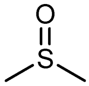

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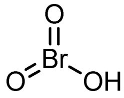
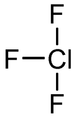


Preferred

Again, some exceptions exist, principally limited to configurations other than tetrahedral and trigonal planar. In a T-shaped configuration, for example, the diagram should be drawn with two of the bonds extending vertically above and below the central atom, and the third bond extending to the left.



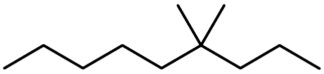
Preferred

There are further restrictions for depicting tetrahedral configuration for atoms with three bonds drawn. Those are discussed elsewhere [6].

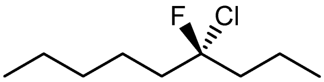
GR-4.1.3 Atoms with four bonds drawn

Atoms with four bonds may be depicted in several different ways, with a preference among these ways determined by context.

When two of the adjacent atoms are each connected to no additional atoms and two of the adjacent atoms are each connected to at least one additional atom, the four bonds should be separated by one 60° angle, an opposing 120° angle, and two 90° angles. Because of the 120° angle, this style will not disrupt the orientation of a chain in which it appears. This style also facilitates the depiction of chiral centers; the two bonds separated by the 60° angle are marked with a solid wedge and a hashed wedge. If the substituents connected to the two bonds separated by the 60° angle are not identical, the graphically larger substituent should be on the right for aesthetic purposes.



Preferred



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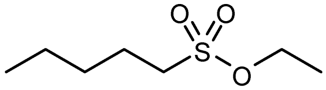

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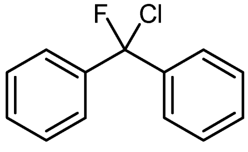

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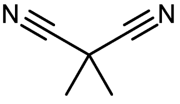
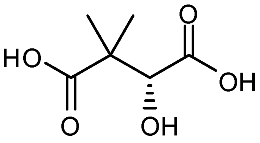
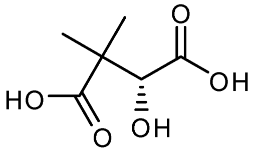


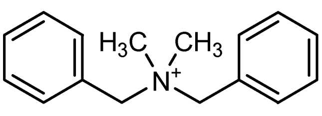
Preferred



Preferred



Not acceptable



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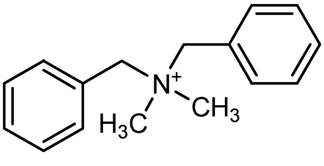
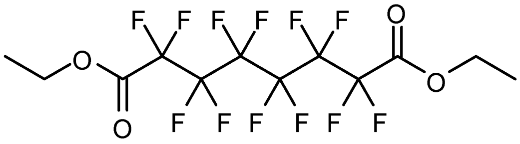


Not acceptable



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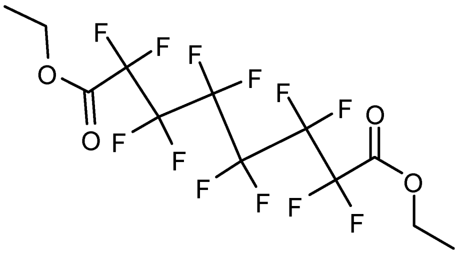
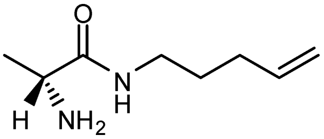
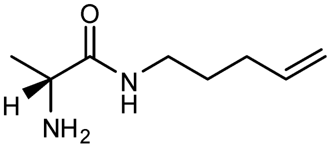


Not acceptable

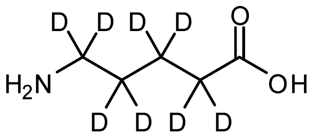
This style should also be used in some cases when three of the adjacent atoms are each connected to no additional atoms and only one adjacent atom is connected to at least one additional atom. Because the 120° angle in this depiction style emphasizes a multiatom chain, it should only be used when an adjacent atom is itself acyclic and can be viewed as part of a larger chain with the atom in question. It is most typically used when exactly one of the terminal substituents is a carbon atom (depicted with a 120° angle separating that substituent from the one with more than one bond) or when two of the terminal substituents are not carbon atoms but identical (depicted with a 60° angle separating the identical substituents).



Preferred



Acceptable



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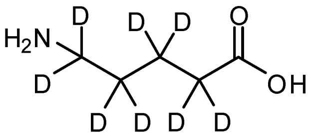
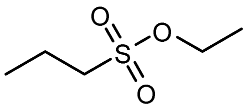
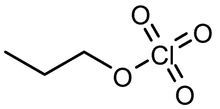


Acceptable

When at least two of an atom's four bonds are double bonds, it is equally preferred for the atom to be depicted with the four bonds separated by four equal 90° angles.

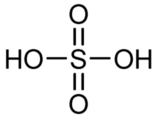


Preferred



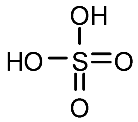
Preferred

If exactly two of the bonds in the style are double bonds (as in sulfonyl groups), those two bonds should usually be drawn opposing each other, with 180° separating them around the central atom. An exception is made if drawing the two double bonds opposite each other would produce unacceptable overlap between other portions of the structure that could be avoided by drawing the double bonds adjacent.



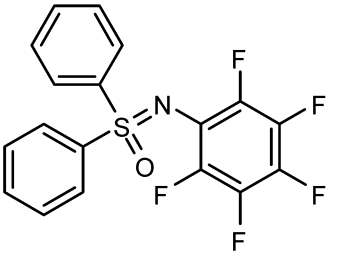
$$\mathrm{HO{-}\underset{\underset{O}{\|}}{\overset{\overset{O}{\|}}{S}}{-}OH}$$

Preferred



$$\mathrm{HO{-}\underset{\underset{O}{\|}}{\overset{\overset{OH}{|}}{S}}{=}O}$$

Not acceptable



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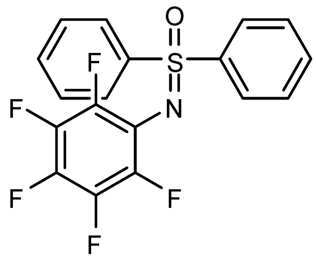
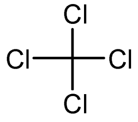


Not acceptable

The style with the four bonds separated by four equal 90° angles should also be used when none of the four adjacent atoms is connected to any other atom. It should additionally be used when every one of the four adjacent atoms is connected to at least two other atoms.



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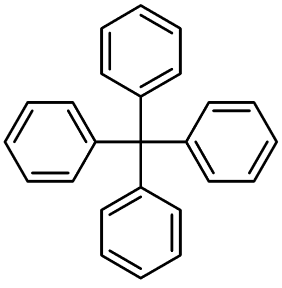
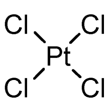


Preferred

The style with four bonds separated by equal 90° angles and with a 45° angle between those bonds and the horizontal axis of the paper should be restricted to square planar complexes.



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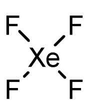
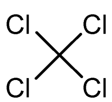
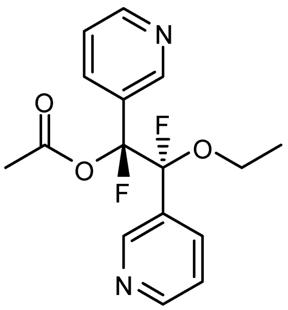


Preferred

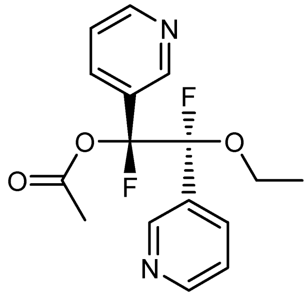


Not acceptable

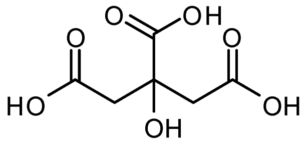
When one of the adjacent atoms is connected to no additional atoms and three of the adjacent atoms are each connected to at least one additional atom, a third style should be used where the smallest substituent is separated from each of its neighbors by a 60° angle and the fourth substituent opposes the smallest substituent, separated from each of its neighbors by 120° angles. When not prohibited due to overlap with another portion of the diagram, the substituent with exactly one bond should be oriented exactly vertically or exactly horizontally.



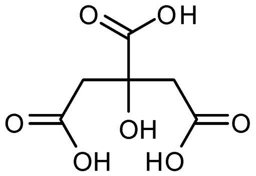
Preferred



Acceptable

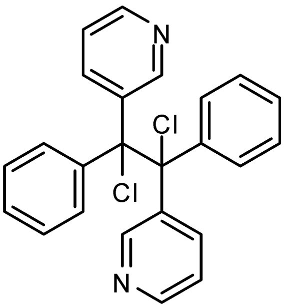


Preferred

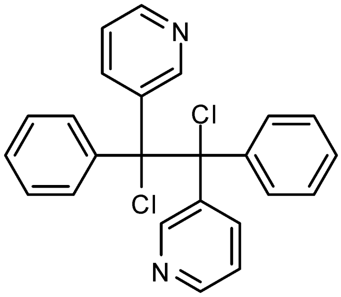


Acceptable

Diagrams are not acceptable if the four bonds attached to a stereogenic atom are aligned to the axes, since such orientations might be interpreted as Fischer projections and are inherently ambiguous.

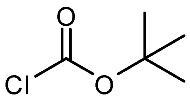


Preferred

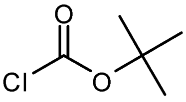


Not acceptable

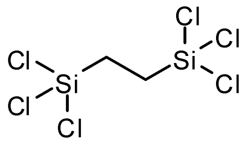
This style should also be used when three of the adjacent atoms are each connected to no additional atoms and only one adjacent atom is connected to at least one additional atom, and when the three adjacent terminal atoms are themselves identical.



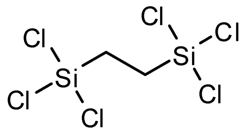
Preferred



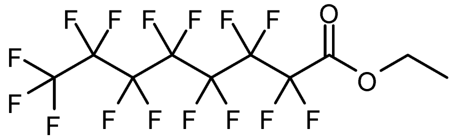
Acceptable



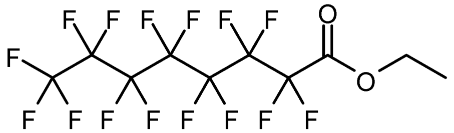
Preferred



Acceptable

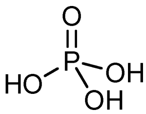


Preferred



Acceptable

A fourth style also may be considered, where the four bonds are separated by one 30° angle, two 105° angles, and one 120° angle. This style is occasionally used to emphasize the tetrahedral geometry of phosphates and phosphate esters (and their arsenic and antimony analogs). The style can also be used in other cases where the tetrahedral geometry is to be emphasized, but it should only be used when two of the substituents are relatively small, graphically, and those substitutents should be placed on the bonds separated by the 30° angle. This style should always be drawn with one of the other bonds exactly vertical or horizontal.



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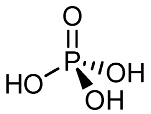
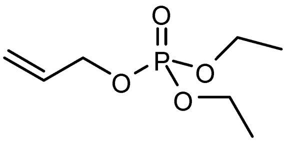
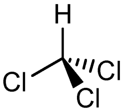


Preferred



Preferred



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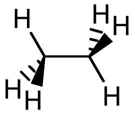


Preferred

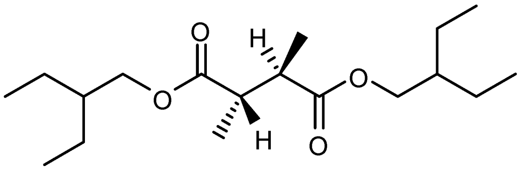
There are further restrictions for depicting tetrahedral configuration for atoms with four bonds drawn. Those are discussed in the recommendations “Graphical representation of stereochemical configuration” [6].

GR-4.1.4 Atoms with more than four bonds drawn

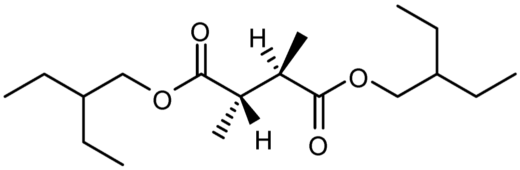
Atoms with more than four bonds are rare in organic chemistry, but more common when dealing with inorganic complexes. If no stereochemical significance is assigned to the bonds, they should most commonly be drawn with one of the bonds directed vertically and the remainder separated by equal angles. If configuration is a concern, the bonds should be drawn in one of the recommended styles for “Graphical representation of stereochemical configuration” [6].

GR-4.1.5 Branching chains should bend outward

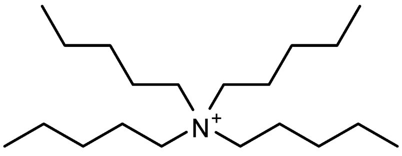
Unconstrained secondary chains that branch off a horizontal chain should be oriented, when possible, so that they bend outward from the graphical center of the structure diagram. Besides improving the general aesthetics of the diagram, this recommendation also helps maximize the diagram’s overall horizontal arrangement, and in many cases will also assist in emphasizing symmetry as described in GR-3.1.4.



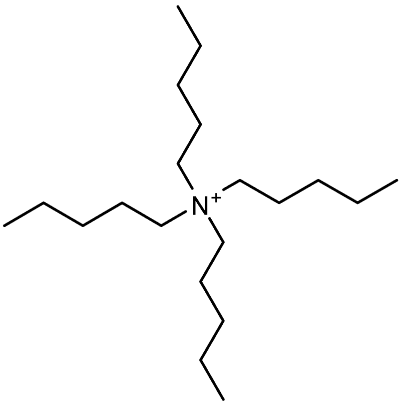
Preferred



Acceptable

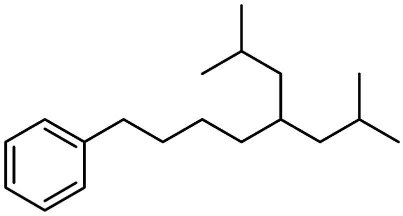


Preferred

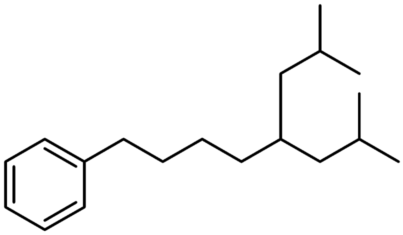


Acceptable

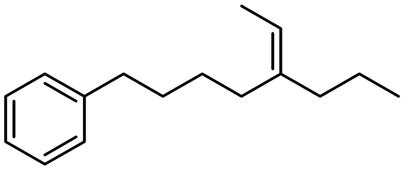
Obviously, a secondary chain may bend in any direction that is necessary, including toward the center of the diagram, when the chain is constrained either by stereochemical configuration or by the need to avoid overlap with other portions of the diagram.



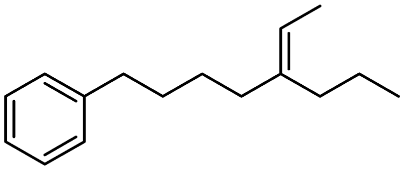
Preferred



Not acceptable



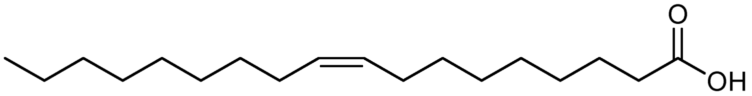
Preferred



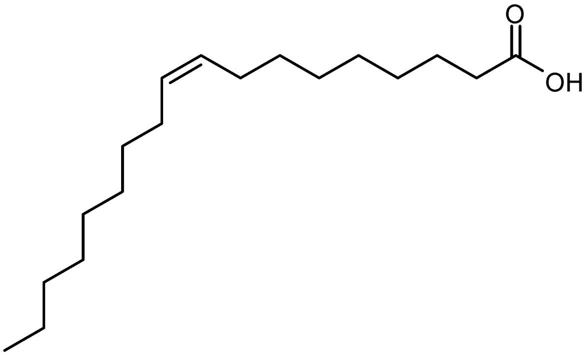
Not acceptable
[when representing the (Z)-stereoisomer at left]

GR-4.1.6 Double bonds in long chains

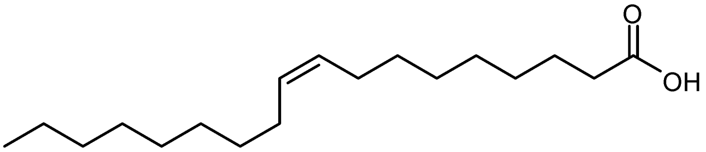
In addition to the styles shown above, there is another style that may be considered when drawing double bonds in long chains when the double bonds are in a *cis* configuration relative to the chain. In this style, the double bond is drawn with 150° angles between it and its attached chain bonds rather than the usual 120°. This style serves to preserve the linearity of the chain, and should only be used when that is desired. It is not acceptable when there is further substitution on the double bond.



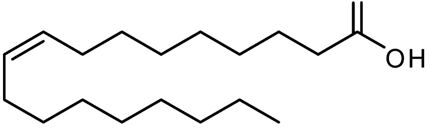
Preferred
[when linearity of depiction is desired]



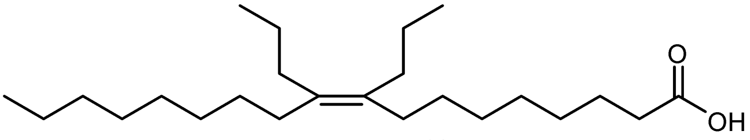
Preferred



Preferred

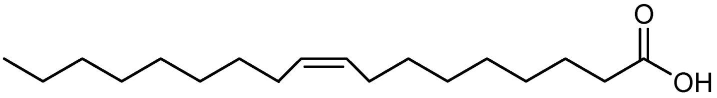


Preferred



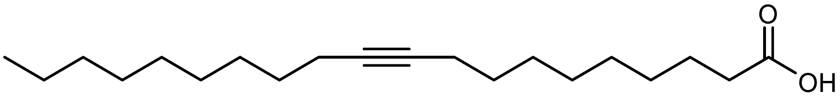
Not acceptable

The similar form with undistorted 120° angles at the double bond and 105° angles to the adjacent chain bonds is acceptable, but not preferred whether or not it has further substituents on the double bond.



Acceptable

Long chains with triple bonds may be depicted in similar ways.



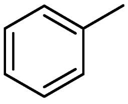
Acceptable

GR-4.2 Bond angles from rings to substituents

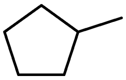
The issues related to bond angles between ring systems and their substituents are very similar to the issues related to chain bond angles (GR-4.1). In many cases, bonds from rings to their substituents may be positioned as if the two neighboring ring bonds described a very short chain, with the substituents being placed as if they were substituents of that chain. There are additionally a few other issues to consider that are specific to rings.

GR-4.2.1 Exterior ring atoms with one substituent drawn

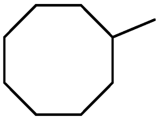
In most cases, exterior (non-fusion, non-bridging, non-bridgehead, non-spiro) ring atoms with a single substituent should be drawn so that the substituent bisects the larger angle formed by that atom's two ring bonds. This is true regardless of the size of the ring or the order of the bond, and also true for nonconvex rings.



Preferred



Preferred



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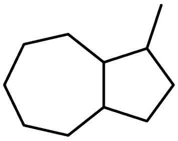

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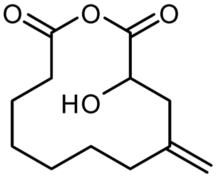
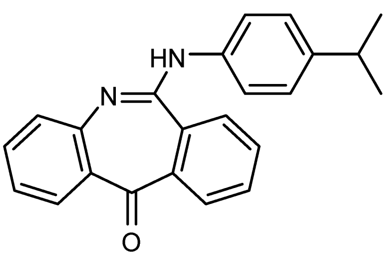


Preferred

As above, in cases where bisecting the adjacent bonds would result in a substituent that is within 5° of being horizontal, vertical, or at another multiple of 30°, the substituent should preferably be adjusted so that it is oriented exactly at the nearest such angle. This most commonly happens at fusions between six- and five-membered rings.



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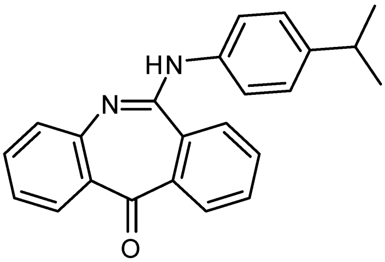

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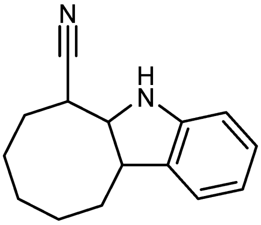

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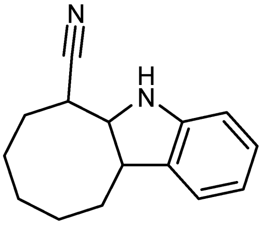
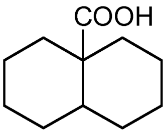


Acceptable

SOFTWARE WARNING: Unlike diagrams that are produced in high resolution (e.g., for a printed publication), diagrams that are displayed on a computer screen are limited to the relatively low resolution of computer monitors. Even at low resolution, bonds that are oriented exactly horizontally or exactly vertically still look crisp. When low-resolution bonds are oriented slightly at an angle, however, it is not possible to draw them smoothly, and they look “jaggy” instead. The overall appearance of low-resolution chemical structure diagrams can be greatly improved by making sure that bonds are aligned exactly horizontally or exactly vertically when possible.

GR-4.2.2 Fusion atoms with one substituent drawn

Ring fusion atoms already have three bonds within the ring system. For external ring fusion atoms, the substituent should preferentially be positioned outside the ring system and oriented so that it bisects the angle between the adjacent bonds.



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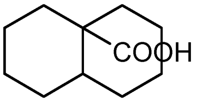
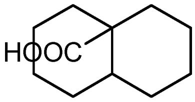
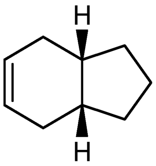


Not acceptable



Not acceptable

As discussed in GR-4.2.1, the substituent should be adjusted so that it is oriented exactly horizontally, vertically, or at another multiple of 30° when bisecting the adjacent bonds would result in a substituent that is oriented within 6° of such an angle. This most commonly happens at fusions between six- and five-membered rings. For substituents with three or fewer atoms, it is acceptable to leave the substituents in their default (unadjusted) position; for larger substituents, the adjustment may be preferable.



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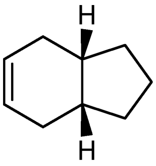

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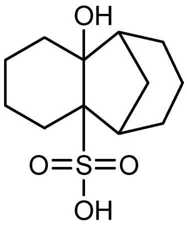

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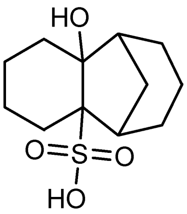
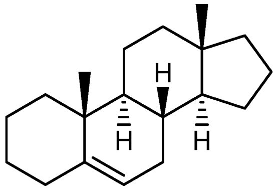


Acceptable

When two substituted fusion atoms are adjacent, placing both substituents outside the ring system will typically cause them to overlap. In those cases, it is better to draw one of the substituents within the ring system. A substituent drawn in this way should preferentially be drawn exactly vertically or horizontally, whichever direction would minimize overlap with other atoms and bonds.



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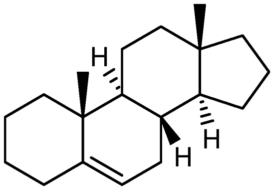
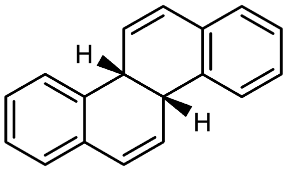


Not acceptable

If a substituted fusion atom is adjacent to an unsubstituted fusion atom, there typically is enough room to orient the substituent either inside or outside the ring system. That substituent should be oriented outside the ring system if all substituents can be oriented outwards, but should preferably be drawn exactly vertically or horizontally if any other substituent is placed within the ring system to avoid conflict with an adjacent substituent.



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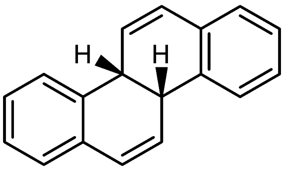

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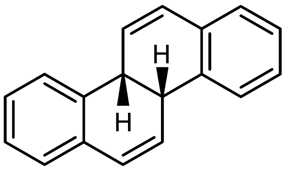

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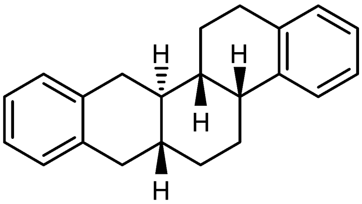

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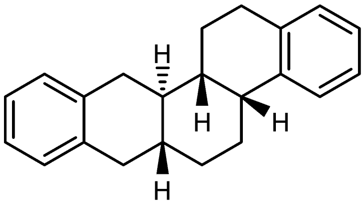
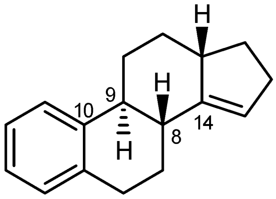


Acceptable

Small substituents on the C-8 and C-9 atoms of steroids should be drawn within the ring system in this fashion even if there are no substituents on the adjacent fusion atoms C-10 and C-14. Certain other natural products [23] also have preferred orientations that place substituents within the ring system.



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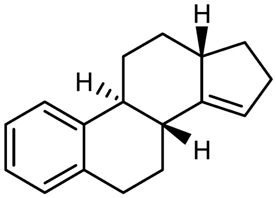
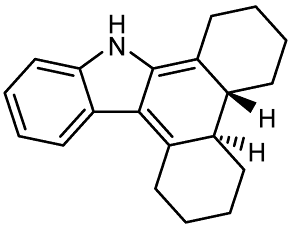


Not acceptable

A substituent should not be oriented within a ring system when attached to a fusion atom that lacks any vertical or horizontal fusion bond. The substituent should be oriented outside the ring system, minimizing overlap as best as is possible. Sometimes, it might be possible to reorient the ring system so that the fusion bonds are vertical; the substituents should certainly be placed vertically if so.



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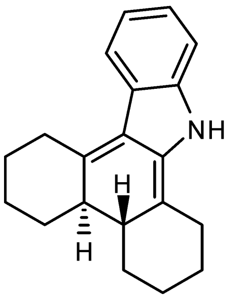

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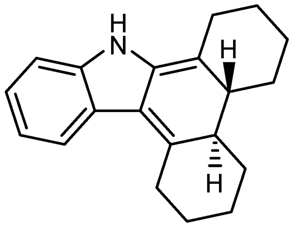
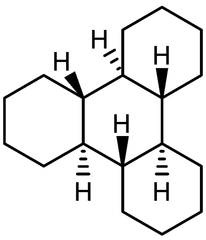


Not acceptable

It is not acceptable to orient two substituents within the same ring if the ring has fewer than eight atoms. One or both of the substituents should be oriented outside the ring system, minimizing overlap as best as is possible.



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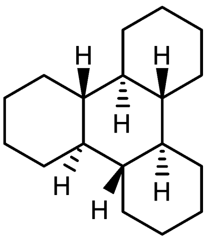

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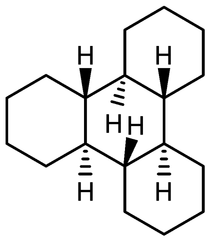
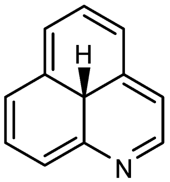


Not acceptable

Substituents on interior fusion atoms have no option other than being drawn within the ring system. As above, such substituents should preferentially be drawn exactly vertically or horizontally, according to the direction that would minimize overlap with other atoms and bonds.



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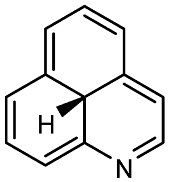
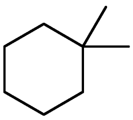


Acceptable

GR-4.2.3 Atoms with two substituents drawn

Ring atoms with two external bonds should normally be drawn with a 60° angle between the chain bonds. This is true regardless of the bond order of those bonds.



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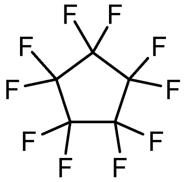

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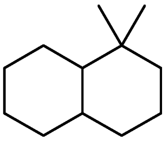

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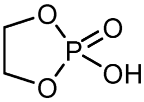

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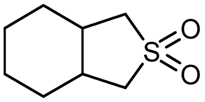
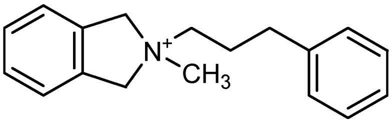
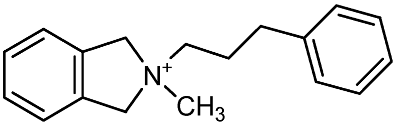


Preferred

In particular, the two substituents should preferably not be positioned so that they evenly subdivide the external angle between the endocyclic bonds.

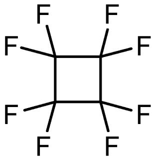


Preferred



Acceptable

Alternatively, for substituents on four-membered rings only, the substituents may be separated by a 90° angle.



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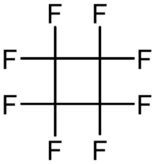
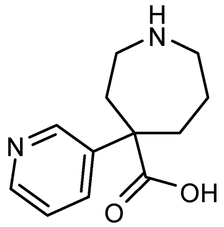


Preferred

In cases where each of the two substituent atoms itself has at least two additional bonds, a 60° angle between the substituents will generally result either in overlap between the substituents or strange distortions to avoid that overlap. In those cases, therefore, the two substituents indeed should evenly subdivide the external angle between the endocyclic bonds as the least unpleasant alternative available.



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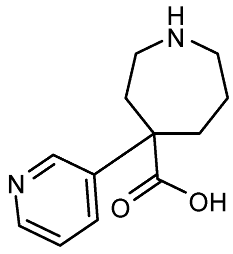

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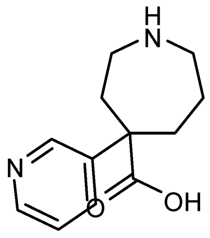
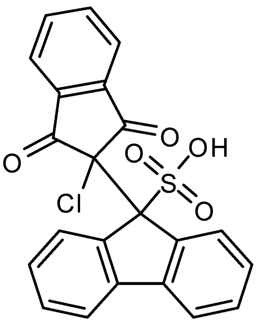


Not acceptable



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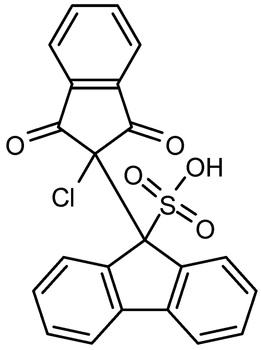

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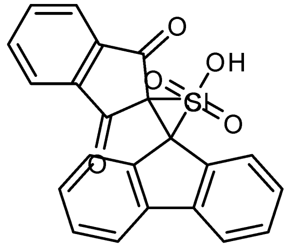
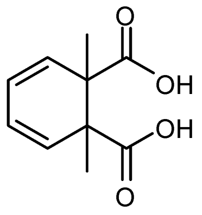


Not acceptable

When the two substituents consist of one single-atom substituent and one multi-atom substituent, and when the two substituents are connected to a six-membered ring, the larger substituent should be oriented outside the ring system so that it bisects the angle of the adjacent bonds and the smaller substituent should be oriented so that it bisects an angle adjacent to the larger substituent. When possible, the smaller substituent should also be oriented exactly vertically or exactly horizontally. This drawing style helps maximize the number of bonds that are depicted at standard ±30° angles.



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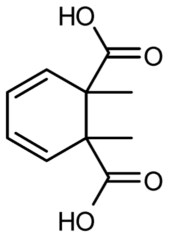
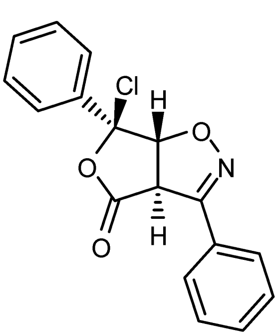


Acceptable

The previous recommendation applies only when the two substituents are attached to a six-membered ring. When the two substituents are attached to rings with other than six members, a 60° separation is preferred even when one substituent is large and one is small.



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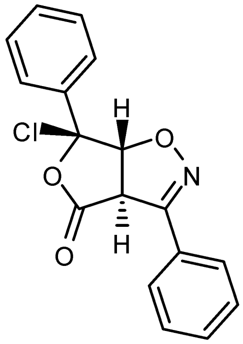

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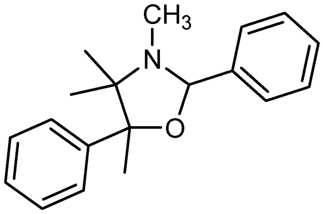

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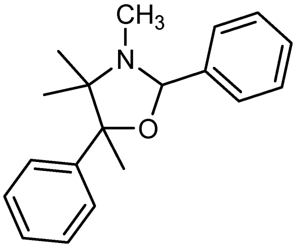

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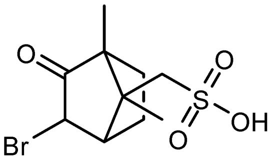

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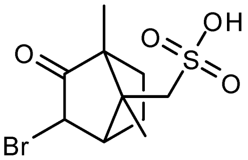
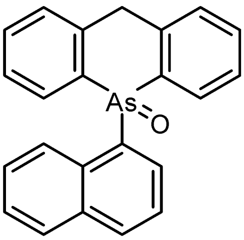


Acceptable

When there is a difference between the two sides of the larger substituent, it is preferable to position the smaller substituent on the less crowded side, although it is acceptable to position it on either side as long as no overlap results (GR-4.3.1).

If the smaller substituent can be placed on either side of the larger one, it is preferable to orient the smaller substituent so that it is exactly vertical or exactly horizontal. If neither side achieves that orientation, the smaller substituent should be oriented to the right or, if that cannot be achieved either, toward the top of the diagram.



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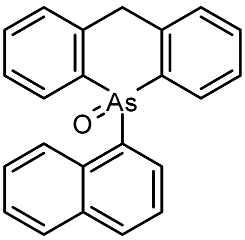

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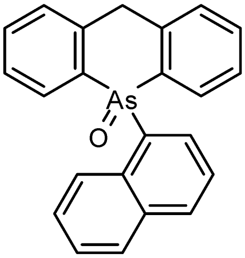

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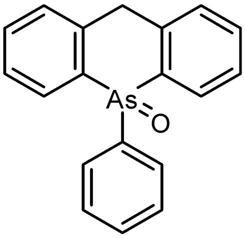
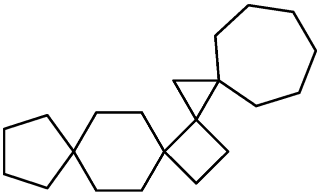


Preferred

GR-4.2.4 Spiro unions

Atoms that form a spiro union between two ring systems should normally be drawn so that the bisector of the angle between the two bonds in one ring is collinear with the similar bisector in the other ring, without distortion of either ring from the shape with which it would be depicted in the absence of the spiro union.



Preferred

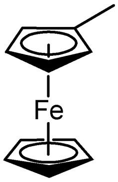
Because individual rings within a spiro system may not be distorted, such systems can quickly become difficult to interpret, particularly in the presence of further substituents on the rings. As always, legibility is of primary importance, and other approaches (GR-4.3.5, GR-4.3.7) may be required to reduce or eliminate overlap that would otherwise be unavoidable.

GR-4.2.5 Atoms with more than two substituents drawn

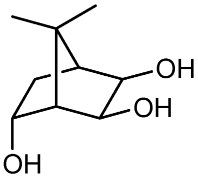
Ring atoms with more than two external substituents are rare in organic chemistry, but more common when dealing with inorganic complexes. If no stereochemical significance is assigned to the bonds, they should most commonly be drawn with substituents separated from each other and from the ring bonds by equal angles. If stereochemical configuration is a concern, the bonds should be drawn in one of the recommended styles for non-tetrahedral configuration [6].

GR-4.2.6 Rings drawn in perspective

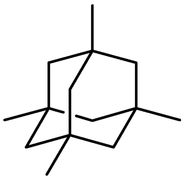
Substituents on rings that have been drawn in perspective [6] should preserve the perspective of those rings. This generally means that such substituents would *not* be drawn to bisect the angles of the ring bonds. Some examples of substituents on rings drawn in perspective are shown.



Preferred



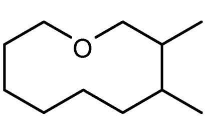
Preferred



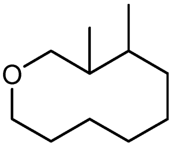
Preferred

GR-4.2.7 Rings with reentrant bond angles

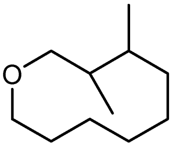
While rings of eight or fewer members are most commonly drawn as convex polygons, larger rings are more appropriately drawn with some reentrant (non-convex) bond angles (see GR-4.2.2). Whenever possible, the ring should be depicted with any substituents positioned on outward-pointing atoms, so that the substituents themselves point outward according to the recommendations above.



Preferred

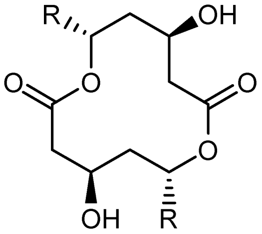


Not acceptable

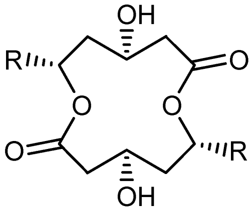


Not acceptable

Special care should be taken when representing stereochemical configuration on reentrant bond angles. As discussed in the tetrahedral configuration recommendations [6], it can be extremely difficult and confusing to interpret wedged bonds and hashed wedged bonds in non-standard orientations. When such stereobonds are placed so that they point outward from a reentrant atom, their proper interpretation can be very difficult indeed.

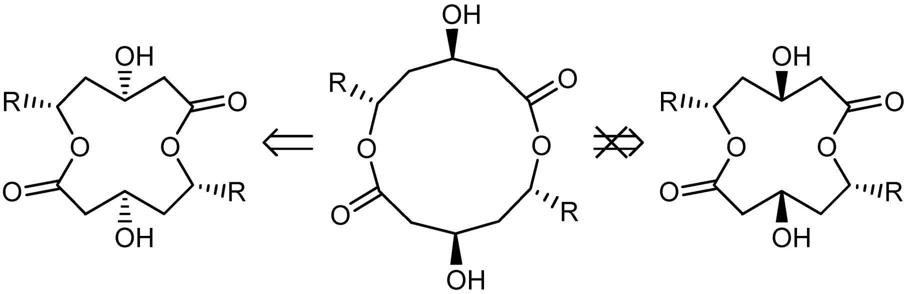


Preferred

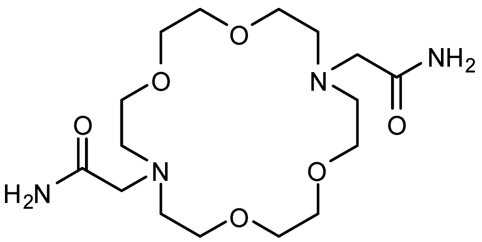


Not acceptable

A second diagram, to help clarify this important point even further:



Substituents on reentrant nitrogen atoms are an exception to the general rule. Many large rings containing heteroatoms can form complexes, making it desirable to orient all of the heteroatoms inwards for emphasis. Since stereochemical configuration is not a concern for those monocyclic nitrogen atoms, it is preferable to select a conformation of the ring that does orient the nitrogen atoms inward, even when resulting in substituents on the reentrant atoms.



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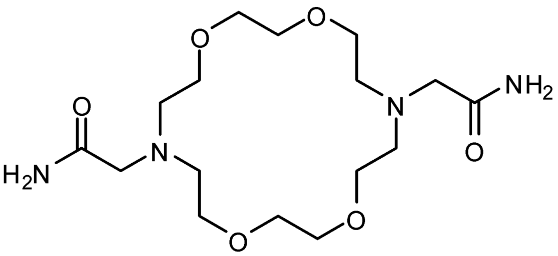
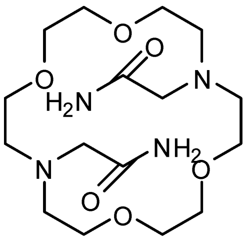
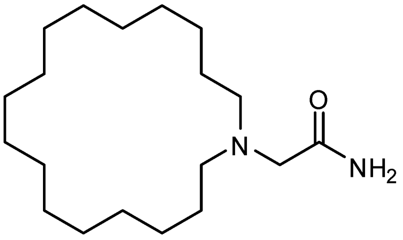


Not acceptable



Not acceptable

The previous exception is limited to cases where there would be a preference to position a substituted atom at a reentrant location even if it was not substituted, and should not be extended more generally. If a large ring is unlikely to form complexes because it contains only a small number of heteroatoms, it is preferable to depict the ring in a way that avoids substituents on reentrant atoms.



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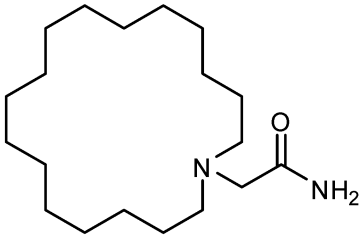


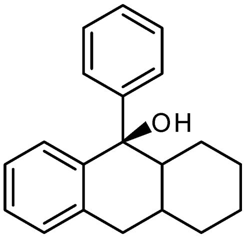
Not acceptable

GR-4.3 Avoidance of overlap between substituents

Since the clarity and legibility of a chemical structure diagram must always have priority over all else, it will often be necessary to consider alternatives to the general recommendations presented in GR-4.1 and GR-4.2 above. In particular, exact overlap between pairs of atoms or bonds is never acceptable. It is usually possible to choose among several possible approaches for avoiding such overlap. Those choices are discussed below. Furthermore, the following recommendations are presented in the order in which they should be considered. The techniques discussed in GR-4.3.2 should not be considered if overlap can be avoided completely using the recommendations of GR-4.3.1, and so on, although any single diagram may require several techniques to be applied to produce a depiction that is legible overall.

GR-4.3.1 Place a small substituent on the other side of a large substituent

For endocyclic atoms with bonds to one large substituent and one small one, GR-4.2.3 recommends that the large substituent be oriented with its bond directly outwards from the ring, and that the small substituent be positioned so that its bond bisects one of the angles adjacent to the bond to the large substituent. There are, however, two such angles. If the position normally recommended by GR-4.2.3 results in overlap that could be avoided by positioning the smaller substituent with its bond along the alternate bisector, then the alternate positioning should be chosen instead.



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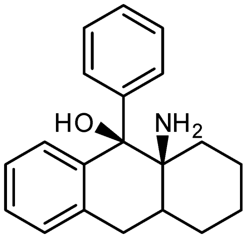

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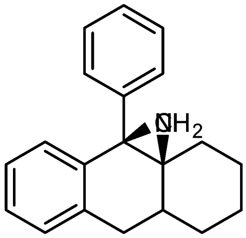
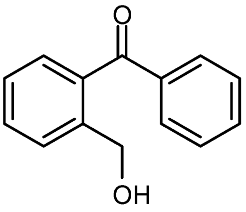


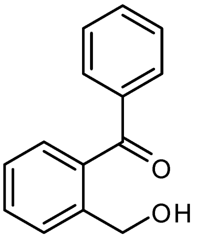
Not acceptable

GR-4.3.2 Rotate about a chain bond

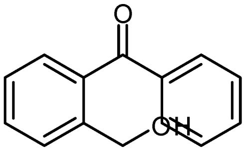
Rotation about a chain bond is perhaps the single most common and most useful technique for removing overlap between substituents. When there are multiple options for choosing a rotation bond, it is preferable to rotate along the bond that results in the smallest change to the overall structure diagram.



Preferred

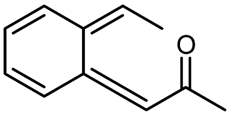


Acceptable

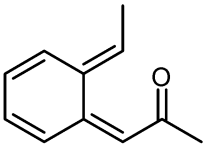


Not acceptable

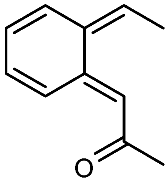
Rotations around stereogenic double bonds must not be considered.



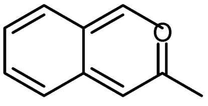
Preferred (see GR-4.3.7)



Wrong
[when representing
the molecule at left]



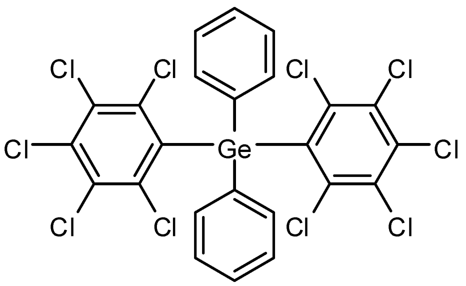
Wrong
[when representing
the molecule at far left]



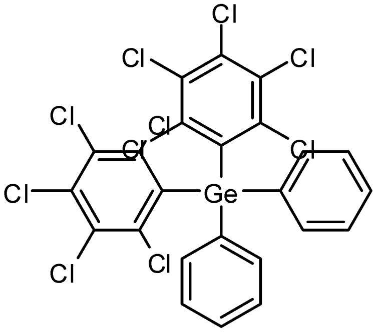
Not acceptable

GR-4.3.3 Swap neighboring substituents

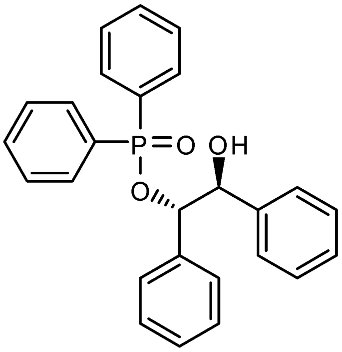
Positioning two large substituents adjacent to each other may result in overlap. One of those substituents should be swapped with a different adjacent substituent if doing so will produce a more legible diagram.



Preferred (see GR-4.3.7)



Not acceptable



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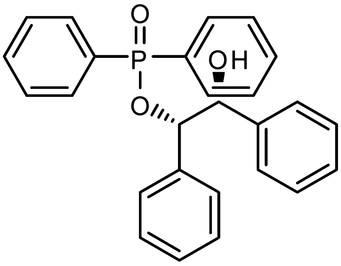
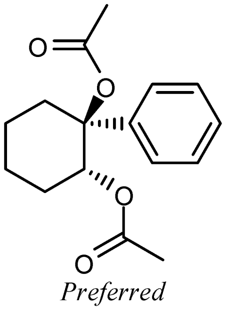


Not acceptable



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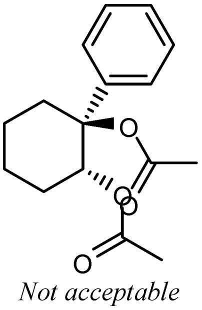

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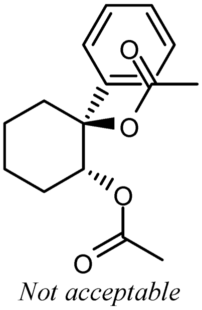
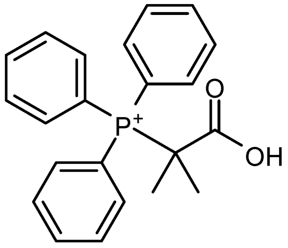
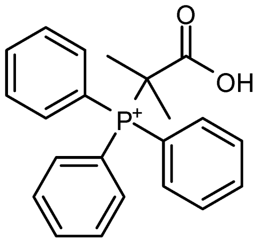


Not acceptable

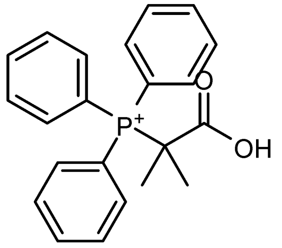
It is not preferred, however, to swap two substituents when the angles to their adjacent (non-swapping) substituents are not equal. In particular, when an atom has substituents separated by 120°, 90°, 30°, and 90°, it is not acceptable to swap either of the pairs that are separated by 90°.



Preferred (see GR-4.3.8)



Acceptable



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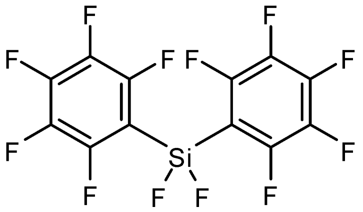
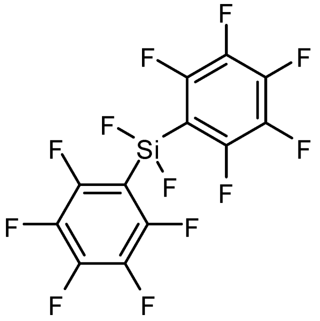


Preferred (see GR-4.3.8)



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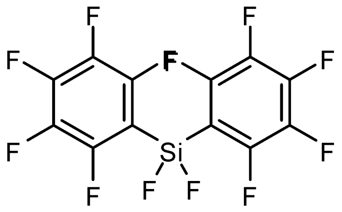
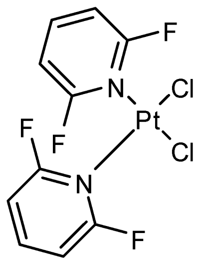


Not acceptable

It is not acceptable to swap substituents if doing so will change the stereochemical configuration of a stereogenic center, such as with a square planar complex.



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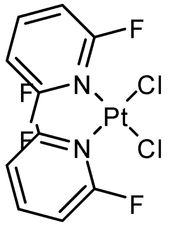
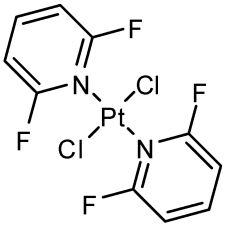


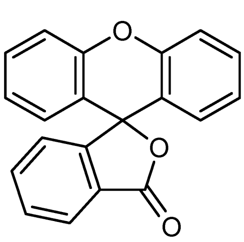
Not acceptable



Wrong
[when representing the molecule at left]

GR-4.3.4 Bend rings at a spiro union

With spiro molecules, it is common for structures to be very crowded. It is far better to distort the spiro union angle than it is to have overlapping atoms and bonds in the other parts of the structure.



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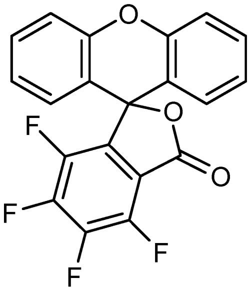

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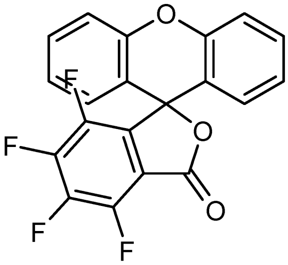
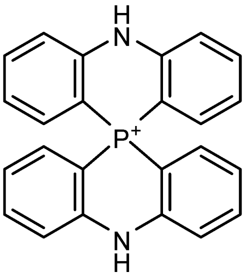


Not acceptable

GR-4.3.5 Stretch rings at a spiro union

When overlap is present as a result of a spiro union and cannot be avoided by distorting the spiro union angle, it may be necessary to distort the ring systems themselves. When such distortion is necessary, all ring systems should be translated outwards from the spiro atom, along with all substituents on those ring systems. This results in lengthening of the bonds to the spiro atom while leaving the other atoms and bonds unaffected.



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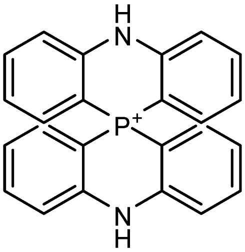
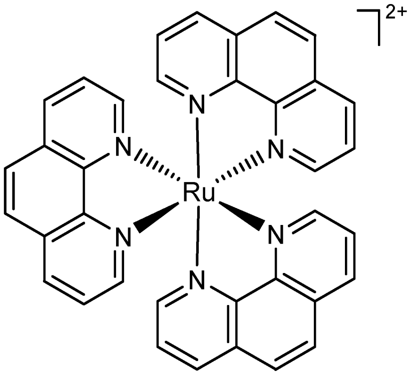


Not acceptable
[when representing the molecule at left]

Inorganic complexes with chelating ligands may be formally considered as having several spiro ring systems sharing the central metal atom. Distortion of these systems may similarly be necessary to avoid overlap.



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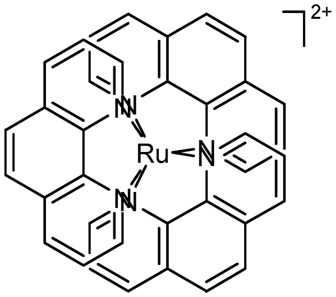
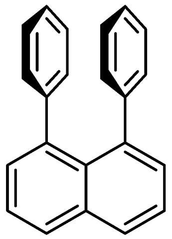


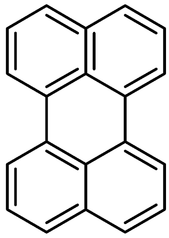
Not acceptable

GR-4.3.6 Change perspective of planar rings

When the bonds of two six-membered rings overlap each other exactly, the simplest method to eliminate that overlap may be to change the perspective of those rings, distorting them along the axis of a substituent bond so that they become narrower and no longer overlap.

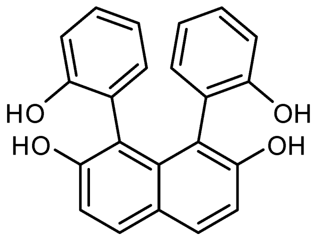


Preferred

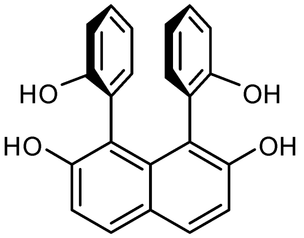


Not acceptable
[when representing the molecule at left]

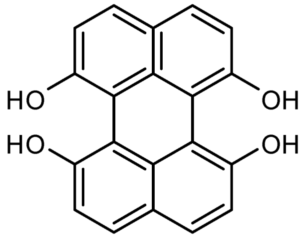
Because changing the perspective of a ring may describe a specific hindered biaryl configuration [6], it is not acceptable to change the perspective of planar rings that have additional substituents. That is to say, it is not acceptable to depict a molecule in such a way that a hindered rotation is implied in cases where the specific stereochemical configuration is not truly known. A different approach, such as changing the angle at a substituent (GR-4.3.8) is preferred in such cases.



Preferred (see GR-4.3.8)



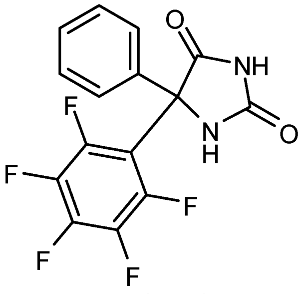
Not acceptable



Not acceptable
[when representing the molecule at left]

GR-4.3.7 Increase the length of a bond

After rotation along a bond (GR-4.3.1), increasing the length of a bond is the most useful single technique for avoiding overlap between substituents. Bonds may be lengthened to avoid overlap, but should not be extended further than necessary.



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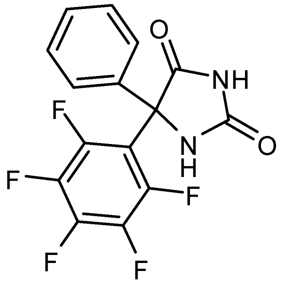
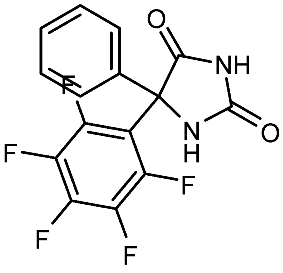
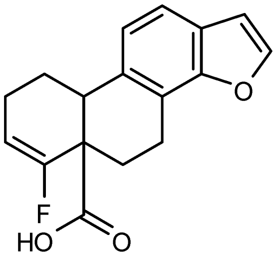


Acceptable



Not acceptable



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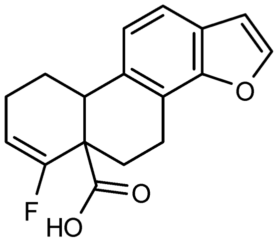
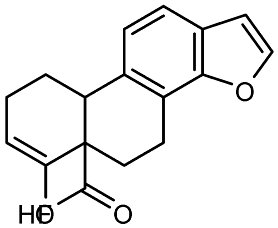
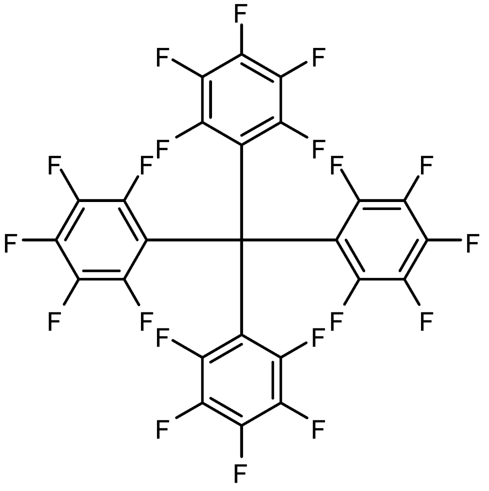


Acceptable

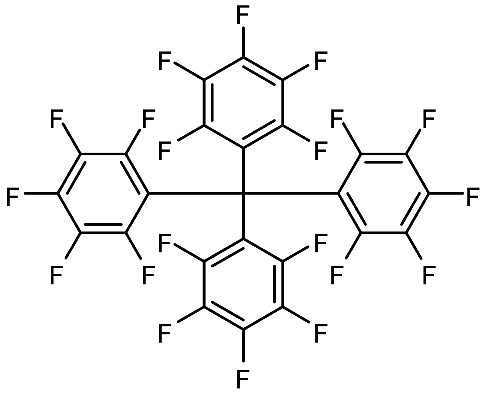


Not acceptable

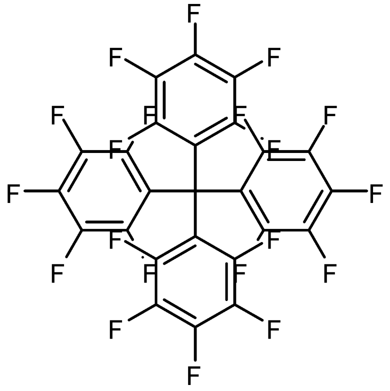
In rare cases, extreme lengthening of bonds (to twice their original length or more) may be the only option for producing a legible diagram. In general, however, extreme lengthening of bonds should be avoided in cases where a smaller bending of bonds (GR-4.3.8) would equally suffice.



Preferred

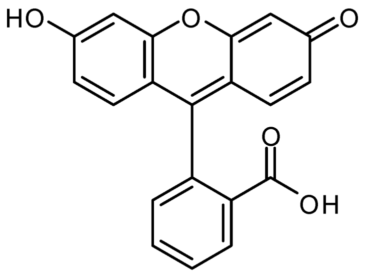


Preferred



Not acceptable

It is particularly important to consider increasing the length of a bond before considering bending bonds at an atom (GR-4.3.8). Stretching a bond will usually produce better-looking diagrams than will be produced by bending bonds at an atom, and will often produce diagrams that are drastically better-looking.



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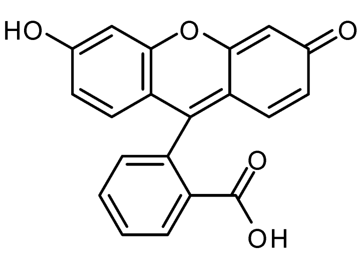
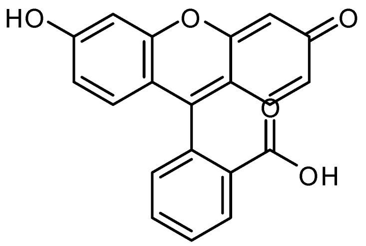
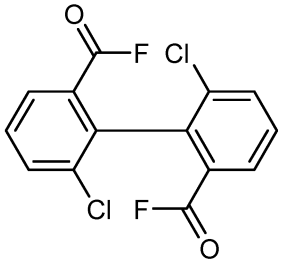


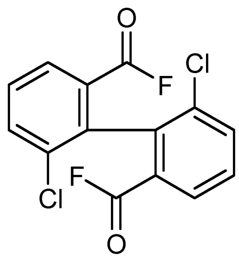
Acceptable



Not acceptable



Preferred



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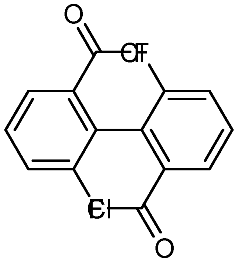
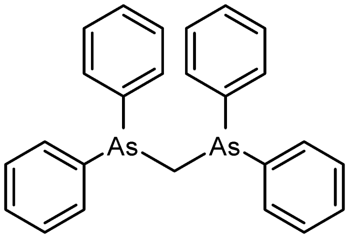
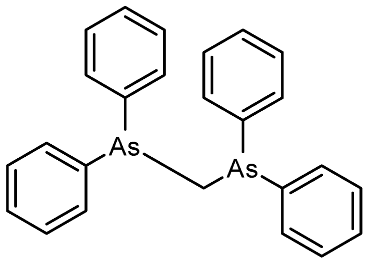


Not acceptable

If two conflicting portions of a chemical structure diagram are visually symmetric (ignoring atom types and bond types) or nearly so, it is preferable to lengthen two bonds equally a smaller amount rather than lengthening one of them a large amount or bending them.



Preferred



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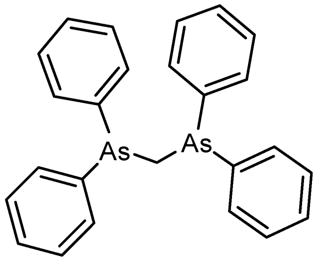

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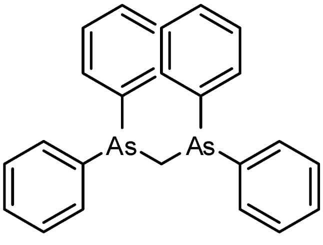
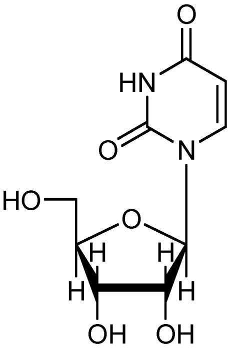


Not acceptable

In nucleosides and nucleotides, the bond connecting the pyrimidine or purine base to the carbohydrate fragment is also typically lengthened as a matter of style specific to those types of molecules.



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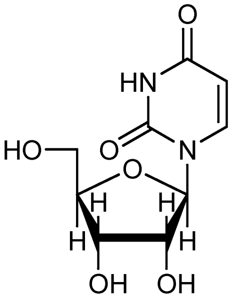
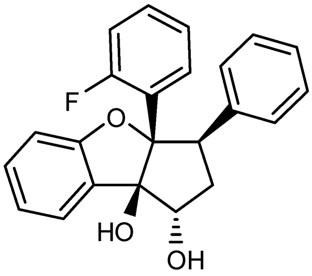


Acceptable

GR-4.3.8 Change angle at a substituent

When no other technique described above can successfully eliminate overlap and produce a legible structure diagram, it may be necessary to rotate an entire substituent.



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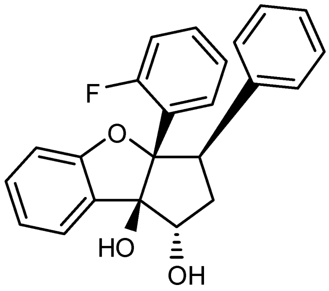

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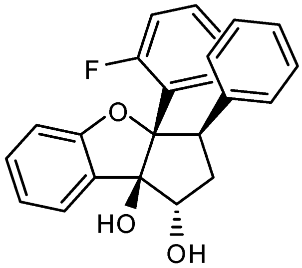
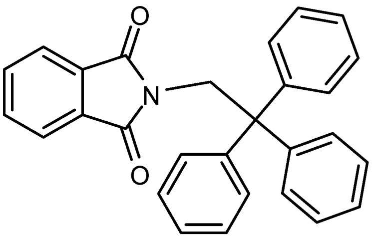
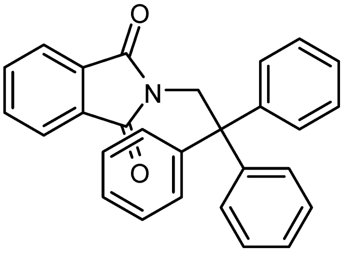


Not acceptable

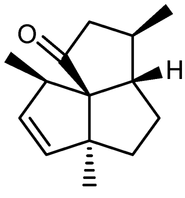


Preferred



Not acceptable

If two conflicting portions of a chemical structure diagram are visually symmetric (ignoring atom types and bond types) or nearly so, it is preferable to bend both of them equally a smaller amount rather than bending one of them a large amount.



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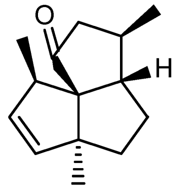

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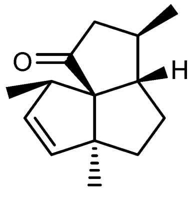

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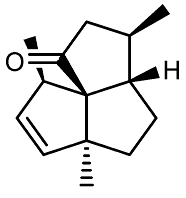

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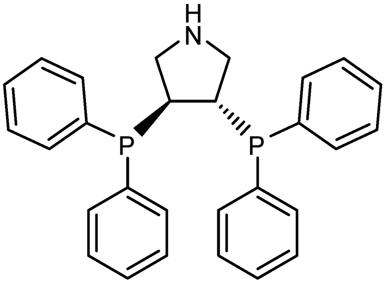
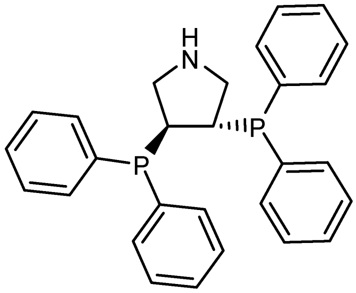


Preferred



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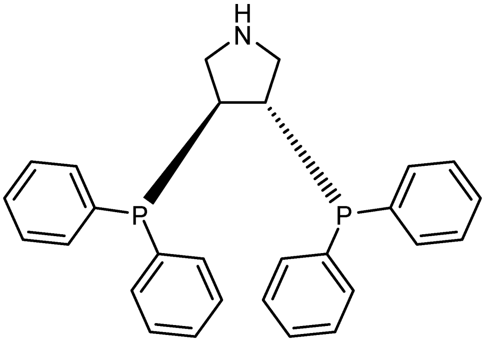
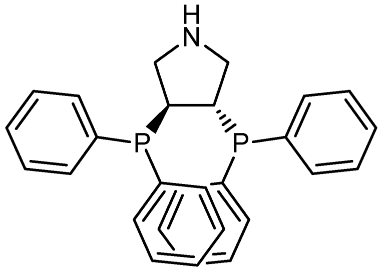


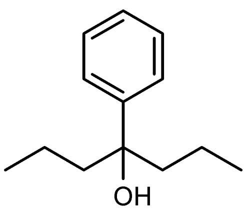
Acceptable



Not acceptable

GR-4.3.9 Rotate one substituent about its neighbors

When an atom has one small substituent in addition to three large substituents that are spaced more or less equally, the small substituent can bisect any of the three angles formed by the large substituents. Although the small substituent may have an orientation that is preferred in the absence of conflicts, it may be rotated to any of the three possible locations if positioning it in its preferred orientation leads to overlap that can be avoided by the rotation.



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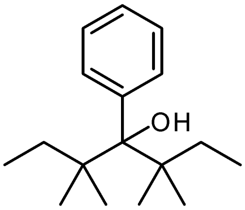
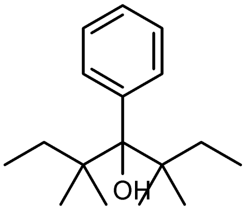


Preferred



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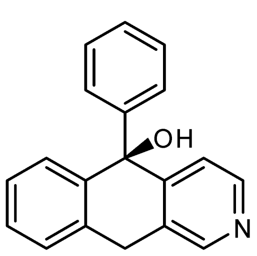

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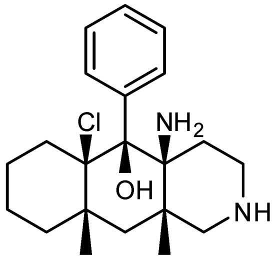
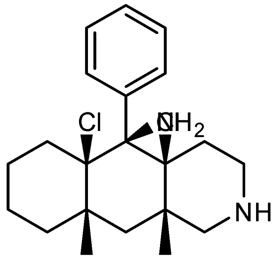
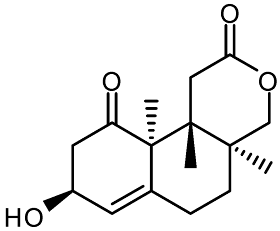


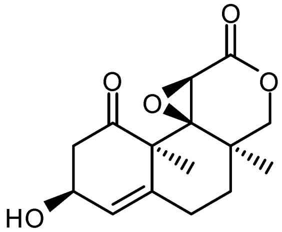
Preferred



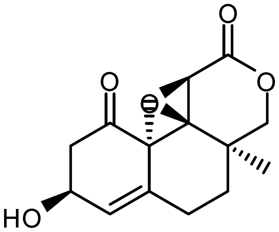
Not acceptable



Preferred



Preferred



Not acceptable

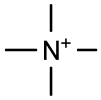
GR-5. CHARGES, UNPAIRED ELECTRONS, AND LONE PAIRS

Charges, unpaired electrons, and lone pairs associated with a chemical structure may be drawn as graphical objects separate from the main structure, or as textual characters within an atom label. In real molecules, charges and unpaired electrons are often delocalized. For this reason, the delocalized charge/unpaired electron representations shown in GR-5.3 and GR-5.7 should be used when the intention is to represent the actual situation as closely as possible. In many cases, however, a localized representation is more convenient, for example, as part of a mechanistic discussion. In such cases, it is appropriate to assign the charge or unpaired electron to a specific atom as discussed in GR-5.1 and GR-5.2.

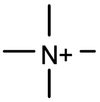
GR-5.1 Charges associated with specific atoms

Charge symbols associated with specific atoms should be positioned so that they are clearly associated with that atom and cannot be misinterpreted as being associated with some other atom. Each charge symbol should be considered as an addition to the corresponding uncharged diagram; the symbol should be placed near its associated atom in a way that best preserves the legibility of the diagram. It is generally not acceptable to modify a diagram to "make room" for a charge symbol. Charge symbols may be entered as text, by typing the appropriate characters as part of an atom label. They may also be positioned as separate objects that can be placed in positions not otherwise available when typing an atom label, such as above or below the element symbol, although it is preferable to place the charge toward the top right of its associated atom if it is possible to do so without sacrificing legibility.

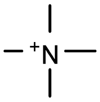
A positive charge is indicated by a plus sign. When assigned to a specific atom, the plus sign should follow that atom's element symbol. If the plus sign is entered as text (see GR-2), it should preferably be superscripted.



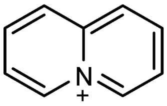
Preferred



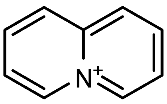
Acceptable



Not acceptable

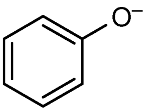


Preferred

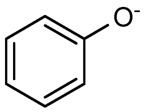


Preferred

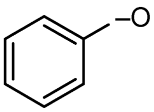
Negative charges are indicated similarly to positive charges, although a minus sign is used instead of a plus sign. A proper en-dash is preferred to a hyphen when possible.



Preferred

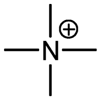


Acceptable



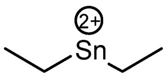
Not acceptable

It is acceptable to use circled symbols for single positive or negative charges, but it is not acceptable to depict multiple charges within a circle.

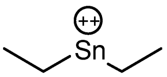


Acceptable

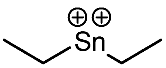
Acceptable



Not acceptable

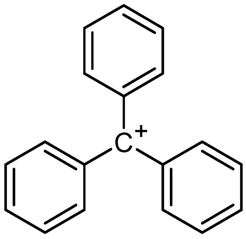


Not acceptable

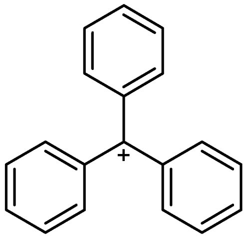


Not acceptable

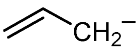
It is also acceptable to omit the atom label for carbon atoms with associated charges, but preferable to include the atom label for clarity.



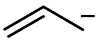
Preferred



Acceptable

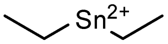


Preferred



Acceptable

If an atom is multiply charged, a number indicating the magnitude of the charge should be included directly before the plus sign. The numeric multiplier should only be used when the magnitude of the charge is greater than one.



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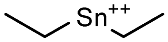
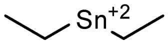
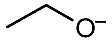


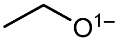
Not acceptable



Not acceptable



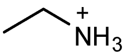
Preferred



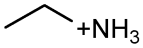
Not acceptable

In an atom label consisting of one non-hydrogen element symbol followed by the symbols for one or more hydrogen atoms, a charge symbol entered as text within the label should preferably be placed after all of the hydrogen symbols. It should not be placed immediately before or after the non-hydrogen element symbol. It is equally preferable to position the charge separately, above or below the non-hydrogen element symbol.

Preferred



Preferred



Not acceptable

Not acceptable

In atom labels containing multiple element symbols or abbreviations, a charge may be placed after the final element symbol in the label. If the label is reversed, the location of the charge symbol should similarly be reversed.

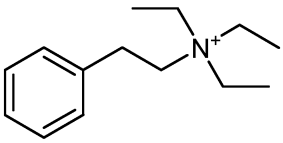
$—COO^-$

Preferred

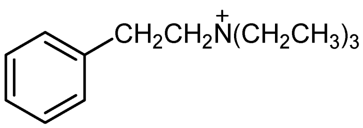
$^-OOC—$

Preferred

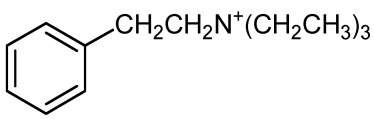
It is not acceptable to position charge symbols within an atom label, after some symbols, and before others. Such labels should preferably be avoided by drawing their atoms and bonds explicitly, or the charge should be positioned separately above or below the single element symbol within the label to which it is associated.



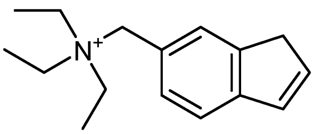
Preferred



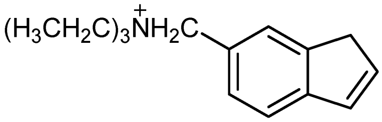
Acceptable



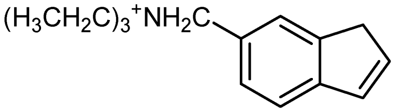
Not acceptable



Preferred



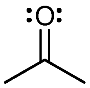
Acceptable



Not acceptable

GR-5.2 Lone pairs

Isolated lone pairs should be positioned, like unpaired electrons, close to the atom with which they are associated. They should normally be positioned exactly above, below, to the left, or to the right of the atom label, with the two dots of the lone pair parallel to the closest side (horizontally if above or below the label, vertically if to the left or the right). Positioning of lone pairs at other angles should be strongly avoided unless it is impossible to do otherwise.



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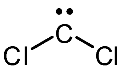

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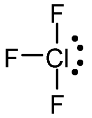
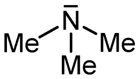
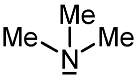


Preferred

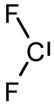
It is not acceptable to represent lone pairs as solid lines, since those lines can easily be misinterpreted as negative charges, textual underlines, or the letter L.



Not acceptable



Not acceptable

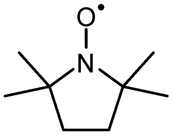


Not acceptable

Lone pairs are also used extensively by Lewis structures. Although that convention is useful for teaching introductory chemistry, the use of Lewis structures outside of educational situations is strongly discouraged.

GR-5.3 Unpaired electrons associated with specific atoms

The depiction of radicals is in most ways similar to the depiction of ions. An unpaired electron that is assigned to a specific atom is indicated by a dot (a “bullet” character when created on the computer). The dot should follow the atom’s element symbol, and it should also follow any hydrogen symbols associated with that atom. If the dot is entered as text, it should preferably be superscripted.



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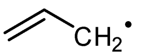

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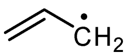
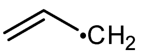


Acceptable



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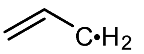
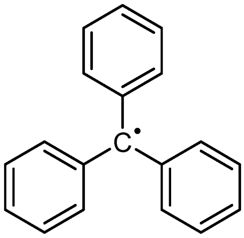


Not acceptable

It is acceptable to omit the atom label for carbon atoms with associated unpaired electrons, but preferable to include the atom label for clarity.



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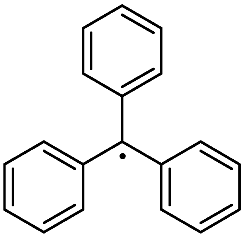
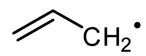
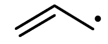


Acceptable



Preferred



Acceptable

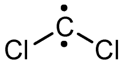
If an atom has more than one unpaired electron, a number indicating the count of unpaired electrons should be included directly before the dot, with both placed toward the top right of the associated atom.

$O_2^{2\bullet}$
Preferred

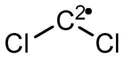
$O_2^{\bullet\bullet}$
Not acceptable

$O_2^{\bullet 2}$
Not acceptable

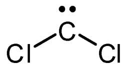
It is equally preferable to emphasize multiple radical character by placing the appropriate number of unpaired electron dots adjacent to the element symbol. However, two dots should be placed next to each other only when intended to represent a lone pair (GR-5.2). When representing two unpaired electrons, the dots must remain well separated, or a numeric multiplier must be used instead, as above.



Preferred
[when representing
two unpaired electrons]



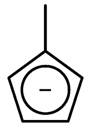
Preferred
[when representing
two unpaired electrons]



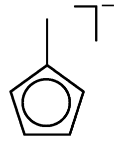
Preferred
[when representing
a lone pair]

GR-5.4 Delocalized charges and unpaired electrons

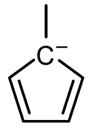
As discussed in GR-6, charges and unpaired electrons that are delocalized across several atoms should be depicted as separate graphical objects centered within the delocalized system. It is equally preferred to depict a “corner” at the top right of the diagram, with the symbol aligned with the top of the “corner” and to its immediate right.



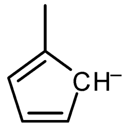
Preferred



Preferred



Not acceptable



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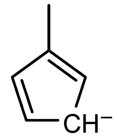
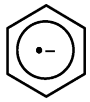


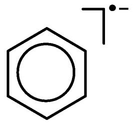
Not acceptable

GR-5.5 Radical ions

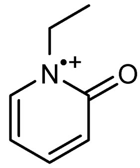
Radical ions should be depicted in similar ways, with the charge symbol immediately following the dot.



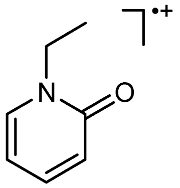
Preferred



Preferred



Preferred



Preferred

Monocharged polyradicals should be depicted with the unpaired electron dot and its associated multiplier enclosed in parentheses to avoid ambiguity about whether the multiplier applies to the charge as well.

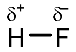
$NO^{(2\bullet)-}$

Preferred

GR-5.6 Partial charges

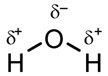
In contrast to formal charges, partial charge indicators typically represent unspecified (and usually non-integral) charge values. They are most commonly used as qualitative indicators of electronegativity or electropositivity. In general usage, partial charge indicators should be omitted from chemical structure diagrams; they should be used only when the author wishes to emphasize the partial charge distribution.

Partial charge indicators may be shown to emphasize the polar nature of certain covalent bonds, to show the charge distribution in a molecule, or to show the atoms participating in hydrogen bonds. The partial charges are designated by symbols δ^- and δ^+ placed near the atom in question (see GR-11). In diagrams of neutral molecules that show partial charges, at least one each of the δ^- and δ^+ symbols must be shown. The δ^- and δ^+ symbols represent unspecified "small quantities" and need not be balanced numerically even in neutral molecules.



$\overset{\delta^+}{H}-\overset{\delta^-}{F}$

Preferred



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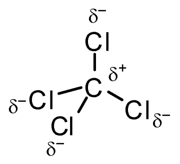
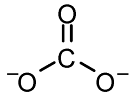


Preferred

The mixing of formal and partial charges in one structure should be avoided. In particular, it is not acceptable to use partial charge indicators to indicate the distribution of a real net charge via resonance.



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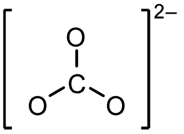
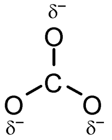
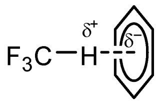


Preferred



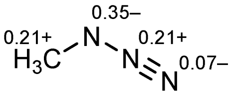
Not acceptable

Partial charge indicators may also be associated with delocalized systems, just as formal charge indicators may be used.



Preferred

Partial charges with specified non-integral values should be depicted analogously to the depiction of integral charges (see GR-5.1).



Preferred

GR-5.7 Polyatomic ions

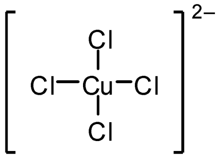
Polyatomic ions add an additional complication. Not only do they often include coordination bonds, but any net charge is usually best represented as delocalized over the entire ion (or a large part of it).

When exact atom-and-bond connectivity is not important, an ion may be best represented by its molecular formula. In accordance with the published recommendations for the nomenclature of inorganic chemistry, the formula should be placed in square brackets, and any charge should be reported as a superscript following the rightmost bracket. For more information about the formatting of formulas, see ref. [13].

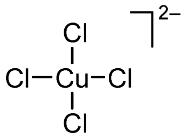
$[CuCl_4]^{2-}$

Preferred

If it is important to depict atoms and bonds explicitly, the ion should be drawn in full without concern for the delocalized charges. That structure should then be enclosed in large square brackets, and again any charge should be reported as a superscript following the rightmost bracket. For single fragments, it is equally preferred to forgo the leftmost bracket and depict simply a "corner" at the top right of the diagram, again with the charge as a superscript following the corner. The full paired brackets should be used in any situation where there is a possibility that the charge may be incorrectly associated with an additional structure diagram to the left of the intended one.

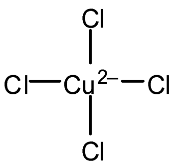


Preferred

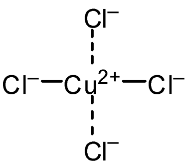


Preferred

Other structural depictions that involve localized charges are undesirable for a variety of reasons and should be avoided.



Not acceptable



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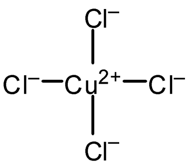
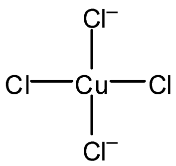


Not acceptable



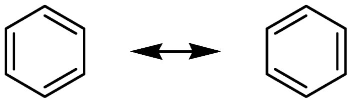
Not acceptable

SOFTWARE CAUTION: When working electronically, it is extremely important to specify delocalized charges appropriately, according to the capabilities of the software program you are using. At the time of writing this document, few chemical software programs are able to interpret delocalized charges, and both of the recommended depictions above would produce undesired results, resulting most likely either in a complete failure to interpret the structure or an incorrect interpretation. Given those weaknesses, software programs appear to most commonly prefer the structural depiction that localizes the negative charge on the metal atom. If you need to store structures of this type in an electronic format, please consult the documentation for the software programs you are using for recommendations on the best methods to use with that package.

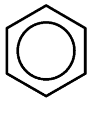
GR-6. AROMATIC RINGS AND OTHER TYPES OF ELECTRON DELOCALIZATION

Standard chemical structure diagrams imply a valence-bond interpretation, with two electrons localized in the general vicinity of a single bond, four electrons near a double bond, and six electrons near a triple bond. It is well known that the physical reality is not that simple, and that many molecules exhibit significant electron mobility.

Possibly the most common class is the collection of molecules characterized as having the characteristic of *aromaticity*. Aromatic molecules have a cyclic π system generally containing $4n + 2$ electrons, for $n = 0, 1, 2$, etc. Benzene is the archetypical example. Conventionally, benzene is commonly drawn with three single bonds and three double bonds, but physically, the six bonds of benzene are indistinguishable from each other. One way to depict this equivalence explicitly is to draw benzene not as a single structure but as a pair of resonance forms:



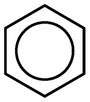
However, benzene is a very simple case. In more complex situations, it is rarely convenient to provide diagrams of all equivalent resonance forms. Instead, a shorthand has been developed that indicates all resonance forms by a curve or circle:



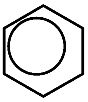
These recommendations discuss preferred usages for these sorts of circles, and by extension, similar curves that represent other types of electron delocalization

GR-6.1 Curves should be drawn uniformly

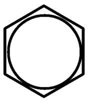
Curves should be drawn to approach all associated bonds at a consistent distance. That means, basically, that a circle should be well centered within its framework of bonds. At its closest approach, the circle should remain separated from each bond by a distance at least equivalent to the width of the bond, and no greater than twice the distance by which a double bond would be specified.



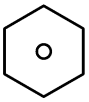
Acceptable



Not acceptable

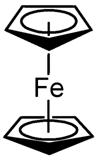


Not acceptable

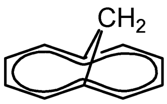


Not acceptable

Additionally, there is no restriction that curves be circular. It is extremely common for curves to be drawn as ellipses when they are associated with ring systems that are viewed in perspective. Curves do not have to be convex either (although non-convex delocalized systems are uncommon). Curves don't even have to be closed: delocalization can also occur in non-cyclic systems such as the allyl radical.



Preferred

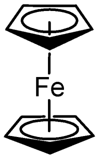


Preferred

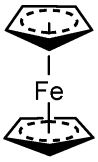
Preferred

GR-6.2 Curves should be solid

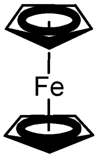
Curves should be drawn as solid lines with the same width as a single bond.



Preferred



Not acceptable

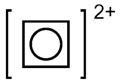


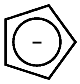
Not acceptable

GR-6.3 Curves represent delocalization

Above all else, curves represent delocalization. Accordingly, they may be used to depict systems that have delocalized electrons.


Preferred


Preferred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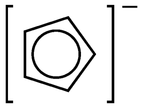
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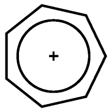
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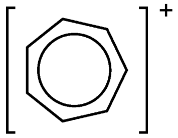
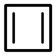

Preferred

Curves should not be used to depict systems whose electrons are primarily localized.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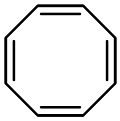
Not acceptable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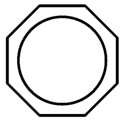
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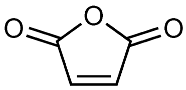
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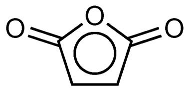
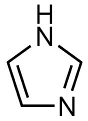

Not acceptable

Furan and pyrrole are examples of systems that can be represented with only one unique arrangement of single and double bonds even though they do have 4*n* + 2 electrons. It is acceptable to depict such systems using curves, but it is preferable to show the localized single and double bonds instead.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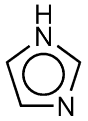
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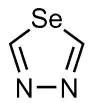
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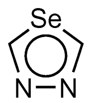
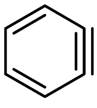

Acceptable

GR-6.4 Curves represent no more than delocalization

Curves only represent the delocalized electrons associated with their adjacent bonds. Most systems will have, at the very least, a σ framework that is not delocalized; it is this framework that is represented by the “single” bonds adjacent to the curve. Structures with additional unsaturation will need further representation. For example, a depiction of the delocalized form of didehydrobenzene would have a “double” bond replacing one of the “single” bonds.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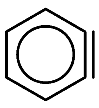
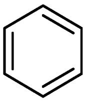

Acceptable

GR-6.5 Curves should only be used when delocalization is being represented

Curves represent delocalization, yet lots of structures have some delocalized elements. Although all such elements could be depicted with curves, there is little gained by doing so. On the contrary, the arbitrary use of curves can draw the viewer’s attention to insignificant portions of a structural diagram, and away from areas that are chemically more important such as an active site or a reactive group. Accordingly, curves should only be used when the delocalization is specifically being highlighted as an important feature of the structure.

When curves are not used, any alternating configuration of double bonds is acceptable within the further constraints discussed in GR-3.5.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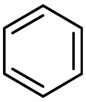
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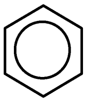
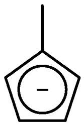

Acceptable

By the same token, the use of curves is preferred for any system that cannot be adequately represented by alternating single and double bonds.



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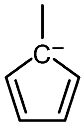

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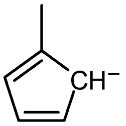

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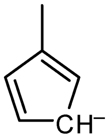
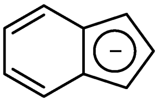


Not acceptable

It is generally not acceptable to use curves in two adjacent fused rings, since such diagrams are at best ambiguous in terms of the character of the shared fusion bond between the two rings. If it is known that there is delocalization over only one ring in a fused ring system, a curve should be used for that ring only.



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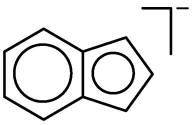


Wrong

GR-7. SALTS AND RELATED FORMS

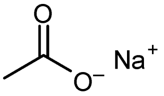
Salts are characterized by having more than one component, most commonly with one or more cationic components accompanied by one or more anionic component. Although such components are physically associated by ionic bonds, they are traditionally depicted on paper as separate, disjoint fragments. So, in addition to all the issues involved with drawing each individual fragment, salts should also be drawn with a consideration of how those fragments should be positioned in relation to each other.

It should be noted that although salts consist of cationic and anionic components, they are not always *drawn* with explicit charges. Many pharmaceuticals, for example, are isolated as hydrochloride salts. It is often reasonable—and, when the site of protonation is variable or uncertain, unavoidable—to draw such molecules with a neutral parent structure and a neutral hydrogen chloride.

Some molecules may be formally drawn with positive and negative charges within a single structural fragment. The discussion here is limited to compounds that are or could be depicted using multiple fragments.

GR-7.1 Depiction of ionic bonds

Structures that are known to be ionic should be depicted as such. They should be drawn with atoms bearing explicit positive and negative charges, and there should be a space (rather than a bond) between those atoms.



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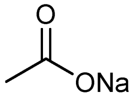

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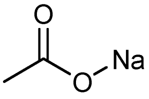
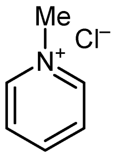


Not acceptable

GR-7.2 Positioning of components

The various components of a salt may be positioned relative to each other in one of two ways. If one of the components consists of a single atom, it may be “paired up” with an oppositely charged atom in a larger component, with the positioning of the larger fragment determined by other considerations as discussed in GR-3. The fragments should be positioned as if there were a single bond between the cationic and anionic centers, even if this requires that the cation be drawn on the right side of the anion. The positioning of the smaller fragment will then usually be determined according to other recommendations (that straight chains should not have arbitrary bends in them, for example).



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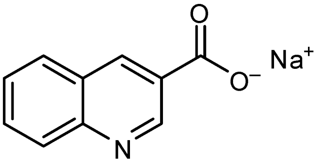

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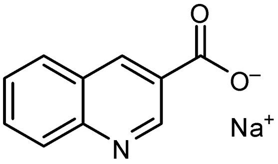
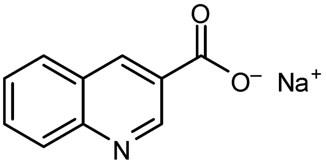


Preferred

Alternatively, the components of a salt may be depicted next to each other. This positioning is acceptable for single-atom components, and preferred for larger ones. If the components are of similar size, positively charged components should preferably be positioned to the left of negatively charged ones; if they are significantly different in size, the larger components should be positioned to the left of the smaller ones.



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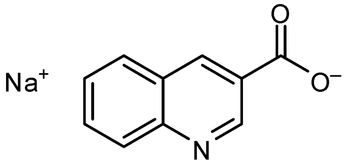
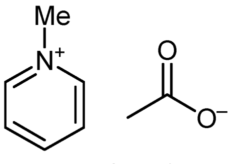


Acceptable



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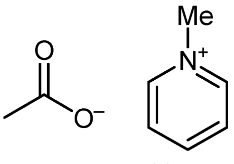
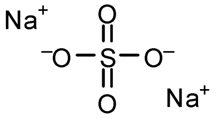


Acceptable

For salts with more than two components, it is preferable to stack several small components vertically if it is possible to do so without exceeding the height of the largest component. It remains equally preferred to position multiple single-atom components near oppositely charged atoms in the larger component.



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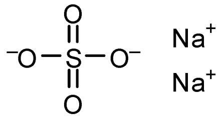

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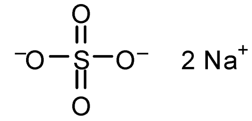

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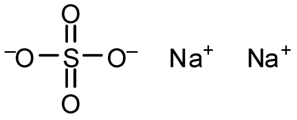
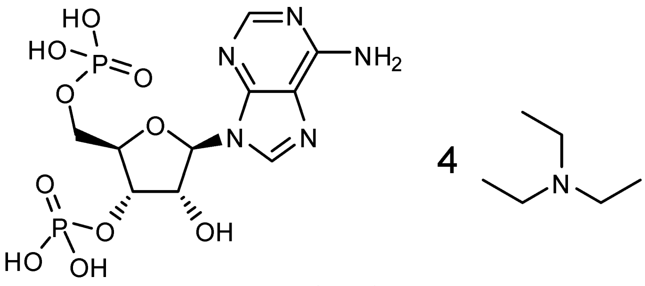


Acceptable

When a salt contains many identical fragments, it is preferable to depict only one of them, with that component preceded by a number that indicates its full stoichiometry. It remains acceptable to depict all of the identical components, of course.

SOFTWARE CAUTION: At the time of writing this document, there are few computer software programs that are able to recognize stoichiometric multipliers. If chemical structure diagrams of multicomponent salts are required for use within an electronic environment, it may be necessary to depict all of the components explicitly.



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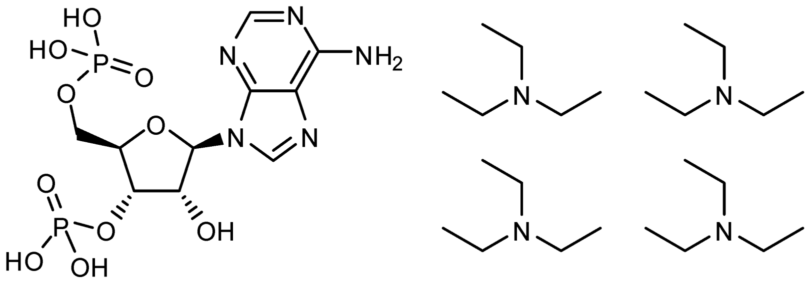
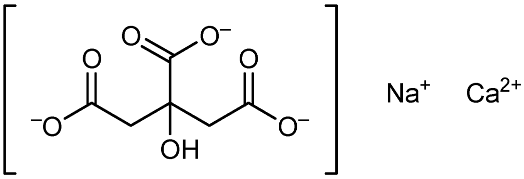


Acceptable

GR-7.3 Salts drawn in unspecified form

In addition to the styles discussed above, an alternative style depicts the ions in structural form, but without any implied association between the ions. This is the preferred form for mixed salts where there is more than one positively charged atom or more than one negatively charged atom, and where the author wishes to treat them separately. In this style, the largest ion(s) should be enclosed in brackets, to emphasize that there is no structural association between it (them) and the other ion(s). The selection of ions to bracket is performed solely based on size, and so the bracketed ion(s) may be positively or negatively charged. The bracketed ions are placed on the left, and the other ions are placed on the right.

The various ions should be clearly separated from each other, but not separated so widely as to seem wholly unrelated. A separation distance roughly equivalent to the structure's average bond length is usually reasonable for most purposes.



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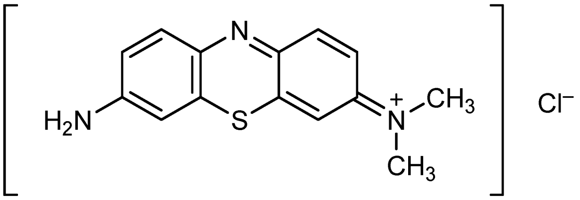
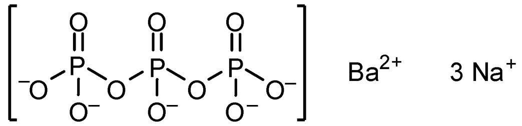


Preferred

When an ion appears more than once, it may be depicted a single time, with an additional numeral present to indicate the repeat count.

If the repeated ion is represented by a molecular formula, the repeat count is placed to the left of the formula in regular-style (non-superscripted, non-subscripted text) and separated from the formula by a space.



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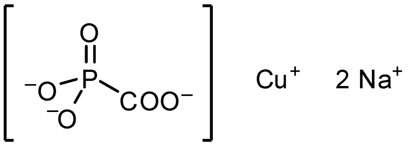
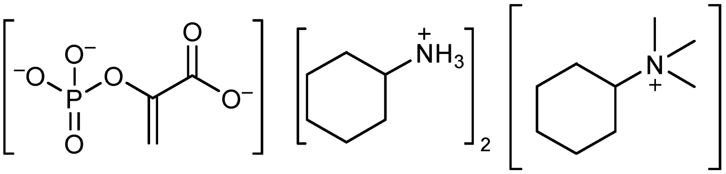


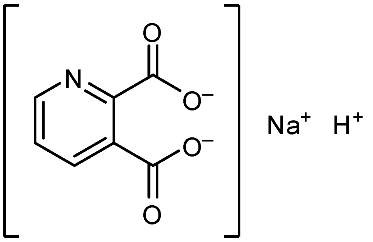
Preferred

If the repeated ion is represented in structural form, it should be enclosed in brackets, and the repeat count should be positioned as a subscript toward the bottom-right of the rightmost bracket of the ion.



Preferred

"Partial" or "acidic" salts would be best drawn in a manner similar to other types of salts.



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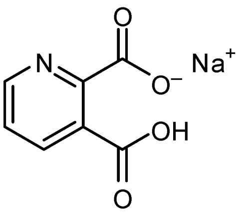
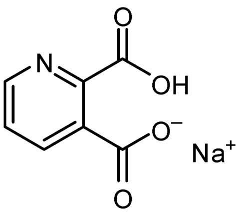
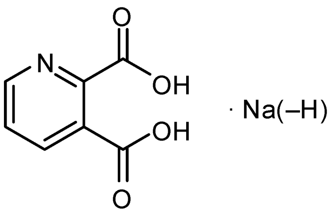


Preferred
[when specific ionization pattern is known]

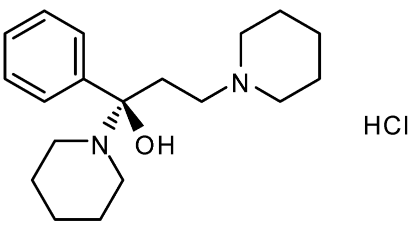


Preferred
[when specific ionization pattern is known]



Not acceptable

Salts drawn as multiple neutral components (such as hydrochlorides) should not have the larger structure enclosed in brackets. The larger structures are drawn to the left, and the smaller ones to the right, with a reasonable separation as discussed above. It is acceptable (but not required) to precede small neutral components by a center-dot if those components are represented as formulas. The center-dot, if present, should be separated from the formula by a space. If a repeat count is required as well as a center-dot, the center-dot should not be separated from the repeat count, but the repeat count should still be separated from the rest of the formula by a space.



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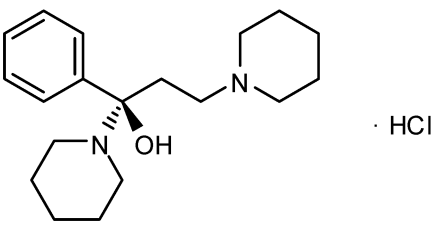


Acceptable

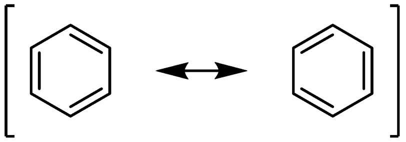
GR-8. DOUBLE BONDS, DATIVE BONDS, AND CHARGE-SEPARATED FORMS

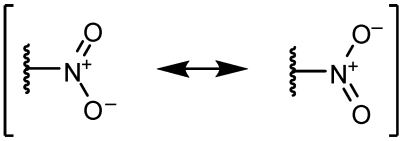
"The nitro problem" is one of the most familiar issues in chemical informatics: How should a nitro group be best represented? Experimentally, the two oxygen atoms are equivalent, so it would make sense to depict them symmetrically. However, any way to depict them symmetrically will either violate the popular "octet rule" or force a double positive charge on the nitrogen atom. Conversely, any attempt to honor the octet rule results in oxygen atoms that appear to be non-equivalent.

Similar problems arise for molecules based on sulfur, phosphorus, and related elements. Furthermore, all of these are fairly common functional groups, and cannot readily be pushed aside as "unusual" cases.

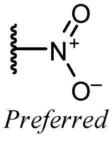
GR-8.1 Nitrogen compounds

In the case of nitrogen compounds, a charge-separated depiction is recommended. While this does not preserve the visual appearance of equivalent oxygen atoms, we feel that it is acceptable by analogy with aromatic structures. Benzene is commonly drawn with three single bonds and three double bonds, but it is understood that all six bonds are actually equivalent due to resonance delocalization between the two localized forms. Similarly, nitro groups should be considered to have both oxygen atoms equivalent through a similar resonance pair.





It is equally preferable, in the case of nitro groups, to avoid entirely the issue of depiction and instead display the functional group using the NO_2 abbreviation as discussed in Table III. As discussed in GR-6, it is acceptable to represent delocalization with a curve when emphasis is needed for that delocalization. Other depiction styles are not acceptable, whether using two double bonds, a dative bond, or further separated charges.



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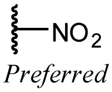
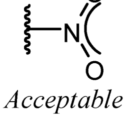
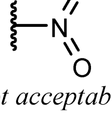


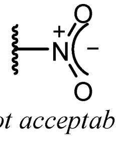
Preferred



Acceptable



Not acceptable



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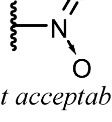

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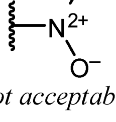

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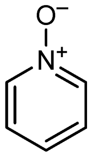

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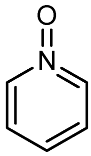

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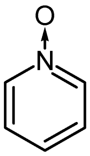
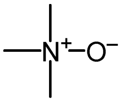
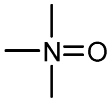


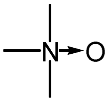
Not acceptable



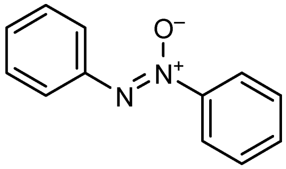
Preferred



Not acceptable



Not acceptable



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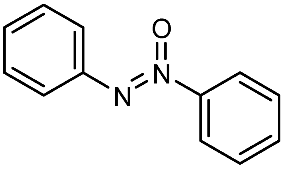

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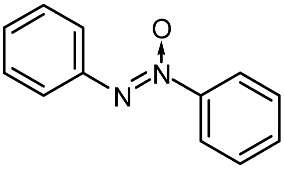
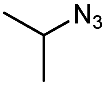
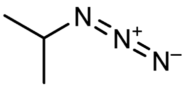


Not acceptable

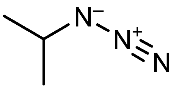
Azides and the structurally similar diazo compounds should preferably be depicted as having two double bonds with a formal negative charge on the terminal atom and a formal positive charge on the atom adjacent to it. It is also acceptable to depict such compounds with a single bond and a triple bond, especially when discussing results that show experimental differences in those bond lengths.



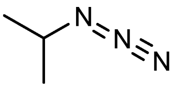
Preferred



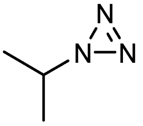
Preferred



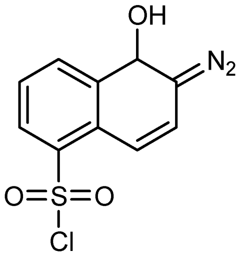
Acceptable



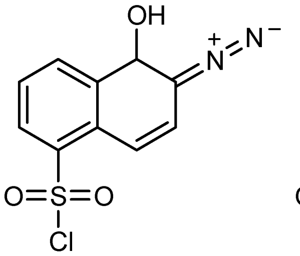
Not acceptable



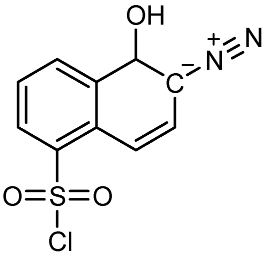
Wrong [when representing 2-azidopropane]



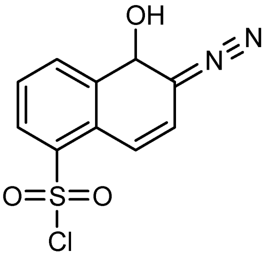
Preferred



Preferred



Acceptable

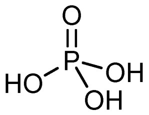


Not acceptable

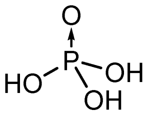
SOFTWARE CAUTION: Although both depiction styles may be used for depicting azides and diazo compounds, different software programs may interpret the two styles as referring to chemically different compounds. It may be necessary to use only the Preferred style when working in electronic environments.

GR-8.2 Phosphates and related Group V compounds

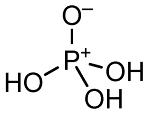
Functional groups containing phosphorus, arsenic, antimony, and bismuth are preferably depicted with normal single and double bonds and without the addition of extra formal charges, even though such representations will violate the octet rule.



Preferred

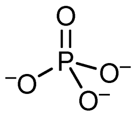


Not acceptable

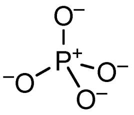


Not acceptable

This depiction style should be preserved even for anions. The four oxygen atoms are chemically equivalent, but that equivalence is commonly understood through resonance.



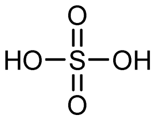
Preferred



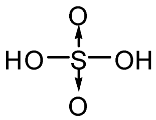
Not acceptable

GR-8.3 Sulfoxides, sulfones, sulfimides, and related Group VI compounds

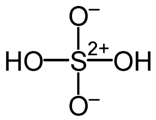
Functional groups containing sulfur, selenium, and tellurium are also preferably depicted with normal single and double bonds and without the addition of extra formal charges, even though such representations will violate the octet rule.



Preferred

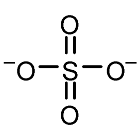


Not acceptable

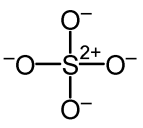


Not acceptable

Again as with phosphorus, this depiction style should be preserved even for anions. The four oxygen atoms are chemically equivalent, but that equivalence is commonly understood through resonance.

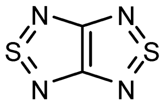


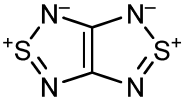
Preferred

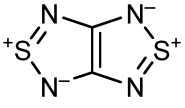


Not acceptable

Similarly, there are some uncommon heterocycles that may be depicted either as zwitterions or with two double bonds to the chalcogen atom. The form with two double bonds is preferred.


Preferred


Not acceptable


Not acceptable

GR-9. VARIABLE ATTACHMENT POINTS AND SUBSTITUENTS

Due to the nature of chemical research and reporting, authors will often need to discuss collections of closely related molecules. In cases where storage space is not a concern, it is generally preferable to depict each molecule individually, for example, as a series of discrete records in a chemical database. However, there are also many cases where storage space is indeed at a premium; this is common in journal articles, for example. Sometimes also it is necessary to refer to the closely related molecules as a single unit; this is common in patents. These guidelines suggest some ways to refer to collections of chemical structures.

In general, variable structures are depicted by providing a parent or "core" structure with marked locations of variability, accompanied by lists of atoms, substructures, or classes of substructures that might be present at each of those marked locations. When the core structure has only one variable location, the total number of structures equals the total number of replacements listed for that location. Core structures with more than one variable location may represent the *combinatorial product* of the number of replacements available for each location. That is to say, a core structure with two variable locations having three possibilities for the first location and seven possibilities for the second location would represent as many as 21 total molecules (the final number of unique molecules may be fewer due to symmetry) if the two locations are considered independently as default. Collections of these types are commonly found in journal articles and are an excellent space-saver when discussing collections of closely related molecules such as are produced in a series of similar reactions.

In addition to listing specific replacements, it is also possible to describe entire classes of substituents, for example, saying that a certain location may contain "an aryl group, or a heteroaryl group of no more than seven atoms". Diagrams that define broad classes of structures such as these are known as Markush structures, after Eugene Markush, the first inventor to include them successfully in a U.S. patent [28]. In structures of this type, it is generally *impossible* to list all possible members of the collection. Markush structures continue to be common in patents, and are increasingly being used to generate combinatorial libraries for electronic analysis.

GR-9.1 Small substituents

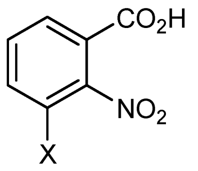
When all variable substituents are small, they can be enumerated as a simple list. The list may be provided as a separate caption near the parent structure, or it may be included as a complex atom label directly in the parent structure itself. When separated from the parent structure, the list should preferably be positioned below or to the right of the parent. If the parent structure is itself part of a larger reaction, the list must be positioned so that it does not interfere with understanding of the larger reaction. That is, it should be positioned below the parent structure rather than to the right of it, for normal horizontal-reading reactions (see GR-11.3 for additional notes on structure-based annotations).

When the variable list is provided separately from the parent structure, the point(s) of variability in the parent should be indicated by an unambiguous label. This label should be chosen so that it cannot easily be confused with other valid element symbols or fragment abbreviations. Traditionally, the letter "R" is widely used, followed by a superscripted number (R^1, R^2, etc.) or prime(s) (R', R'', etc.) if necessary to distinguish different groups. It is not acceptable to use a letter followed by a subscripted number, since subscripted numbers are more commonly used to indicate repeat counts, and confusion between the two is inevitable. Other common symbols include X, Z, and G. Unless otherwise specified, multiple sites within a single diagram are considered to be independent (that is, the representation includes all combinatorial products).

A label may also be used without an explicit list of allowed substituents. Such labels may be used to indicate that substitution is permissible or likely, without specifying anything about the substituents themselves. If more than one substituent is indicated on the structure and those substituents may be different, unique labels (R^1, R^2, etc.) should be used to emphasize the possibility of that difference.

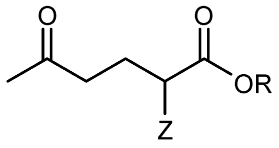
Most commonly, variable substituents are connected to the parent structure by only one bond. Variable substituents connected to more than one bond should only be used when all fragments within the variable list are monoatomic or otherwise symmetric in terms of substitution.

In the absence of an external connection point drawn explicitly on the members of the variable list, each item in that list is assumed to connect to the parent structure according to the standard rules of valence, or by the first atom in the item if more than one atom has free valences.



X = OMe, Me

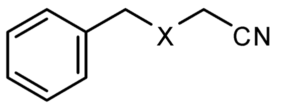
Preferred



$Z = NH_2$, NCO

R = Pr, allyl

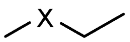
Preferred



$X = NH, O, S, CH_2$

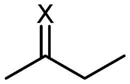
Preferred

Variable lists that also imply changes to bonding patterns are extremely confusing to the reader and are therefore not acceptable.



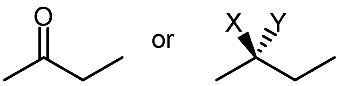
X = C=O
CHOH
CHCl
CHN_3
$CHNH_2$

Preferred



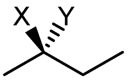
X = O
OH, H
Cl, H
H, N_3
H, NH_2

Not acceptable



X = OH, Y = H
X = Cl, Y = H
$X = H, Y = N_3$
$X = H, Y = NH_2$

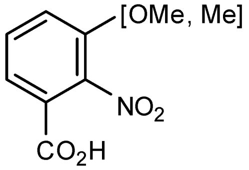
Preferred



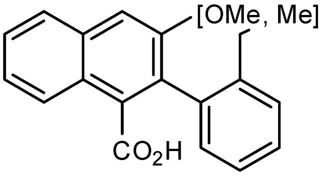
X, Y = O
X = OH, Y = H
X = Cl, Y = H
$X = H, Y = N_3$
$X = H, Y = NH_2$

Not acceptable

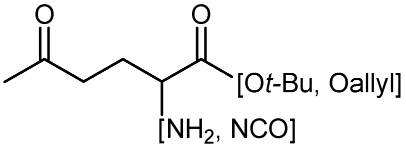
When the variable list is provided directly within the parent structure as an atom label, each list should be enclosed in brackets to make it clear that the terms are associated. This should only be considered for small lists that can be provided without impinging on other portions of the parent structure.



Acceptable

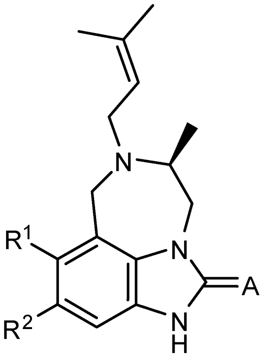


Not acceptable



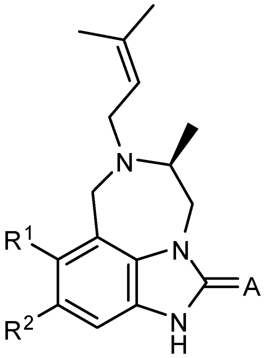
Acceptable

Unadorned lists are simplest to understand and should always be preferred to textual descriptions of the variable substituents.



A = S, O
R^1 = Cl, F, Me, pyridin-2-yl, OMe, H, CN
R^2 = H, Cl

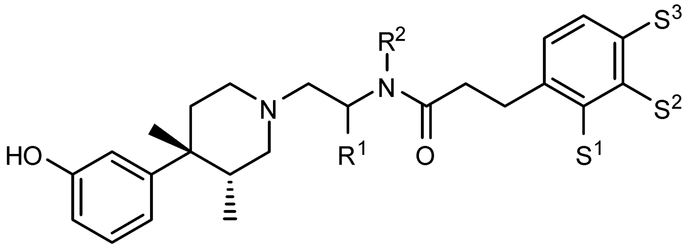
Preferred



A is S or O, R^1 can be Cl, F, methyl, pyridin-2-yl, methoxy, H, or CN, and R^2 can be H or Cl

Not acceptable

Large collections of small substituents may often be most conveniently presented in tabular form, especially when the substituents are not independent.



Compd.	R^1	R^2	S^1	S^2	S^3	% inhib.
...						
8	iPr	H	H	H	OH	71
9	iPr	H	H	H	OH	11
10	iPr	H	H	H	H	28
11	iPr	H	H	OH	H	20
12	iPr	H	OH	H	H	25
13	iPr	H	H	H	OH	6
14	iPr	H	H	H	OH	15
15	iPr	H	H	H	F	26
16	iPr	H	H	OH	OH	31
17	iPr	H	H	OCH_3	OH	42
18	iPr	H	H	H	OCH_3	16
19	H	H	H	H	OH	11
20	CH_3	H	H	H	OH	20
21	H	CH_3	H	H	OH	0
22	CH_3	CH_3	H	H	OH	1
23	Ph	CH_3	H	H	OH	7

Preferred [29]

Parent structures with a substituent that is attached at one of several ring atoms may be depicted by drawing that substituent attached to a bond that extends into the center of a ring. In printed works, it is assumed that the substituent may then be attached to any of the ring atoms as is allowed by normal bonding rules. When working in electronic formats, it may be possible to specify that the substituent can be attached to certain of the ring atoms and not to others, depending on the capabilities of the software being used. If more than one substituent may be independently connected to various ring atoms, the bonds attached to those substituents should both extend toward the center of the ring, but should not themselves be connected to each other.

SOFTWARE CAUTION: Variable lists of all sorts pose many problems for interpretation by computer software. At the time of writing this document, even the simplest forms can be recognized by only a few software programs, and extended variable lists are not supported by any software. Although these forms are extremely compact and can be a boon to printed publication, it will usually be necessary to draw all forms explicitly when using current programs.

GR-9.2 Predefined substituent classes

Sometimes a substituent can be defined only by describing the general class to which it belongs. Some classes are common enough that specific labels have traditionally been used to define them. When used without accompanying text to further describe the substituents, the labels in Table GR-9.1 should only be used to represent the specific substituent classes listed.

Table GR-9.1 Structural labels that refer to a specific class of substituents.

Alk	alkyl
Alkyl	alkyl
Ar	aryl
Aryl	aryl
E	electrophile
EWG	electron-withdrawing group
M	metal
Nu	nucleophile
Q	heteroatom (not hydrogen, not carbon)

Use of those labels in conjunction with accompanying descriptive text should be avoided. However, if descriptive text is used with one of these labels, it should be used only to further restrict one of the listed classes (“Ar = halogen-substituted aryl”) and should not be used to describe an entirely unrelated set of substituents (“Ar = methyl, ethyl, or propyl”).

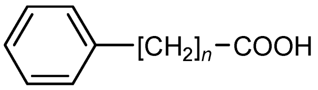
If more than one of these labels is required in a given structure, they may be differentiated by the use of superscripted numbers or primes as described above.

The use of the “Ar” label should be strongly avoided in any context where it might possibly be interpreted to represent an argon atom. Since argon forms few molecules, contexts of this sort are exceedingly uncommon.

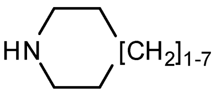
The “R” label has in some cases been used to indicate alkyl substituents, and in other cases to indicate non-hydrogen substituents. However, it is more frequently used in the fully generic sense to indicate “some unknown substituent” without further restriction. Similarly, “X” has been used to represent halogen atoms or, sometimes, also halogen-like substituents such as tosyl. We recommend that these labels be used either in conjunction with descriptive text (“R = alkyl”) or in the fully generic sense.

GR-9.3 Variable chain length and ring size

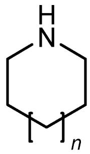
It is often convenient to specify that a chain or ring must be present, but that its actual length or size may vary. This may be accomplished by specifying the ring or chain atom, generally CH_2, within brackets, then by following the brackets by a subscripted range of values to indicate the minimum and maximum number of those atoms that may be present. Only homogenous chains should be represented in this way. If multiple element types or unsaturated bonds may be present, they should be represented outside of the variable section or another type of notation should be used entirely.



Preferred



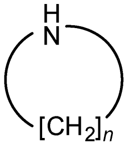
Preferred



Preferred

It is also acceptable to use curved lines to emphasize that the number of atoms within a ring is variable or unknown.

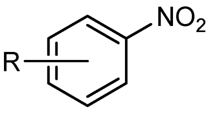
SOFTWARE CAUTION: At the time of writing this document, there is no software that supports the use of curved bonds. Although this representation is acceptable for general depiction, it must be considered not acceptable in cases where the resulting diagram will be further modified in electronic format.



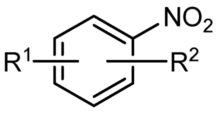
Acceptable

GR-9.4 Variable attachment location

In addition to allowing the type of attachment to vary, it may also be convenient to indicate that the attachment's *location* is variable as well. This type of notation should be restricted to substituents that are known to be bonded to a specific ring, but at an unspecified or unknown atom of that ring. The substituent will always replace a hydrogen atom on one of the ring atoms, and cannot be bound to any atom that lacks an attached hydrogen atom. Unless explicitly specified otherwise, such diagrams imply that the substituent may be bonded to any ring atom that has an attached hydrogen atom. Similarly, if more than one such substituent is present for a given ring, the bonding of each substituent is independent of all of the others. In other words, all permutations of bonding are represented by the single diagram.



Preferred
[representing any of five molecules (three unique molecules)]



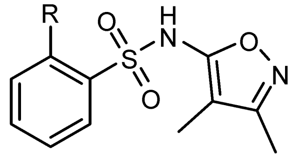
Preferred
[representing any of 20 molecules (10 unique molecules)]

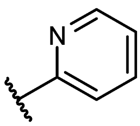
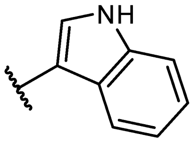
SOFTWARE CAUTION: When working electronically, it is extremely important to specify the variable attachment correctly, according to the capabilities of the software program you are using. If the variable attachment is specified incorrectly, the structure may be interpreted as two disjoint fragments, with the variable bond being interpreted as a normal bond to a carbon atom. In addition to losing the intended variability, this misinterpretation will also add an additional CH_4 to the structures perceived formula: CH_3 for the "methyl group" at the center of the ring, and one more H for the location in the ring that was not substituted as intended.

GR-9.5 Large substituents

Graphically large substituents and large collections of substituents are most conveniently described in tabular form.

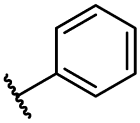
SOFTWARE CAUTION: At the time of writing this document, there is no software that is able to interpret this sort of tabular data. Nonetheless, it remains as an acceptable way of depicting large substituents and large collections of substituents in printed form, even if it may be necessary to draw all individual molecules explicitly if they are to be further modified by computer software.



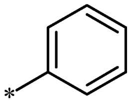
Compd.	R
1	Ph
2	
3	

Preferred [30]

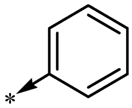
In cases where the external connection points must be indicated for the variable substituents, such indication should be unambiguous. Some attachment types are shown:



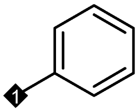
Preferred



Not acceptable



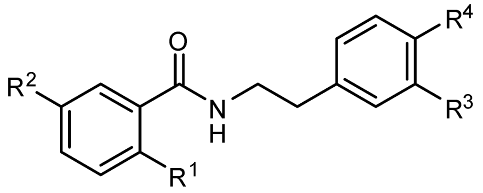
Not acceptable

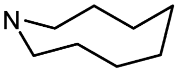
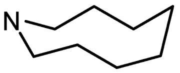
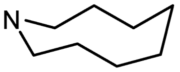
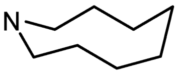


Not acceptable

Philosophically, an external connection point represents a "null" atom. That is, the associated bond is connected only to one atom. When the full structure is enumerated, the site represented by the external connection point is filled by an atom in the parent structure.

When a structural fragment is drawn with explicit bonds, the location of its attachment point should be shown explicitly. The attachment point should not be implied simply by the absence of a hydrogen atom on a drawn structure.



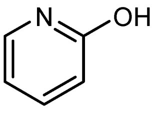
Compd.	R^1	R^2	R^3	R^4
1		Cl	H	COOH
2		Cl	OEt	COOH
3	H	Cl	H	COOH
4		H	H	COOH
5		Cl	H	H

Not acceptable [31]

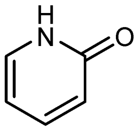
The point of attachment should not be indicated in a subtle manner such as by varying the length of a bond.

GR-10. TAUTOMERS

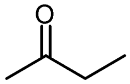
Graphical representations of molecules that can undergo tautomeric rearrangements always represent the single tautomer as drawn. This is consistent with IUPAC recommendations on chemical nomenclature [13,20].



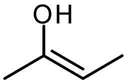
Preferred



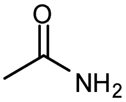
Preferred



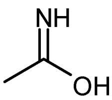
Preferred



Preferred



Preferred



Preferred

GR-11. ANNOTATIONS

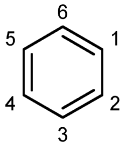
Annotations are bits of text that are closely associated with the atoms and bonds of a structure but not chemically meaningful themselves. They may describe something about the structure, or they may simply provide a convenient label. In either case, they should be close enough to the subject of interest that they are clearly associated, and far enough from other objects that the nature of the association is not confused.

SOFTWARE CAUTION: Some software programs may have special ways to create annotations so that they remain associated with their target objects, or so that they may be indicated as having a specific meaning. If you are using annotations in an electronic environment, you may want to take advantage of the features that your chemical drawing software offers in this area.

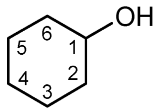
GR-11.1 Atom-based annotation

Annotations that describe a specific atom should be positioned close to that atom. Some common atom-based annotations include atom numbering and stereochemistry indicators.

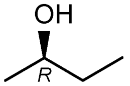
Atom-based annotation is generally positioned in the largest open space near the atom, since there is less chance that the annotation will be interpreted as referring to another object if there are fewer objects nearby. When annotating several atoms in a ring system, it is also common to place the annotations within the ring. Annotations describing the stereochemical configuration of an atom will generally be placed opposite one of the atom's wedged or hashed wedged bonds.



Preferred



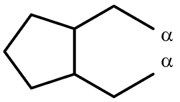
Preferred



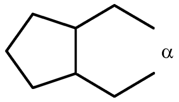
Preferred
[when desired to show stereodescriptor]

Annotations should be clearly separated from the atom in question, whether it has a label or represents an unlabeled carbon atom. However, they should also be closer to the atom in question than to any other atom. Typically, atom-based annotations will be separated from the atom by a distance on the order of half the height of a "C" or an "H" in the font used for atom labels, but that distance may vary according to the aesthetics of the chemist. As a practical matter, the indicator will rarely be separated from its atom by as much as the full height of a "C" or an "H" in the font used for atom labels.

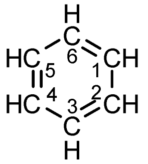
Annotations should also be visually different from regular atom labels. Typically, they will be drawn smaller. They may also be drawn in a different font, style, or color. If numeric indicators are drawn smaller than regular atom labels, then care should be taken when positioning them to the right or left of an existing atom label, lest they be mistaken for element repeat counts or isotopic labels.



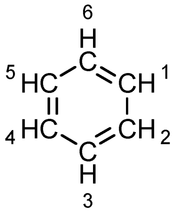
Preferred



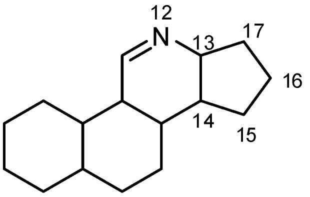
Not acceptable



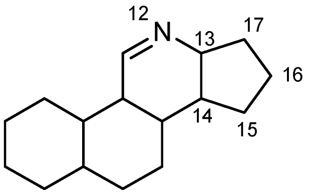
Preferred



Not acceptable



Preferred



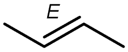
Not acceptable

GR-11.1.1 Asterisks

Asterisks have traditionally been used in several contexts: not only to indicate the presence of a stereogenic center, but also to specify isotopic labeling or excited states. Accordingly, the use of an asterisk as an indicator for any one of those items (including as an indicator of stereogenic centers) is potentially misleading and should be avoided. Any use of the asterisk should be undertaken with extreme care, and should generally be accompanied by additional descriptive text that explains its meaning in that specific context.

GR-11.2 Bond-based annotation

Many of the issues relating to atom-based annotation also apply to bond-based annotation. Graphical stereodescriptors are a common example of bond-based annotation. Annotations associated with a bond are generally positioned near the midpoint of the bond.



Preferred

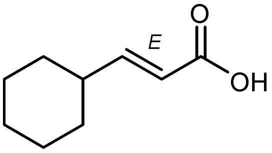
GR-11.3 Structure-based annotation

Annotations describing an entire structure are probably the most common sort of annotations. Nearly every structure depicted in a journal article will be identified by a letter or number nearby.

Structure-based annotation should be clearly associated with a specific structure. It should be positioned so that it is closer to the target structure than to any other structure, but it should also be positioned far enough away from the structure that it is not likely to be interpreted as an annotation of a single atom or bond within the structure. Typically, that means that it will be separated from the closest part of the structure by a distance at least equal to half of the bond length used in the structure, and no further than twice as far as the structure's bond length.

These annotations should be visually different both from atom labels and from atom- and bond-based annotation (if present). Typically, structure-based annotation will be drawn in a font that is the same size as or larger than the structure's atom labels. The font, style, or color may also be different.

Structure-based annotations will usually be placed below the structure. They will sometimes appear to the left or right instead, but that positioning should be avoided in reaction schemes where there are other structures to the left or right.



21

Preferred

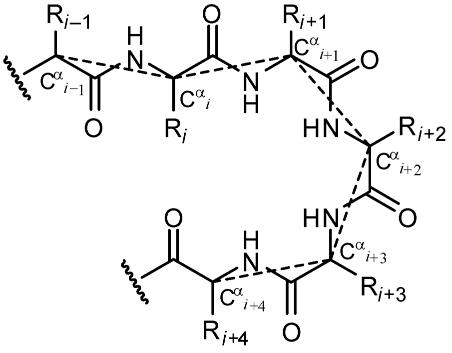
GR-12. PSEUDOBONDS

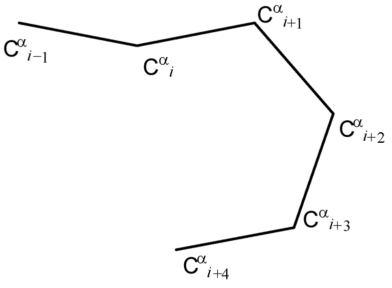
A *pseudobond* can be defined as a graphical linkage between two atoms that are not directly bound to each other chemically. Pseudobonds should be always drawn in a fashion that is clearly distinguishable from regular covalent bond. Pseudobonds are used to simplify representation of complex structures such as macromolecules or coordination compounds.

SOFTWARE CAUTION: At the time of writing this document, there are few computer software programs that are able to recognize pseudobonds of any sort. If chemical structure diagrams of such molecules are required for use within an electronic environment, it may be necessary to eschew pseudobonds and instead depict all of the atoms and bonds explicitly.

GR-12.1 Biological macromolecules

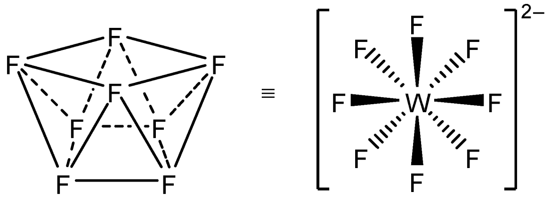
The representation of biological macromolecules often is simplified so only some of the "backbone" atoms connected with pseudobonds are shown. This method is especially useful for representation of secondary structure. For instance, a polypeptide backbone is often represented as a set of Cα–Cα pseudobonds [32]. For nucleic acids, several variants were suggested, such as pseudobonds between P and C4' atoms in RNA [33] or between phosphate 3' oxygen atoms in DNA [34].



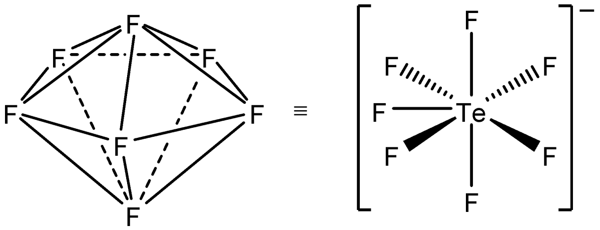


GR-12.2 Coordination polyhedra

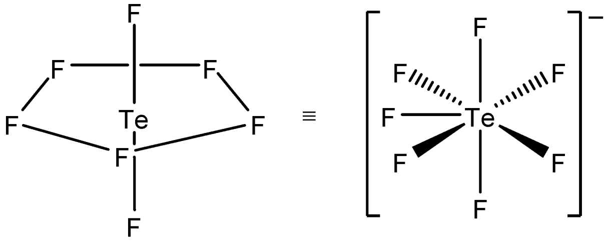
In representations of coordination geometries, a different kind of graphical convention is often used. Configurations with seven or more ligands are most commonly depicted as polyhedral solids, where pseudobonds connect the donor atoms of ligands and the central atoms are not shown. It is not acceptable, however, to represent some coordination geometries (*TBPY*-5; *PBPY*-7) with the equatorial plane shown with pseudobonds, while the axial ligands are linked to the central atom with "real" bonds.



Preferred



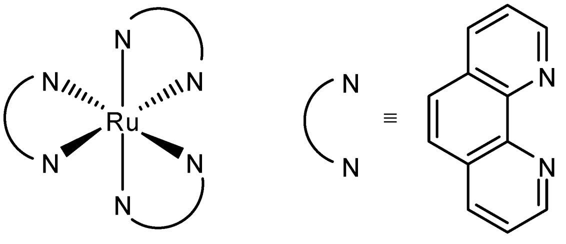
Preferred



Not acceptable

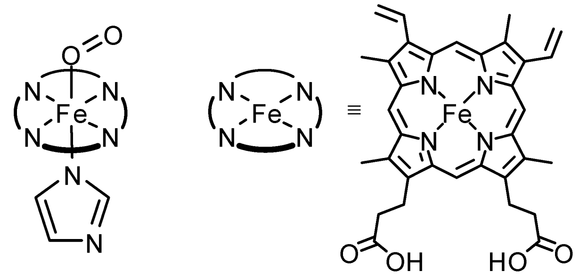
GR-12.3 Connectors

A connector is a variant of pseudobond used for schematic representation of molecules such as polydentate ligands where only a few atoms or groups are explicitly labeled. The connectors are usually drawn as curved bonds between atoms (groups) of interest.

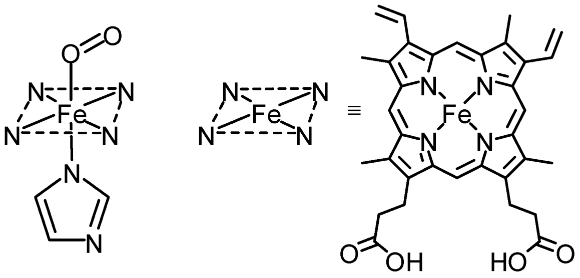


Preferred

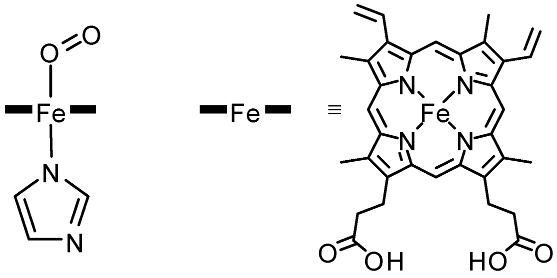
Tetrapyrrole-metal complexes are often schematically represented as “wheels” with four spokes (i.e., each connector is a 90° segment). Such representation is acceptable and sometimes even preferred to detailed depiction of tetrapyrrole ligand, since there is no confusion between real bond (linear) and pseudobond (curved).



Preferred



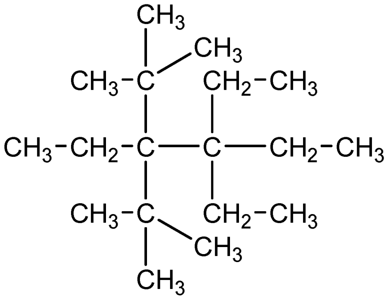
Acceptable



Not acceptable

GR-13. LINEAR DRAWING STYLE

When presented in the “linear” drawing style, acyclic chains are drawn exclusively with horizontal and vertical bonds. Accordingly, their use is limited to those structures that truly can be represented using only horizontal and vertical bonds. Extremely congested structures, for example, are not suitable to this drawing style.



Not acceptable

Additionally, atoms with more than four attached bonds cannot be represented in this style. Accordingly, this style should be used to represent only relatively simple structures. Some further points are discussed below, and unless otherwise indicated, all other issues relating to chains in general (see GR-3.2, etc.) would apply to the linear drawing style as well.

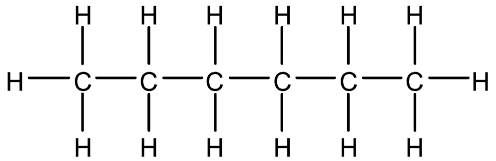
The linear drawing style is used primarily in introductory educational environments where it is necessary to keep the diagrams as simple as possible. It should be considered as not acceptable for general usage.

GR-13.1 Atoms should be labeled

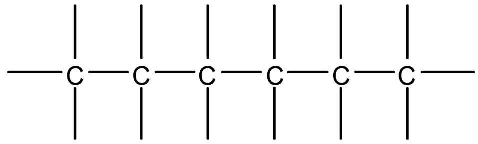
Because there is no "bend" in the chain of bonds, all atoms, including carbon and hydrogen atoms, should always be labeled explicitly.

$CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$

Preferred



Acceptable



Not acceptable

GR-13.2 Bonds should be sufficiently long

The standard bond length used when drawing the structure should be long enough that the bonds are not obscured by the atom labels. This is much more of a problem in this drawing style than in the "chain" style because it is much easier for a horizontally oriented atom label to obscure a horizontal bond than a bond at an angle.

$CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$

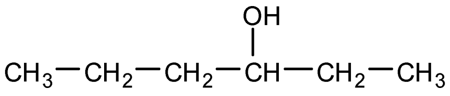
Preferred

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$

Not acceptable

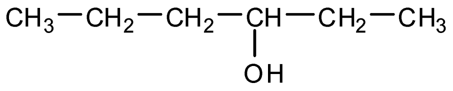
GR-13.3 Substituents should preferentially be upwards

A substituent on a non-terminal atom should preferentially be positioned above that atom, rather than below.



$$CH_3-CH_2-CH_2-\overset{\displaystyle OH}{\overset{|}{CH}}-CH_2-CH_3$$

Preferred

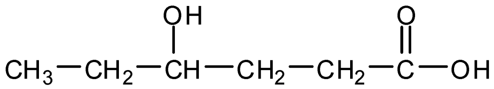


$$CH_3-CH_2-CH_2-\underset{\displaystyle OH}{\underset{|}{CH}}-CH_2-CH_3$$

Acceptable

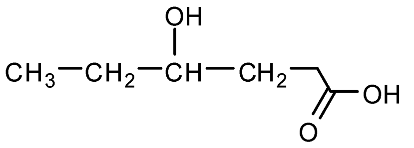
GR-13.4 Structure drawing styles should be consistent

If the linear drawing style is used for part of a structure, it should be used for the entire structure. Similarly, a group of related structures should be consistent in the style that is used among them.



$$CH_3-CH_2-\overset{\displaystyle OH}{\overset{|}{CH}}-CH_2-CH_2-\overset{\displaystyle O}{\overset{\|}{C}}-OH$$

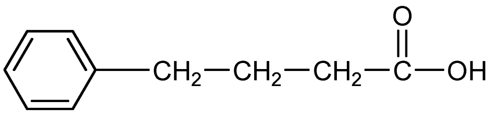
Preferred



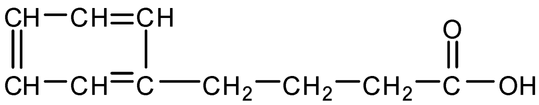
Not acceptable

GR-13.5 Rings are always drawn as rings

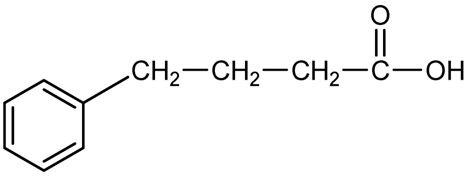
There is no equivalent of the linear style for use with cyclic structures. Any ring system should be drawn as a ring system, even if the rest of the structure is drawn using the linear drawing style. However, any bonds connecting the ring to the linear portion of the structure should remain horizontal or vertical.



Preferred



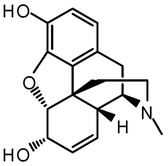
Not acceptable



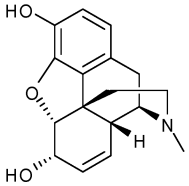
Not acceptable

TABLE I. SAMPLE DRAWING STYLES FOR PUBLICATIONS

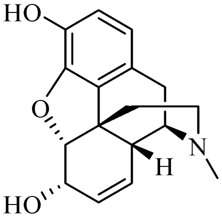
The following diagrams demonstrate a selection of drawing styles that are used or have recently been used in various printed publications. All of these diagrams may be considered "preferred", despite the wide variation in text (GR-0.3), bond lengths (GR-1.1), bond widths (GR-1.2), bond patterns (GR-1.3), and spacing of multiple bonds (GR-1.6). In each case, the combination of individual styles produces a diagram that is wholly legible, and that is more important than the specific numeric value of any single property.



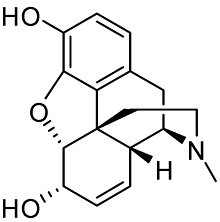
Morphine
Journal of
Heterocyclic Chemistry



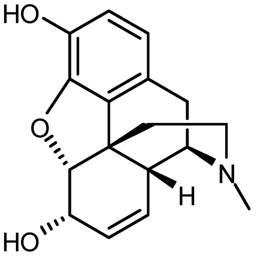
Morphine
Royal Society of Chemistry
publications



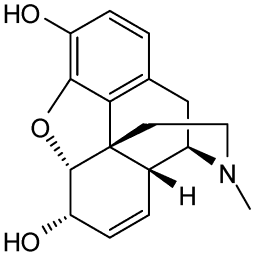
Morphine
Journal of
Molecular Modeling



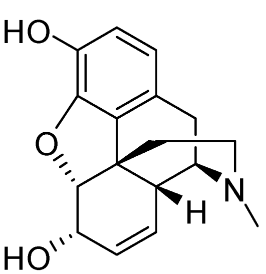
Morphine
American Chemical Society
publications



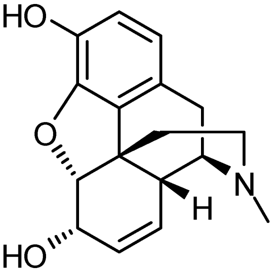
Morphine
Advanced Synthesis
& Catalysis



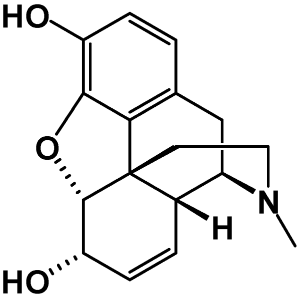
Morphine
Verlag Helvetica
Chimica Acta



Morphine
Wiley publications



Morphine
Journal of the
Chinese Chemical Society



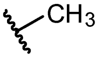
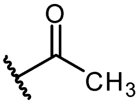
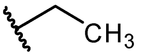
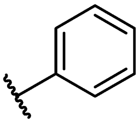
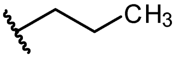
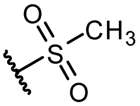
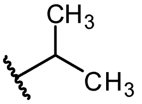
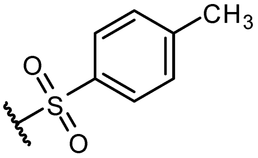
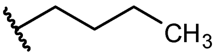
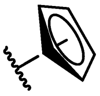
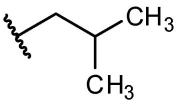
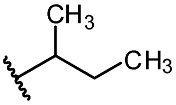
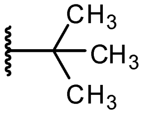
Morphine
Phytomedicine

TABLE II. STRUCTURAL ABBREVIATIONS

The following nicknames (with capitalization as shown) may be used without further explanation to refer to the structure fragments shown. In all cases, the nicknames should be used to refer only to the specific structures shown, without further substitution and without the presence of further charges, unpaired electrons, or non-natural isotopy.

Authors are welcome to create their own abbreviations as well, but any abbreviations not included in the list below should be defined clearly when they are used (see GR-2.2).

Several of the abbreviations listed below include portions of the text in italics. The italicization shown is the preferred formatting of those abbreviations. However, the corresponding forms without italicization are also acceptable.

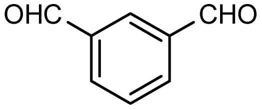
Abbreviation	Full structure	Abbreviation	Full structure
Me		Ac (†)	
Et		Ph	
Pr (†)		Ms	
iPr		Ts	
Bu		Cp (‡)	
iBu			
s-Bu			
t-Bu			

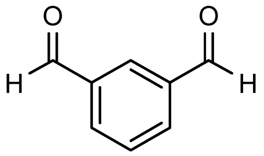
(†) The text used by the Ac and Pr abbreviations is identical to the element symbols for actinium and praseodymium, respectively. Those abbreviations should be used only in organic contexts where they are unlikely to be mistaken as element symbols.

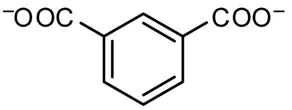
(‡) The Cp abbreviation may be used only when bonded to a metal atom.

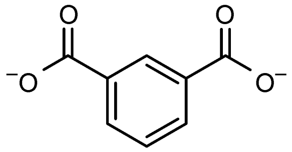
TABLE III. COMMON CONTRACTED ATOM LABELS

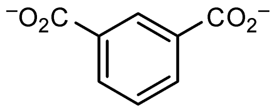
Some very common contracted labels cannot be interpreted with a simple application of valence rules, but also need some implicit charges to be added. Others may represent slightly unusual bonding patterns. The labels shown below, along with their corresponding chalcogen analogs, may be freely used within contracted labels; however, since they all have only a single point of attachment, the textual strings shown below should always be the last (or only) text within a label or within a parenthesized portion of a label. (The central rings and metal atoms in the examples below are provided simply as scaffolds to which these labels are attached. Both left-to-right and right-to-left forms of the label are shown.)

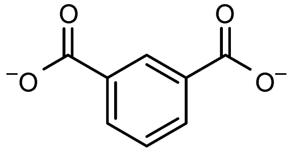


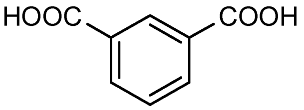


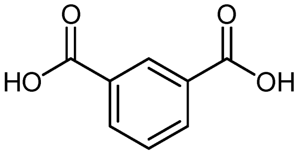


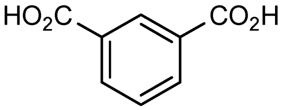


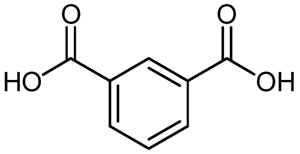


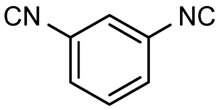


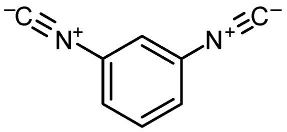


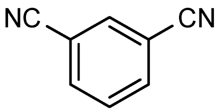


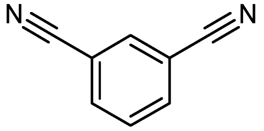


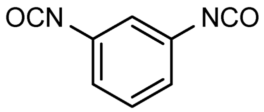


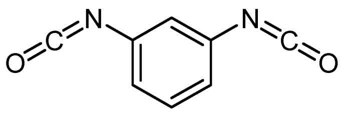


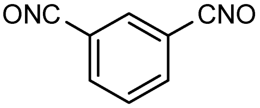


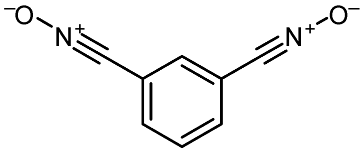


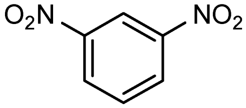


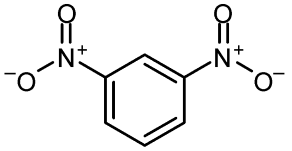


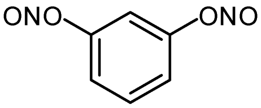


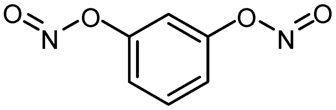


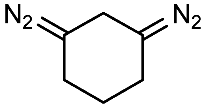


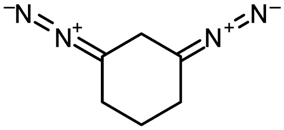


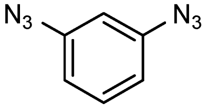


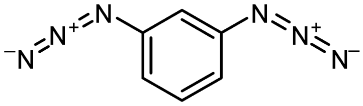


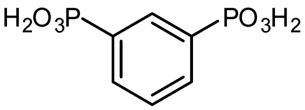


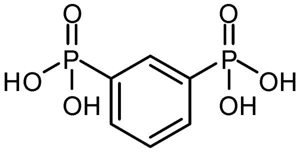


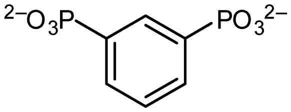


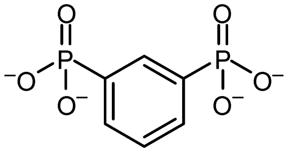


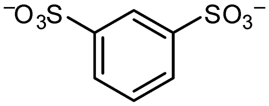


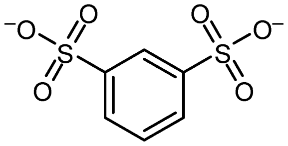


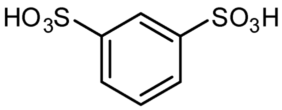


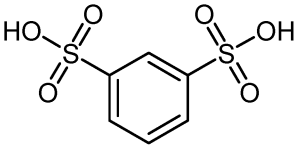


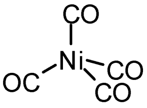


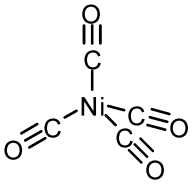












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