

INTERNATIONAL UNION OF PURE AND
APPLIED CHEMISTRY, CHEMICAL
NOMENCLATURE AND STRUCTURE
REPRESENTATION DIVISION

**GRAPHICAL
REPRESENTATION OF
CONFIGURATION
(Draft IUPAC
Recommendations 2005)**

Developed by the Task Group for Graphical
Representation Standards for Chemical
Structure Diagram:

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Abstract.

The configuration of compounds is determined by the relationship of atoms in three dimensional space, yet chemical structures are most commonly depicted in two dimensional media such as printed publications or computer screens. Recommendations are provided for the display of three-dimensional stereochemical information in two-dimensional diagrams in ways that avoid ambiguity and are likely to be well-understood by all viewers. Examples are provided for all types of stereochemical configuration, with explanation of which styles are preferred and which should be avoided.

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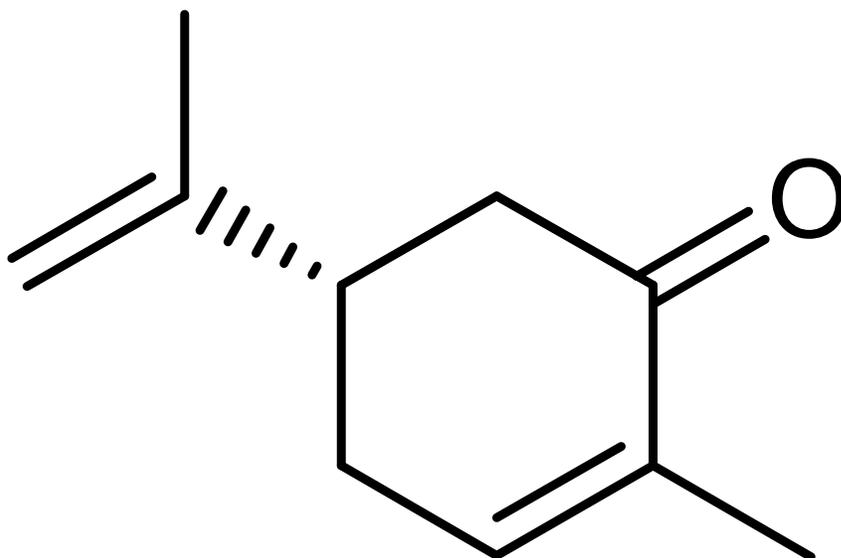
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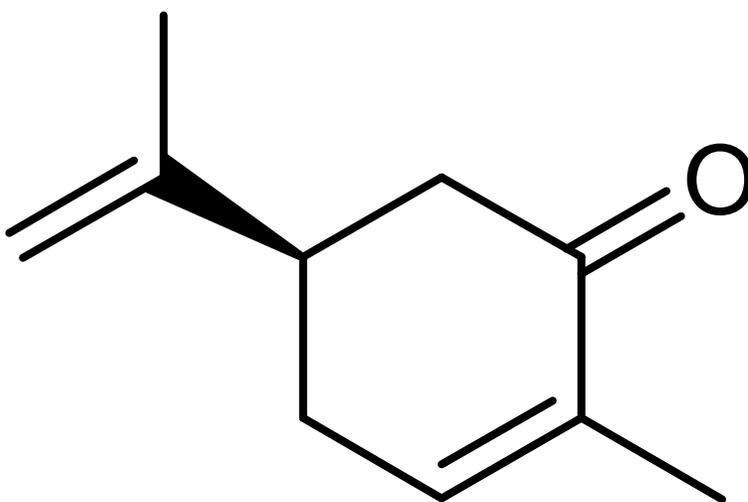
NB Only a few sections of the draft IUPAC recommendation have been included in this poster – sections in *italics* have been omitted from the poster

ST-0. INTRODUCTION

Stereochemistry is the aspect of chemistry concerned with the different spatial arrangement of atoms in molecules and compounds and the effect that those differences have on their physical properties and reactivity. The significance of stereochemistry even in everyday life is famously demonstrated by the two isomers of carvone, where the (*S*)-(+)-form of carvone provides the odor of caraway while the (*R*)-(-)-form instead smells like spearmint.



(*S*)-carvone (caraway)



(*R*)-carvone (spearmint)

Chemical structures are inherently three dimensional, but they are commonly depicted on two dimensional media such as printed paper or electronic computer displays. Any depiction of a three-dimensional object on a two-dimensional surface is going to require some level of distortion.

ST-0.1 Overview

Throughout this publication are numerous examples of chemical structures drawn in styles that are labeled as “preferred”, “acceptable”, “not acceptable”, or occasionally “wrong”. Since the depiction of chemical structures is something of an art form and will likely remain so, it is worthwhile to clarify the meaning of those terms as they are used here.

The styles labeled as “preferred” show how the configuration of a structure should best be indicated 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. Steroids, for example, must be drawn in a specific fixed orientation [1]. A complex structure might need to be distorted in order to avoid overlap in other parts of the diagram. Bridged ring systems can be particularly interesting, since the topology of the ring system itself can force its bonds into orientations that are not otherwise seen in acyclic systems. Solid wedged and hashed wedged bonds should not be placed between two atoms that are both asymmetric except when literally unavoidable; that restriction alone accounts for many of the exceptional cases in this publication. 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 substance other than the one intended.

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 so on.

This publication extends and supersedes the section titled “Graphic Representation of Three- Dimensional Structures” in the earlier publication on the Basic Terminology of Stereochemistry [2]. Only issues related to the depiction of stereochemistry are discussed here; a future publication is planned that will make recommendations regarding non-stereochemical aspects of chemical structure depiction.

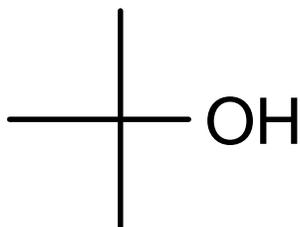
ST-0.2 Plain bonds

All single bonds attached to nonstereogenic atoms should normally be drawn as plain bonds, that is, as simple thin lines that are not bold or dashed or hashed or wavy or adorned in any other way. The use of stereobonds (\blacktriangleleft , ||||| , — , ||||| , ---- , etc.) at nonstereogenic atoms should be avoided.

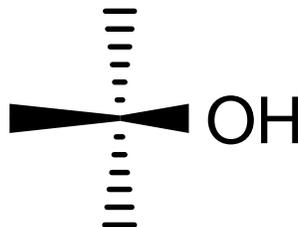


It is always acceptable to use stereobonds when emphasizing three-dimensional configuration, whether the associated atoms are stereogenic or not. For example, solid wedged bonds and hashed wedged bonds might be used when designating the *pro-R* and *pro-S* substituents on a prochiral tetrahedral center, or when depicting *syn*, *gauche*, or *anti* conformations of a torsion angle. This does not contradict the previous paragraph, as prochiral centers and torsional angles are in fact not normally emphasized as such. The use of solid wedged bonds and hashed wedged bonds in nonstereogenic environments is outside the scope of these recommendations.

Plain bonds should be used for nonstereogenic atoms even though the atom's substituents are not physically coplanar.

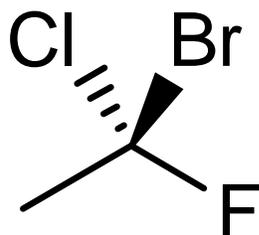


Preferred

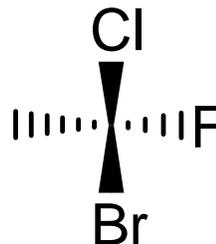


Not acceptable

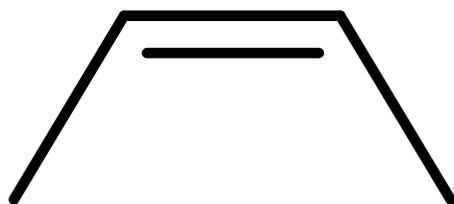
When attached to stereogenic atoms, plain bonds indicate the set of bonds that is to be considered as being in the plane of the paper. Other solid wedged or hashed wedged bonds are considered to extend above or below this plane. As a general rule, structures should be drawn to maximize the number of plain bonds, although there are exceptions (particularly for inorganic complexes with coordination numbers greater than four).



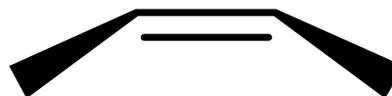
Preferred



Acceptable



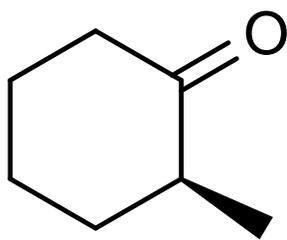
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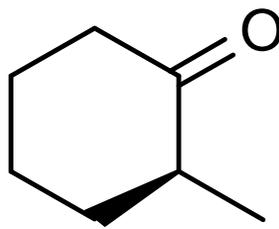
Acceptable

As discussed above, it is always acceptable to use solid and hashed wedged bonds when emphasizing the perspective of three-dimensional configuration, even if an alternate representation is possible that uses fewer stereobonds.

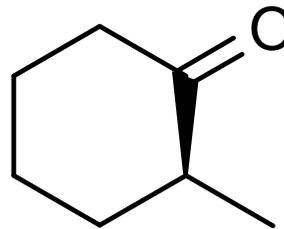
Simple rings and fused ring systems should be drawn using plain bonds within the rings. If configuration is to be indicated with hashed wedged and solid wedged bonds, those bonds should be restricted to acyclic substituents. This is true even though in most cases the ring atoms will not all be coplanar; the implied coplanarity should be considered on a per-atom basis only, just as with acyclic compounds. Depiction of a solid wedged or hashed wedged bond within a ring is acceptable only in cases where no reasonable alternative is available (as in a spiro fusion, see ST- 1.3, or) or where all acyclic neighbors are themselves stereogenic (ST-0.5).



Preferred



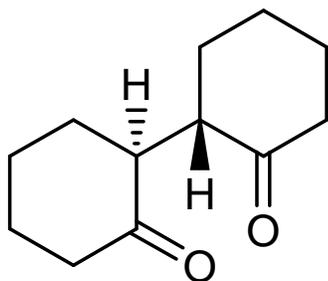
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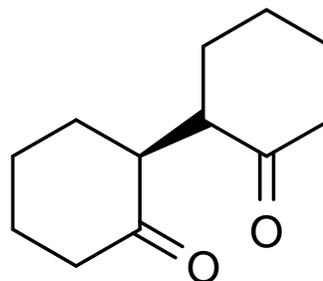
Not acceptable

ST-0.5 Stereobonds between stereocenters

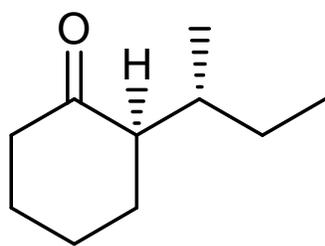
Stereobonds between stereocenters should be avoided at all costs. This was stated above but bears repeating because it is so important.



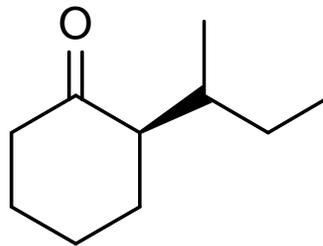
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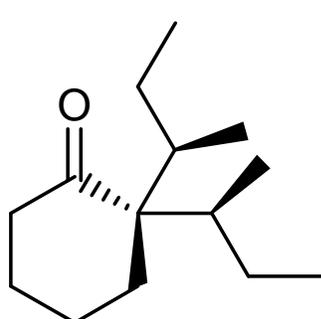
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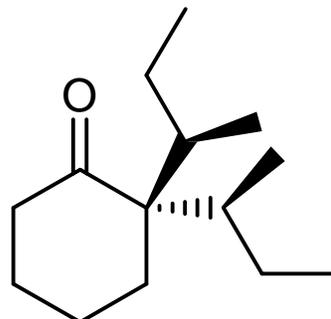
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Not acceptable

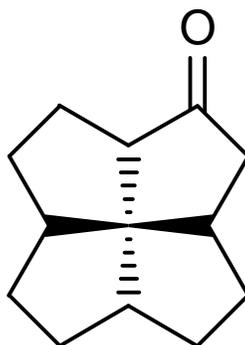


Preferred



Not acceptable

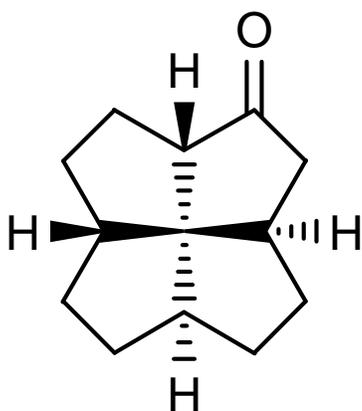
In rare cases — for example when one stereocenter is completely surrounded by four other stereocenters — a stereobond must be present between two stereocenters. There is no ideal solution in such cases, as some ambiguity is unavoidable. In this case, like the others, only the atom at the narrow end of a stereobond should be considered as having a specified configuration.



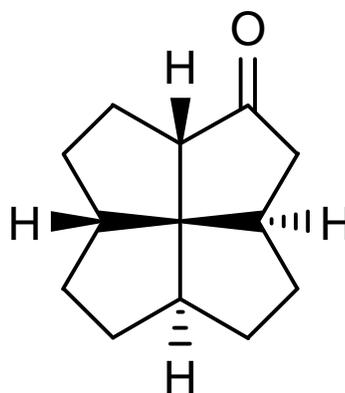
Acceptable

If the central atom has a specific configuration and the surrounding atoms also have specific configurations,

additional stereobonds must be added to the surrounding atoms. It is preferred to select a depiction style for the central atom that has as few stereobonds as possible, since that will eliminate completely any ambiguity regarding the intended configuration at some of the adjacent atoms.



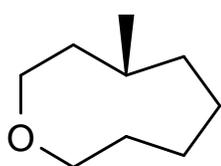
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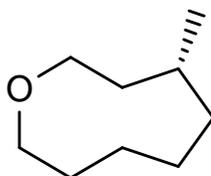
Preferred

ST-1.4 Tetrahedral centers at re-entrant atoms

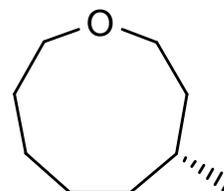
Although small ring systems are generally drawn as convex polygons, larger rings containing nine or more atoms are preferentially drawn as non-convex polygons, with two or more atoms “pointing inward” relative to the rest of the ring. As discussed above, it is not acceptable to depict tetrahedral stereochemistry at re-entrant atoms when any other option is available.



Not acceptable

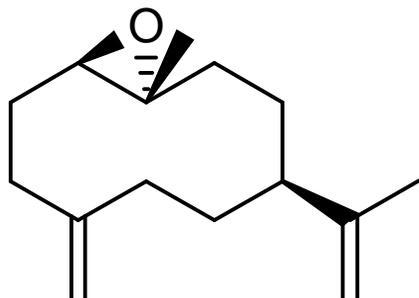


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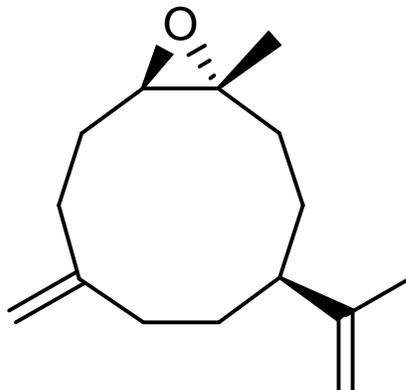


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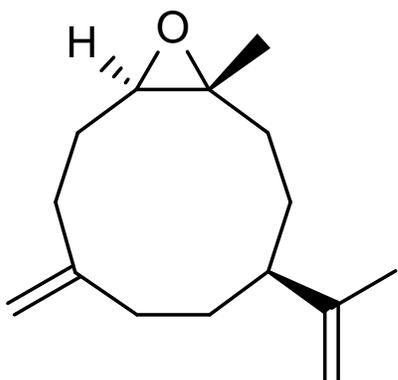
Epoxides have commonly been depicted in ways that incorporate solid wedged bonds or hashed wedged bonds at re-entrant angles. Such depiction styles are not acceptable.



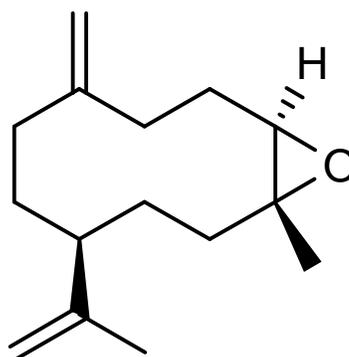
Not acceptable



Acceptable

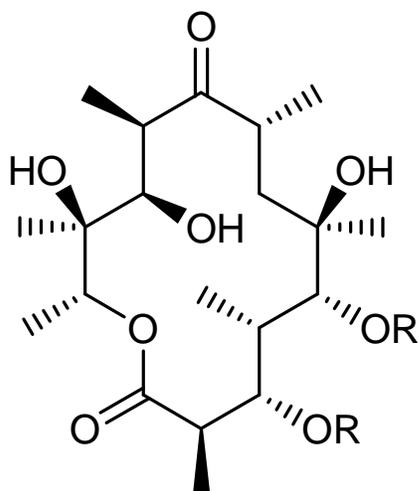


Preferred

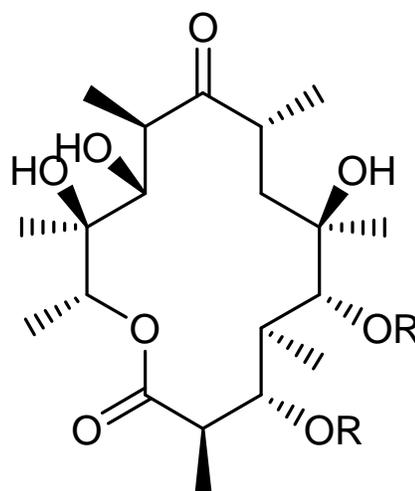


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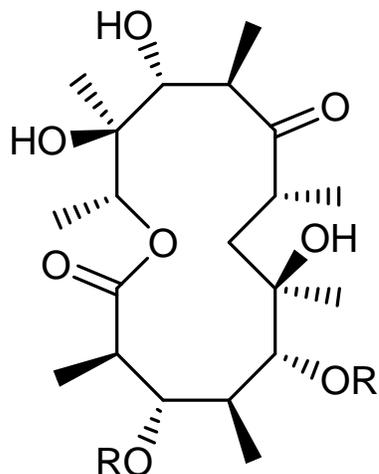
In some cases there are few appealing alternatives to having stereogenic atoms at some re-entrant positions. A classic example is the core ring of the antibiotic Erythromycin A, shown below. Traditionally, that ring has been depicted with 120° angles at each atom of its 14-membered ring, which results in two stereogenic centers at re-entrant atoms. In such a case, the substituents at the re-entrant atoms should be oriented inwards to the ring as well. It would be preferable to depict the ring in a way that did not require any stereogenic centers at re-entrant atoms.



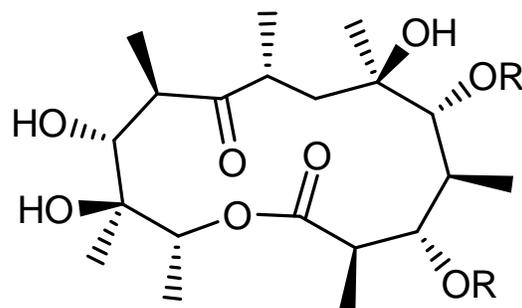
Acceptable



Not acceptable



Acceptable



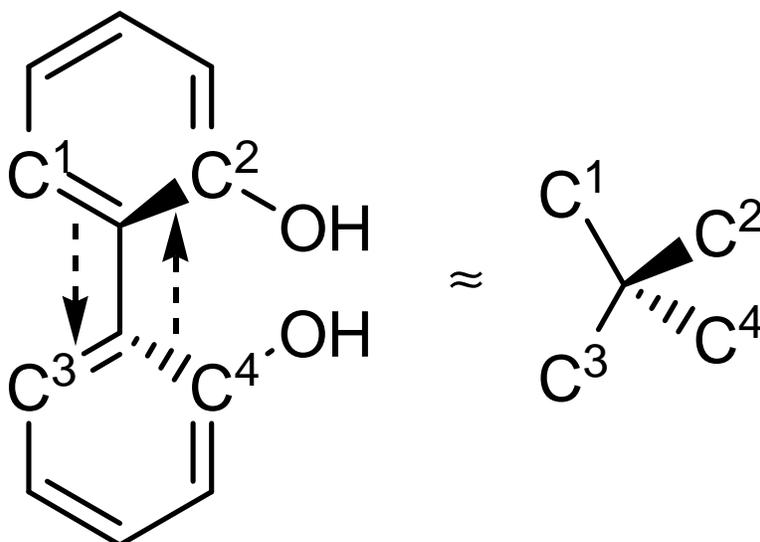
Acceptable

The examples above also demonstrate that solid wedged bonds must be converted to hashed wedged bonds and vice versa when a re-entrant atom is converted to a more-standard convex environment.

ST-1.7 Hindered biaryls

Hindered biaryls (such as 2,2'-disubstituted 1,1'-binaphthyl) represent yet another case of axial chirality. The additional substituents in this system constrain the aromatic rings so that they can no longer rotate freely, and such systems are

described as having “hindered rotation”. As with cumulenic systems with an even number of double bonds, the stereogenic unit in hindered biaryls can be viewed as a distorted tetrahedron. It can be interpreted by “squeezing out” the rotatable bonds joining the two ring systems in the viewer’s mind, and considering the four isolated substituents. As with cumulenic systems, this “squeezing out” should be used only to understand this configuration as a distorted tetrahedron and cannot be used to determine absolute Cahn-Ingold-Prelog (CIP) stereodescriptors.



All biaryls with at least three substituents in the *ortho* positions have hindered rotation, as the *ortho*-substituents inhibit coplanarity at least to some extent.

Hindered biaryls should always be drawn with hashed and wedged bonds within the aryl rings and directly connected to the single bonds about which they rotate. Additional bonds within the aryl systems may also optionally be drawn with solid wedged or hashed wedged bonds.