GRAPHICAL REPRESENTATION OF CONFIGURATION

(IUPAC Recommendations 2005)

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Graphical Representation of Configuration
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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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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.

![Carvone Isomers](image)

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. Chemical information, however, has traditionally been communicated using two-dimensional media such as the printed page and more recently the computer screen. The problems associated with the communication of three-dimensional information in two-dimensional media are far from unique to chemistry. The introduction of perspective, for example, was one of the hallmarks of
early Renaissance artwork. Although the use of perspective is commonplace today in pictorial images, it is less commonly used in conjunction with symbolic information: mapmakers use contour lines to indicate elevation or varying shades of blue to indicate ocean depth.

In chemistry, the need to show the true three-dimensional molecular architecture in two-dimensional media has given rise to a variety of structure drawing conventions. One convention depends on perspective to convey spatial relationships, just as a pictorial image would. The use of perspective in structure drawing is discussed here, but in its own section. By far the most common way to represent spatial configurations in chemical structures is through the insertion of special bond types — bold, hashed, dashed, and/or wedged — into an otherwise planar depiction of a chemical structure. Each special bond type would indicate the spatial arrangement of two atoms in relation to each other, usually specifying that one or the other atom was closer to or further from the viewer relative to the plane of the diagram. The proper use of hashed wedged and solid wedged bonds occupies the majority of these recommendations.

Historically, the varying conventions for depiction of configuration have caused confusion among chemists. Any one diagram may or may not have had a single interpretation either by the chemist who viewed the information or, as is now becoming more important, by the computer into which the information was stored. This publication contains a self-consistent series of recommendations for the unambiguous depiction of molecules in two dimensions using standards that are for the most part understandable by both human and machine.

**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.

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 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.

Some structural depictions are described as being formally correct, formally incorrect, or formally ambiguous, referring to whether a depiction might possibly represent the intended
configuration from a strictly logical or formal analysis. For example, it is formally incorrect to depict a tetrahedral configuration using four wedged bonds connected to a central atom. Such a depiction would imply that all four substituents are on the same side of the central atom (all “nearer” the viewer relative to the plane of the diagram), whereas the geometrical definition of a tetrahedron precludes such an arrangement. The formal correctness of a structural depiction is related to the acceptability of the depiction, but the two are not exactly the same. Some depictions may be formally incorrect but still preferred because of long-standing convention. Other depictions may be formally correct but not acceptable. Discussions of formal correctness are included principally in cases where the correctness and the acceptability are different.

Several of the depiction styles include descriptions with specific angular measurements. For the sake of readability, angular measurements 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 “linear” should be interpreted as “forming an angle between 170° and 190°”. In other words, two bonds that look nearly linear should be treated as exactly linear, even that is not exactly true for their actual geometric relationship.

Similarly, any mention of bonds being “adjacent” refers to their appearance in the two-dimensional representation. Any bond in a physical (three-dimensional) tetrahedron 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.

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. There are other valid ways to represent structures including Newman projections, ball-and-stick models, and many others. These recommendations should not be overgeneralized as applying to anything beyond the “standard” two-dimensional chemical structure diagrams.

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 (–, ––, –––, –—, etc.) at nonstereogenic atoms should be avoided.

![Preferred](Preferred.png) ![Not acceptable](Not acceptable.png)

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.

\[
\text{OH} \quad \text{Preferred} \quad \text{OH} \quad \text{Not acceptable}
\]

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).

\[
\begin{align*}
\text{Cl}_2\text{Br} & \quad \text{F} \\
\text{Preferred} & \quad \text{Acceptable}
\end{align*}
\]

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. Again, however, such exceptions should be considered only when necessary to accommodate some other aspect of the diagram and are not preferred in the general case.

\[
\text{Acceptable}
\]

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).

\[
\begin{align*}
\text{Preferred} & \quad \text{Not acceptable} & \quad \text{Not acceptable}
\end{align*}
\]

**ST-0.3 Hashes, dashes, and wedges**

Structural diagrams that depict configuration must be prepared with extra care to ensure that there is no ambiguity. As discussed above, plain lines depict bonds approximately in the plane of the drawing. Bonds to atoms above the plane should be shown with a solid wedge (starting
from an atom in the plane of the drawing at the narrow end of the wedge). A bold bond \( \overline{\text{---}} \) has sometimes been used instead of a bold wedge but is not recommended.

Unfortunately, bonds below the plane of the drawing have historically been represented in many different ways. Each of those representations has involved a bond drawn with small line segments either parallel (\( \overline{\text{-----}} \)) or perpendicular (\( \overline{\text{\cdot\cdot\cdot\cdot}} \)) to the main axis of the bond. The two schools of thought that prefer the use of a hashed wedge bond \( \overline{\text{\cdot\cdot\cdot\cdot}} \) assign it two directly opposite interpretations — one school says that the atom at the narrow end should be considered in the plane of the paper, while the other says that the atom at the wide end should be so considered. Additionally, a dashed line \( \overline{\text{-----}} \) is often used also to represent a partial bond, delocalization, or a hydrogen bond. The biggest problem is that there is no way to intuit an author’s desired meaning from a chemical structure drawing alone. For these reasons, chemical structure diagrams should be created so as to avoid these sorts of bonds when doing so will not otherwise compromise the clarity of the drawing, and solid wedged bonds should be preferentially used instead.

Although a solid wedged bond can often be used instead of a hashed wedged bond by drawing the structure slightly differently (as above), that situation is far from universal. There are many cases where the use of a hashed bond produces a more aesthetic structure. One common situation happens with ring systems, where it is often preferable to draw an explicit hydrogen with a hashed bond rather than put a solid wedge on a ring bond. Another common situation arises when showing a series of enantiomers or diastereoisomers where the contrast between the solid and hashed types directly emphasizes the chemical differences.

In cases where such below-the-plane bonds are required, there is no option that will please everyone. Earlier recommendations \[2\] proposed the use of an unwedged hashed bond \( \overline{\text{\cdot\cdot\cdot\cdot}} \), but today such bonds are in fact encountered in the literature least frequently of all options. This document now recommends the use of a hashed wedged bond \( \overline{\text{\cdot\cdot\cdot\cdot}} \) interpreted in a sense similar to the solid wedged bond (starting from an atom in the plane of the drawing at the narrow end of the wedge). This recommendation is made primarily because the hashed wedge is easier to analyze visually than the unwedged type, particularly when it is used in a sense similar to the wedged bold bond. Strictly speaking, unwedged bold and hashed lines show that both atoms are above or below the plane of the drawing (as is used in Haworth drawings of carbohydrates). If these bonds are used to convey chirality, they require extra effort to determine which atoms are truly asymmetric and which are not. The wedged hashed bond contains more — and more useful — information than the unwedged version. While the use of an unwedged hashed bond is often unambiguous, such a bond is not always unambiguous, and in the rare cases that cannot avoid having a hashed bond between stereocenters (see below), the unwedged version will never be unambiguous.

Additionally, the consistent use of a wedged bond is simpler: in each case, the sharp end of the bond shows the stereogenic center, and there is no need to analyze both ends to figure out what was intended. After careful consideration, it appears that the only responsible recommendation is that only the hashed wedged bond be used when representing below-the-plane bonds.

Admittedly, strong cases can be made in favor of other systems. A system based entirely on a perspective-based analysis is possibly the most popular of these other systems. In a perspective-based analysis, more-distant objects are always perceived as smaller than objects that are nearer. Accordingly, a wedged bond is interpreted as extending above the plane of the paper from the narrow end to the wide end, and extending behind the plane of the paper when considered from
the wide end to the narrow end. Lin et al. [3] have shown that a system of this type can be internally self-consistent and can be used to represent most types of tetrahedral configurations. Unfortunately, it cannot be used in all cases. Since this system always specifies the configuration of atoms at both ends of every wedged bond, it cannot be used to depict, for example, a tetrahedral center of known configuration connected to four other centers of unknown configuration. Additionally, the One-Wedge system as described by Lin et al. eliminates the use of a hashed wedge bond entirely, thereby discarding a very popular drawing style widely used for many years. This simplification has some appeal in terms of simplicity of usage, but the benefits of a hashed bond — in particular, the ease with which a hashed bond can be distinguished from a bold bond at a quick glance — are too great to eliminate.

Others have recommended a perspective-based analysis that preserves the use of a hashed bond. The scheme described earlier, where a hashed wedged bond would be interpreted as “down” from the wide end to the narrow end, is a perspective-based approach. Unfortunately, this system not only suffers from the same weaknesses as the One-Wedge approach above, but additionally results in a scheme where a solid wedged bond and a hashed wedged bond — while looking quite different — actually represent exactly the same concept [4].

The responsible recommendation is to reject a perspective-based approach, and rather to interpret the bonds as more-abstract graphical objects. To summarize, a solid wedged bond should be interpreted as projecting above the plane of the paper from the narrow end to the wide end (with the wide end being nearer to the viewer), and a hashed wedged bond should be interpreted as projecting below the plane of the paper, also from the narrow end to the wide end (with the wide end being further away from the viewer).

\[
\text{Preferred}
\]

That said, it is possible to use the other bond types in ways that are unambiguous. In particular, any type of hashed bond is unambiguous when connected to an atom with no other substituents (a hydrogen atom, a chlorine atom), no other non-hydrogen substituents (a hydroxy group, an amino group), or at most one other non-hydrogen substituent (an ethyl group, an ethoxy group). In each of those cases, a viewer would have no difficulty in understanding that the hashed bond projects below the plane of the paper from the other atom to that atom. Accordingly, both the unwedged hashed bond and the hashed wedged bond with reverse directionality are acceptable when used exclusively in those cases.

\[
\text{Acceptable}
\]

However, anyone using bonds of these types should be aware that they are not the most common bond types used to represent behind-the-plane configuration. At best, an author using these types may cause a moment of confusion as a reader figures out which convention was intended. In extreme cases, a reader might actually interpret the structure incorrectly — for example, by interpreting an unwedged hashed bond in the convention where it would represent
relative (and not absolute) configuration, as discussed above. Fortunately, such cases are rare. The hashed wedged bond (interpreted from the narrow end to the wide end) remains preferred.

Because the unwedged hashed bond is visually non-directional, it absolutely must not be used when connecting two stereocenters. (See also ST-0.5.)

Not acceptable

The dashed bond should be reserved for the indication of partial bonding of various types, including hydrogen bonding. It should not be used to represent configuration.

Not acceptable

**ST-0.4 Wavy bonds**

If configuration is unknown, this can be indicated explicitly by a wavy line \( \sim \sim \sim \). The waves in such a line may be rounded or angular, but they should be of constant amplitude. The use of “wedged wavy” bonds is discouraged.

In most cases, a wavy bond is conceptually identical to a plain bond, and a plain bond should be used instead. Wavy bonds are most often used in general usage when an author wants to place special emphasis on the unknown nature of the configuration at a specific position; the wavy bond would usually be accompanied by additional explanatory text in that case.

Preferred Acceptable

Historically, wavy bonds have frequently been used to represent a mixture containing several enantiomers or diastereoisomers. That is reasonable, since the configuration of any arbitrary structure within such a mixture is indeed unknown. It is preferred to use a plain bond to depict a mixture, just as it is preferred when depicting single structures. If the nature of the mixture needed further emphasis, a wavy bond would remain acceptable for mixtures as well.

Some specific classes of compounds have further conventions for depiction of unspecified configuration within those classes. In steroid nomenclature, for example, atoms 8, 9, 10, 13, and 14 are always assumed to be in standard configuration unless explicitly denoted with a wavy bond [1]. In Haworth projections of carbohydrates, the anomeric carbon is frequently indicated with a wavy bond when representing a mixture of anomers [5]. These usages of a wavy bond should not be extended to structures outside those classes.
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.

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.
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.

**ST-0.6 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 for stereochemistry) 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.

**ST-0.7 CIP stereochemical indicators**

Absolute stereochemical configuration can be described using descriptors derived from the Cahn-Ingold-Prelog (CIP) priority rules. While quite powerful, the CIP rules can also be difficult for even skilled chemists to interpret correctly. CIP descriptors may certainly be present in a diagram to indicate the absolute configuration, but should never be used as a replacement for proper stereochemical representation (hashed wedged and solid wedged bonds). Obviously, if a CIP stereodescriptor is included in a diagram, extra care should be used to ensure that it is accurate.
ST-1. TETRAHEDRAL CONFIGURATIONS

Saturated carbon atoms exist in tetrahedral configurations. Accordingly, the accurate representation of tetrahedral configuration is critical in organic chemistry.

ST-1.1 Tetrahedral depictions with four explicit bonds

When depicting tetrahedral configuration around a stereogenic atom, the following depictions may be considered. Each of these depictions may be freely rotated in the plane of the paper without affecting the configuration being represented.

As discussed above, solid wedged bonds are preferred to hashed wedged bonds. If there are no other constraints on the orientation of the structure (as there would be, for example, in steroids), it would be preferred to position the structure so that it has the maximum number of solid wedged bonds.

Also, if any pair of non-identical substituents attached to a single atom is arranged horizontally, the graphically larger substituent should be to the right of the smaller one for aesthetic purposes. In this context, “graphically larger” refers to the size of the substituent within the drawing itself: An “OH” atom label is graphically larger than an “I” atom label because it consists of two characters rather than one, even though the iodine atom might be physically larger than the hydroxy group in terms of van der Waals radius.

Several of these depiction styles have three plain bonds, which in other cases would imply that those bonds are coplanar. In reality, tetrahedral configurations can never have three coplanar bonds. The use of three plain bonds in these cases is simply a matter of convention, and chemists will readily be able to understand the true tetrahedral nature of the center when any of the preferred or acceptable depiction styles is used.

ST-1.1.1

Two plain bonds, one solid wedged bond, and one hashed wedged bond, with the two plain bonds depicted as adjacent and separated by less than 180° (ideally, 120° as shown here). Since the two plain bonds are depicted as adjacent, the hashed wedged and solid wedged bond will also necessarily be depicted as adjacent, and they should be separated by less than the separation between the plain bonds (ideally, 60° as shown here).

The bisectors of the A-B and C-D angles should preferably be collinear. If they are not collinear, the depiction is still acceptable, but not preferred.
It may be noted that these depictions are not geometrically accurate in the strictest sense. If a tetrahedral center were positioned so that it was viewed orthogonal to the plane described by substituents A, B, and the central atom, then substituent D would completely obscure substituent C or vice versa. Nonetheless, chemists have long been trained to ignore that subtlety, and this remains among the preferred representations of tetrahedral configuration.

**ST-1.1.2**

Two plain bonds, one solid wedged bond, and one hashed wedged bond, with the two plain bonds depicted as adjacent and separated by 180°. Since the two plain bonds are depicted as adjacent, the hashed wedged and solid wedged bond will also necessarily be depicted as adjacent.

This depiction represents a see-saw configuration rather than a tetrahedral one and is not acceptable for representing tetrahedral configurations.

**ST-1.1.3**

Two plain bonds, one solid wedged bond, and one hashed wedged bond, with the two plain bonds depicted as adjacent and separated by greater than 180°. Since the two plain bonds are depicted as adjacent, the hashed wedged bond and solid wedged bond will also necessarily be depicted as adjacent, and are positioned within the smaller angle described by the plain bonds.

This depiction represents a square pyramidal configuration rather than a tetrahedral one and is not acceptable for representing tetrahedral configurations.

**ST-1.1.4**

Two plain bonds, one solid wedged bond, and one hashed wedged bond, with the two plain bonds separated by other than 180° and not depicted as adjacent.

These depictions are formally ambiguous and cannot be interpreted with certainty. They should never be used. Historically, they have been used in several situations that can sometimes be interpreted without certainty, but alternate acceptable representations are possible in all of those cases.
When depicting substituents at bridgehead atoms, some chemists have been tempted to depict the substituent atom using the wedged bond style that is opposite to the one used for the bridging bonds, apparently on the assumption that “if the bridge goes ‘up’, then the other substituent must go ‘down’.” In fact, if the ring system is oriented in the plane of the paper and the bridging bonds are oriented upwards, then the substituents are oriented upwards as well. Such structures should be depicted with substituents that use the same bond type as the bridging bonds. The substituents may also be depicted using plain bonds.

When depicting substituents at fusion atoms, one acceptable orientation of the substituent is vertically upwards/downwards from the atom, even if that places the substituent within the ring system (this is particularly common for steroids). Wedged bonds placed in this orientation may conflict with an opposite wedge on another of the fusion bonds. In such a case, that other fusion bond should be depicted using a plain bond.

When depicting substituents to rings drawn in perspective, some chemists have been tempted to use solid wedged bond and hashed wedged bonds to indicate the substituents’ positions relative to the ring without regard to their positioning in the diagram. The use of solid wedged bonds and hashed wedged bonds should always take into consideration the actual orientation of each substituent as drawn.

ST-1.1.5
Two plain bonds, one solid wedged bond, and one hashed wedged bond, with the two plain bonds separated by 180° and not depicted as adjacent.

These depictions represent square planar configurations rather than tetrahedral ones and are not acceptable for representing tetrahedral configurations.

**ST-1.1.6**

![Preferred](image1)

Three plain bonds and one wedged bond, with each pair of plain bonds separated by less than 180° (ideally, 120° as shown here). The wedged bond can be positioned in any orientation but will usually bisect one of the other angles as shown here. Additionally, the substituent D at the end of the wedged bond should generally be among the graphically smallest of the four.

Since in this style the drawing implies that the central atom is coplanar with substituents A, B, and C, it is technically incorrect in the strictest sense. In preference it should only be used for cases where the central atom is in a fused or bridged ring system.

![Preferred](image2)

When at least two of the central atom’s substituents are acyclic, the first recommendation above, with two plain bonds, one solid wedged bond, and one hashed wedged bond, is preferred.

![Preferred](image3)

![Preferred](image4)

![Acceptable](image5)

![Acceptable](image6)

![Acceptable](image7)

![Acceptable](image8)

![Acceptable](image9)

![Acceptable](image10)
Three plain bonds and one wedged bond, with one pair of plain bonds separated by 180° or more and the wedged bond positioned within that largest space between plain bonds.

This depiction style should be used with caution. It is a preferred style when substituents A, B, and C are all part of the same ring system. In depiction of ring systems, the constraints of the ring system determine the positioning of the three plain bonds and those constraints take precedence over other matters.

This depiction is an acceptable style when two of the plain bonds are within a ring. There would likely be a more preferred way of representing a tetrahedral stereocenter of this type, but this depiction is unambiguous.

This depiction is also an acceptable style when the wedged bond is itself within a ring system. This style is used primarily when the ring system is shown in perspective, with the wedged bond helping to indicate that perspective.

This depiction style must not be used when all four substituents are acyclic, since structures of this sort are ambiguous and cannot be interpreted reliably.

ST-1.1.8

Wrong

Wrong

Wrong

Wrong
Three plain bonds and one wedged bond, with one adjacent pair of plain bonds separated by 180° or more and the wedged bond not positioned within that largest space between plain bonds.

These depictions represent see-saw or square pyramidal configurations rather than tetrahedral ones and are not acceptable for representing tetrahedral configurations.

**ST-1.1.9**

\[
\begin{array}{cccc}
A & B & C & D \\
\text{Not acceptable} & \text{Not acceptable} & \text{Not acceptable} & \text{Not acceptable}
\end{array}
\]

Three bonds of the same wedged type (solid wedged or hashed wedged) and one bond of another type (the opposite wedge type, or plain), with each pair of identically wedged bonds separated by less than 180° (ideally, 120° as shown here). The fourth bond can be positioned in any orientation but will usually bisect one of the other angles as shown here.

Although these depictions are formally unambiguous, they should be avoided due to the overabundance of wedged bonds.

**ST-1.1.10**

\[
\begin{array}{cccc}
A & B & C & D \\
\text{Not acceptable} & \text{Not acceptable} & \text{Not acceptable} & \text{Not acceptable}
\end{array}
\]

\[
\begin{array}{cccc}
A & B & C & D \\
\text{Not acceptable} & \text{Not acceptable} & \text{Not acceptable} & \text{Not acceptable}
\end{array}
\]

Three bonds of the same wedged type (solid wedged or hashed wedged) and one bond of another type (the opposite wedge type, or plain), with one adjacent pair of identically wedged bonds separated by 180° or more and the fourth bond positioned within that largest space between the identically wedged bond bonds.

These depictions are formally ambiguous and cannot be interpreted with certainty. They should never be used.

**ST-1.1.11**

\[
\begin{array}{cccc}
A & B & C & D \\
\text{Acceptable} & \text{Acceptable} & \text{Acceptable}
\end{array}
\]

Two bonds of the same wedged type (solid wedged or hashed wedged) and one bond of another
type (the opposite wedge type, or plain), with each adjacent pair separated by 90°, and with alternating bond types.

This depiction style is not preferred, but it is still acceptable.

**ST-1.1.12**

Two bonds of the same wedged type (solid wedged or hashed wedged) and one bond of another type (the opposite wedge type, or plain), with each adjacent pair separated by other than 90°, and with alternating bond types.

Although these depictions are formally unambiguous, they can be extremely confusing to the reader due to their infrequent use in the published literature. They should be avoided.

**ST-1.1.13**

Two solid wedged bonds and two hashed wedged bonds, with each adjacent pair of bonds separated by less than 180°, and with similar bond types depicted as adjacent.

This depiction represents a square planar configuration rather than a tetrahedral one and is not acceptable for representing tetrahedral configurations.

**ST-1.1.14**

Two solid wedged bonds and two hashed wedged bonds, with one pair of identically-wedged bonds separated by 180° or more and with the other pair positioned within the smaller angle described by the first pair.

These depictions represent square pyramidal configurations rather than tetrahedral ones and are not acceptable for representing tetrahedral configurations.

**ST-1.1.15**

Two wedged bonds of the same type (either solid wedged or hashed wedged) and two plain bonds, with each adjacent pair of bonds separated by 180° or less, and with similar bond types
depicted as adjacent.
These depictions are formally ambiguous and cannot be interpreted with certainty. They should never be used.

**ST-1.1.16**

```
  A  B  D  C
  A  B  D  C
Wrong  Wrong
```

Two wedged bonds of the same type (either solid wedged or hashed wedged) and two plain bonds, with the pair of plain bonds separated by more than 180°, and with the wedged bonds positioned within the smaller angle described by the first pair.

These depictions represent square pyramidal configurations rather than tetrahedral ones and are not acceptable for representing tetrahedral configurations.

**ST-1.1.17**

```
  A  B  D  C
  A  B  D  C
  A  B  D  C
Wrong  Wrong  Wrong  Wrong
```

Four wedged bonds of the same type (either solid wedged or hashed wedged) positioned at any angles.
These depictions represent square pyramidal configurations rather than tetrahedral ones and are not acceptable for representing tetrahedral configurations.

**ST-1.1.18**

```
  A  B  D  C
  A  B  D  C
  A  B  D  C
  A  B  D  C
Not acceptable  Not acceptable
```

One plain bond and two wedged bonds of the same type (either solid wedged or hashed wedged), each pair separated by less than 180°, and a fourth bond of the opposite wedged type positioned between the two similar wedged bonds.

Although these depictions are formally unambiguous, they should be avoided due to the overabundance of wedged bonds.

**ST-1.1.19**

```
  A  B  D  C
  A  B  D  C
  A  B  D  C
  A  B  D  C
Not acceptable  Not acceptable  Not acceptable  Not acceptable
```

One plain bond and two wedged bonds of the same type (either solid wedged or hashed wedged) and a fourth bond of the opposite wedged type positioned between the two similar
wedged bonds, with any adjacent pair of bonds separated by 180° or more.

Although these depictions may represent square planar, square pyramidal, or see-saw configurations, they should be avoided regardless due to the overabundance of wedged bonds. These configurations will be formally ambiguous in some combinations of bond angles.

**ST-1.1.20**

![Diagram](image)

Not acceptable

One plain bond and two wedged bonds of the same type (either solid wedged or hashed wedged), each adjacent pair separated by less than 180°, and a fourth bond of the opposite wedged type not positioned between the two similar wedged bonds.

Although these depictions are formally unambiguous, they should be avoided due to the overabundance of wedged bonds.

**ST-1.1.21**

![Diagram](image)

Not acceptable Not acceptable Not acceptable Not acceptable Not acceptable Not acceptable

One plain bond and two wedged bonds of the same type (either solid wedged or hashed wedged) and a fourth bond of the opposite wedged type not positioned between the two similar wedged bonds, with any adjacent pair of bonds separated by 180° or more.

Although these depictions may represent square planar, square pyramidal, or see-saw configurations, they should be avoided regardless due to the overabundance of wedged bonds. These configurations will be formally ambiguous in some combinations of bond angles.

**ST-1.2 Tetrahedral depictions with three explicit bonds**

The drawing of a stereocenter containing a hydrogen atom will generally appear less encumbered if that substituent is omitted. Tetrahedral atoms with one hydrogen substituent can usually omit the hydrogen (this is a change from earlier recommendations [2]), but it is always acceptable to depict the hydrogen explicitly. Structures depicted with explicit hydrogens are less ambiguous than those with implicit hydrogens; however, the rigorous display of all explicit hydrogens also adds to the overall congestion of a diagram and can quickly render a depiction illegible even for moderately sized structures.

Hydrogens should be omitted from tetrahedral atoms only when the resulting structure is unambiguous. In this context, it means that a substituent at the end of the wedged bond should have a maximum of two non-hydrogen substituents including the wedged bond itself. It is also acceptable to omit the hydrogen in cases where the substituent has more than two non-hydrogen substituents as long as the substituent itself is nonstereogenic. Care should be taken in that case, however, that the substituent cannot possibly be interpreted as being asymmetric, and should generally be limited to common small substituents such as unsubstituted rings, tert-butyl groups, and so on.
Hydrogens must not be omitted when the other substituent is itself asymmetric, since stereobonds must be avoided between two stereocenters when any alternative is available.

A trigonal pyramidal atom may be considered as similar to a tetrahedral atom having three explicit bonds, where the position of the fourth “bond” in the case of a trigonal pyramidal atom is occupied by a lone pair rather than an implicit hydrogen atom. Depictions of trigonal pyramidal atoms are discussed more fully in ST-2.5.

When depicting tetrahedral configuration around a stereogenic atom with three explicitly drawn bonds, the following configurations may be considered.

**ST-1.2.1**

Two plain bonds and one wedged bond, with the pair of plain bonds separated by less than 180° (ideally, 120° as shown here) and the wedged bond opposing the A-B angle. Additionally, the substituent C at the end of the wedged bond should generally be among the graphically smallest of the three.

The wedged bond should preferably be collinear with the bisector of the A-B angle. If it is not collinear, the depiction is still acceptable, but not preferred.

The implied hydrogen or lone pair in this depiction is assumed to be behind the C substituent, thus:
ST-1.2.2

Two plain bonds and one wedged bond, with the pair of plain bonds separated by less than 180° and the wedged bond positioned within the smaller space between plain bonds.

The implied hydrogen or lone pair in this depiction is assumed to be opposite the A-B angle relative to the C substituent. This leads to the observation that the absolute stereochemistry of a tetrahedral configuration depicted with two plain bonds and one wedged bond is unchanged regardless of where the wedged bond is positioned, thus:

Preferred

This depiction style should be used with caution. It is the preferred style when substituent C is a bridgehead bond of a bridged ring system. In depiction of ring systems, the constraints of the ring system determine the positioning of the three bonds and those constraints take precedence over other matters.

Acceptable

When substituents A and B are both within the same non-perspective ring, and the A-B angle is re-entrant (pointing “inward” relative to the ring), this depiction style is not acceptable and should be avoided. In such cases, it will never be clear to the user whether the wedged bond was intended to be interpreted in its normal sense or whether it was intended to be interpreted relative to the
plane of the ring as depicted — and the two senses would result in opposite stereochemical configurations. This is discussed further in ST-1.4.

**ST-1.2.3**

Two plain bonds and one wedged bond, with the pair of plain bonds separated by 180°.

These depictions represent T-shaped configurations rather than tetrahedral ones and are not acceptable for representing tetrahedral configurations.

**ST-1.2.4**

Two plain bonds and one wedged bond, with the wedged bond separated from one of its adjacent plain bonds by 180° or more.

These depictions are acceptable but not preferred. They are most commonly used when the two plain bonds are within a ring displayed in perspective. As discussed in ST-3, it is preferred to use exclusively plain bonds in perspective diagrams, but the use of solid wedged and hashed wedged bonds within a perspective diagram remains acceptable.

If these depictions are used, the implied hydrogen is assumed to be positioned in the largest free angle:

**ST-1.2.5**

Acceptable
One plain bond, one solid wedged bond, and one hashed wedged bond, with the plain bond separated from one of its adjacent wedged bonds by 180° or more.

These depictions are acceptable, but not preferred because they can typically be drawn with fewer wedged bonds. If these depictions are used, the implied hydrogen is assumed to be positioned in the largest free angle:

\[ \text{A} \bigtriangleup \text{B} \bigtriangledown \text{C} = \text{A} \bigtriangleup \text{B} \bigtriangledown \text{C} \]

**ST-1.2.6**

One plain bond, one solid wedged bond, and one hashed wedged bond, with the plain bond separated from both of its adjacent wedged bonds by 180° or less.

These depictions represent trigonal planar configurations rather than tetrahedral ones and are not acceptable for representing tetrahedral configurations.

**ST-1.2.7**

One plain bond and two wedged bonds of the same type (either solid wedged or hashed wedged) positioned at any angles.

Although these depictions are formally unambiguous, they should be avoided due to the overabundance of wedged bonds. In addition, these depictions can be difficult to interpret due to issues similar to those discussed in ST-1.2.2. If these depictions were used, the implied hydrogen would be assumed to be opposite the A-B angle relative to the C substituent:

\[ \text{A} - \text{B} - \text{C} = \text{A} - \text{H} - \text{B} = \text{A} - \text{H} - \text{B} = \text{H} - \text{B} - \text{C} \]

\[ \text{A} - \text{B} - \text{C} = \text{A} - \text{H} - \text{B} = \text{A} - \text{H} - \text{B} = \text{H} - \text{B} - \text{C} \]
**ST-1.2.8**

Two wedged bonds of the same type (either solid wedged or hashed wedged) and one wedged bond of the opposite type, with all pairs of adjacent bonds separated by 180° or less.

These depictions represent trigonal planar configurations rather than tetrahedral ones and are not acceptable for representing tetrahedral configurations.

**ST-1.2.9**

Two wedged bonds of the same type (either solid wedged or hashed wedged) separated by 180° or more and one wedged bond of the opposite type positioned within the smaller angle described by the first two bonds.

Although these depictions are formally unambiguous, they should be avoided due to the overabundance of wedged bonds.

**ST-1.2.10**

One solid wedged bond and one hashed wedged bond separated by 180° or more and one wedged bond of either type positioned within the smaller angle described by the first two bonds.

These depictions are formally ambiguous and cannot be interpreted with certainty. They should never be used.

**ST-1.2.11**

Three wedged bonds of the same type (either solid wedged or hashed wedged), with all pairs of adjacent bonds separated by 180° or less.

Although these depictions are formally unambiguous, they should be avoided due to the overabundance of wedged bonds.
ST-1.2.12

Three wedged bonds of the same type (either solid wedged or hashed wedged), with one pair of adjacent bonds separated by 180° or more.

These depictions are formally ambiguous and cannot be interpreted with certainty. They should never be used.

ST-1.3 Stereogenic atoms in rings

Because of the importance of rings in organic chemistry, it is generally best to keep the ring system(s) as uncomplicated as possible while also preserving the clarity of any individual stereogenic atoms within those rings.

Asymmetric ring atoms with a single non-hydrogen exocyclic substituent should usually be drawn with a wedged bond to that substituent and with the hydrogen implicit. The wedged bond should be positioned so that it is parallel with the bisector of the angle between the two other ring bonds on that atom. However, also see below for a discussion of avoiding stereobonds between stereocenters.

Preferred

Asymmetric ring atoms with two simple exocyclic substituents should be drawn with a wedged bond to one substituent and a hashed bond to the other. The two exocyclic bonds should be positioned so that the bisector of the angle between them is collinear with the bisector of the angle between the ring bonds, and the angle between the exocyclic bonds should ideally be close to 60°.

Preferred

If one of the exocyclic substituents is complex, it is best to connect it to the ring with a plain bond. The plain bond in that case should itself bisect the angle between the ring bonds, and the remaining substituent, regardless of stereochemical nature (solid wedged or hashed wedged bond), should be positioned to maximize legibility. Typically, that final substituent would be positioned outside the ring and near the bisector of the angle between one of the ring bonds and the larger exocyclic substituent.
Asymmetric ring fusion atoms should be drawn with hashed wedged or solid wedged bonds to the exocyclic substituent at the fusion atom whenever possible. If necessary, an implicit hydrogen should be made explicit in order to provide an exocyclic substituent to bear the hashed wedged or solid wedged bond. When one of the fusion bonds is oriented vertically and the exocyclic substituent is graphically small (such as a hydrogen or a methyl group, or even such physically larger substituents as a phenyl group represented with a graphically small “Ph” atom label), the exocyclic substituent is also preferentially oriented vertically and opposite to the vertical fusion bond. This orientation is preferred even if it results in the substituent being placed within the ring system, and is particularly common in the depiction of steroids and other natural products.

Asymmetric spiro fusions are treated similarly to a ring with two exocyclic substituents. The two bonds associated with one of the rings in the spiro fusion should be drawn as plain bonds, while the two bonds associated with the other ring should be drawn with one solid wedged bond and one hashed wedged bond.

In asymmetric spiro fusions involving rings of different sizes, the solid wedged and hashed wedged bonds are usually associated with the smaller ring.

Asymmetric spiro fusions involving rings of the same size are often depicted with one ring distorted toward the spiro axis. In such cases, the solid wedged and hashed wedged bonds should be associated with the distorted ring.
Asymmetric spiro fusions that are themselves adjacent to other stereogenic atoms should be represented using one of the other preferred or acceptable depiction styles for tetrahedral configurations, so that wedged bonds are not depicted with stereogenic atoms on both ends.

Atoms participating in both regular and spiro fusions should similarly be drawn with one solid wedged and one hashed wedged bond. Those two bonds should be the ones that do not participate in a regular ring fusion. The two bonds that do participate in a regular ring fusion should remain plain.

Atoms participating in both regular and spiro fusions that are themselves adjacent to other stereogenic atoms should be represented using one of the other preferred or acceptable depiction styles for tetrahedral configurations, so that wedged bonds are not depicted with stereogenic atoms on both ends.

**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.
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.

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.
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-1.5 Tetrahedral stereocenters connected to a double bond**

Tetrahedral stereochemistry requires a tetrahedral arrangement of ligands around a central point. It does not require that all of those ligands be connected to a central atom using single bonds. It is perfectly reasonable to have one or more ligands connected to the central atom using higher-order bonds. This is most commonly seen with chiral sulfoximides, phosphates, and related compounds, each of which is commonly drawn with one or more double bonds. Stereocenters of this type should be indicated by the appropriate placement of bold and/or hashed wedged bonds connecting the central atom to the singly-bonded ligands. Although wedged and hashed double bonds have appeared in the literature, they are rarely required for chemical clarity, and their use is infrequent enough to be confusing to the casual viewer.

**ST-1.6 Cumulenes with an even number of double bonds**

Cumulenes with an even number of double bonds can be considered as systems with a chiral axis or possessing axial chirality. Four substituents of an even cumulenic system form a distorted tetrahedral arrangement and can be viewed as similar to an atomic center, except with double bonds inserted in the middle and connecting two pairs of substituents. These systems can be interpreted by “squeezing out” the double bonds in the viewer’s mind, and considering the four isolated substituents, but this sort of “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.

\[ X \cdots C \cdots Y \approx X \cdots W \cdots Z \]
These stereogenic units should be drawn using rules similar to those for regular atomic centers discussed above with a difference that stereobonds may not be used on both ends of the cumulenic system.

![Preferred and acceptable stereogenic units for cumulenic systems](image)

It is unambiguous to depict a cumulenic system with three plain bonds and one hashed or wedged bond, so that depiction style is acceptable. It is, however, fairly unusual to have a plain bond on the same end of a cumulenic system as a solid wedged bond or a hashed wedged bond. This depiction style should be limited to cases when one of the atoms adjacent to the cumulenic system is itself asymmetric, in which case it is desirable to avoid drawing a stereobond between the cumulenic system and a second stereocenter.

![Acceptable and not acceptable stereogenic units for cumulenic systems](image)

**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.

![Hindered biaryl structure](image)

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. Preferably, one ring system of each pair should be drawn exclusively with plain bonds, and the other should be drawn with two solid wedged bonds, one directly connected to the rotating bond and one opposite. In even-membered systems, the bond between the solid wedged bonds should be depicted as bold and unwedged if it does not itself participate in a ring fusion.

The configuration of the biaryl system should not solely be represented by solid wedged and hashed wedged bonds to other ring substituents that are distant from the rotatable bond.
**ST-1.8 Fischer projections**

Fischer projections are characterized by one or more asymmetric centers surrounded by four plain bonds arranged in a plus-shaped pattern, with multiple adjacent asymmetric centers aligned vertically. They were originally proposed \[6,7\] for the depiction of carbohydrates, and they remain acceptable for the depiction of carbohydrates and their derivatives [5].

\[
\begin{array}{c}
\text{CHO} \\
\text{H} \\
\text{HO} \\
\text{H} \\
\text{H} \\
\text{OH} \\
\text{CH}_2\text{OH}
\end{array}
\quad
\begin{array}{c}
\text{CHO} \\
\text{HO} \\
\text{H} \\
\text{H} \\
\text{OH} \\
\text{OH} \\
\text{CH}_2\text{OH}
\end{array}
\]

*Acceptable*  *Acceptable*

The use of Fischer projections in non-carbohydrates is problematic. Any drawings of this type are necessarily ambiguous since it is unclear if the author of the drawing intended to make a Fischer projection or simply happened to draw a diagram in that orientation. Structures depicted in the style of Fischer projections are likely to be recognized as such when they contain at least two acyclic stereogenic centers oriented vertically, although such interpretation is not guaranteed. Structures containing a single stereogenic center pose even greater problems since it is often convenient to separate the four ligands by equal angles whether or not a single stereoisomer is intended.

\[
\begin{array}{c}
\text{Cl} \\
\text{Br} \\
\text{F} \\
\text{I}
\end{array}
\quad
\begin{array}{c}
\text{Cl} \\
\text{Br} \\
\text{F} \\
\text{I}
\end{array}
\quad
\begin{array}{c}
\text{Cl} \\
\text{Br} \\
\text{F} \\
\text{I}
\end{array}
\]

*Fischer-like depictions of small non-carbohydrates are ambiguous*

Accordingly, although Fischer projections of carbohydrates are acceptable, similar depictions of non-carbohydrates should be used only when the viewer of the diagram is certain to understand that the diagram was intended to represent a Fischer projection. Fischer projections should be avoided where ambiguity is possible, including when used in computer applications.

In an earlier document [8], a related depiction style was discussed in which asymmetric centers were aligned horizontally instead of vertically. That style is no longer preferred, and should not be used outside the context of polymers in any case.

\[
\begin{array}{c}
\text{CH}_3
\end{array}
\quad
\begin{array}{c}
\text{H} \\
\text{H}
\end{array}
\quad
\begin{array}{c}
\text{HOH}_2\text{C} \\
\text{OH} \\
\text{OH} \\
\text{OH}
\end{array}
\]

*Preferred*  *Acceptable*  *Not acceptable*

It is also worth noting that Fischer projections are the only representations of stereochemistry that are not invariant with respect to rotation in the plane of the paper. A Fischer projection rotated 90° represents the enantiomer of the original unrotated structure; in all other cases, a rotated diagram is identical to a non-rotated one.
These comments do not apply to the assorted variants of Fischer projections that have one or more wedged or hashed bonds on each stereocenter. Those can readily be interpreted according to the same rules used for interpreting wedged and hashed bonds in other (non-Fischer) cases.

ST-1.9 Haworth projections

Haworth projections, like Fischer projections, are used primarily in depicting carbohydrates and related compounds such as inositols. These diagrams are characterized by a ring system viewed “in perspective”, with wedged and/or bold bonds. There are several subtypes of Haworth projections, including variations with and without hydrogens and variations with and without the bottom-most ring bond drawn as bold. The wedges may also be omitted entirely.

It is also acceptable to depict the acyclic carbon atoms in a Fischer projection when the main carbohydrate ring is depicted in a Haworth projection.
Diagrams of this type can be ambiguous in many ways. Even when wedges are present, only two of the four or five asymmetric ring atoms are situated at the narrow ends of wedges. In six-membered rings, one of the stereogenic atoms isn’t attached to a wedge at all, either at the wide or the narrow end. When wedges are omitted, matters only get worse.

Any drawings of this type are necessarily ambiguous since it is unclear if the author of the drawing intended to make a Haworth projection or simply happened to draw a diagram in that orientation. Accordingly, these depictions should be used only when the viewer of the diagram is certain to understand that the diagram was intended to represent a Haworth projection. Haworth projections should be avoided where ambiguity is possible, including when used in computer applications.

An alternative to Haworth projections would be to draw the ring system according to standard conventions for depicting structures within a plane. In the context of carbohydrate chemistry, this “from above” drawing style is also known as the Mills depiction [9].

**ST-1.10 H-Dot/H-Dash/H-Circle**

The use of the H-Dot, H-Dash, and H-Circle symbols remains strongly deprecated. These symbols have been used to indicate the position of a hydrogen atom at a ring fusion, with the dot form representing a hydrogen above the plane of the ring and the dash or circle form representing a similar hydrogen below the plane of the ring.
Unfortunately, the dashes and especially the dots and circles are often very subtle and can be easily overlooked. When clarity is important, they should be avoided.

Even when used, H-Dots, H-Dashes, and H-Circles are meaningful only when positioned on unsaturated ring-fusion carbon atoms containing a single exocyclic hydrogen substituent. They should never be used in any other circumstances.

**ST-2. NON-TETRAHEDRAL CONFIGURATIONS**

Although tetrahedral configurations are by far the most common type of stereochemistry among organic compounds, they are not the only type to consider. Many other configurations exist, primarily among inorganic structures, and several of them are fairly common.

In the recommendations to follow, atom labels have been omitted from the structural diagrams at the ligand positions so that the orientation of the bonds may be seen most clearly. Traditionally, an unlabeled atom represents a carbon atom to organic chemists, but the unlabeled ligands here may represent any sort of structure, certainly including a carbon atom, but also potentially a hydrogen, a halogen, or any other element type. These recommendations are concerned only with the geometry of the central atom, generally labeled with an “M” below. They apply regardless of the types of ligands, and regardless of whether the ligands are discrete entities (chelating substituents, for example, would have one or more ligating atoms linked to each other, either directly or through other atoms).

The depictions in this section labeled as “preferred” have been selected in order to satisfy two primary goals: they must be recognizable to most chemists, and they must not be readily confused with any other conformation. Thus, a depiction of a square pyramidal configuration must clearly indicate the pyramidal arrangement of its four ligands, and at the same time it must not suggest that the ligands might be arranged in a planar or tetrahedral configuration instead. In consequence, the depictions here follow many of the general precepts regarding the use of perspective to represent configuration that are discussed more fully in ST-3.

In accordance with the IUPAC revision of the Nomenclature of Coordination Compounds [10], polyhedral symbols that are tied to the presence of lone pairs (e.g. $TBPY$-3, $TBPY$-4) are no longer recommended.

**ST-2.1 Linear**

**Polyhedral symbol $L$-$2$**

**Number of ligands: 2**

Linear configurations have two ligands diametrically opposite to each other, separated by exactly 180°. Although depiction styles are discussed here, for practical purposes the only important detail is that the ligands be drawn in a linear fashion, as implied by this configuration.
Isolated linear systems should be drawn horizontally, vertically, or at a 30° angle rising or descending from left to right. Linear fragments that are part of larger compounds should be positioned according to the needs of the larger system.

Because of their simplicity, many well-known linear systems can be represented succinctly using formulas rather than explicit atoms and bonds.

### ST-2.2 Angular Polyhedral symbol: A-2 Number of ligands: 2

Angular configurations have two ligands that are separated from each other by any amount other than 180°. Although depiction styles are discussed here, for practical purposes the only important detail is that the ligands not be drawn in a linear fashion, as implied by this configuration name.

Isolated angular systems should be drawn horizontally, with one bond extending upwards at a 30° angle rising from left to right, and the other bond extending downwards at the opposite angle. Angular fragments that are part of larger compounds should be positioned according to the needs of the larger system.

Because of their simplicity, many well-known angular systems can be represented succinctly using formulas rather than explicit atoms and bonds.
ST-2.3 T-shaped Polyhedral symbol: TS-3 Number of ligands: 3

T-shaped configurations have three ligands, so they must be clearly differentiated not only from trigonal pyramidal and trigonal planar configurations, but also from tetrahedral configurations that are drawn with an implicit hydrogen on the central atom. Although the T-shaped configuration does not technically need a depiction style of its own since all atoms are coplanar, it is useful to specify a recommended style to distinguish it from the other three-coordinate configurations. In other words, the recommended styles for a T-shaped configuration are not recommended for any of the other configurations.

Because they may also be mistakenly viewed as representing a tetrahedral configuration with one missing ligand, depictions of T-shaped configurations must clearly distinguish themselves from tetrahedral depictions with, for example, an implicit hydrogen on the central atom. Accordingly, these configurations must never be drawn with implicit ligands. All three ligands must be drawn so that they are connected to the central atom by explicit bonds, and the central atom must clearly be labeled as a single atom (that is, as “Br” versus “BrCl”, for example).

Furthermore, it is understood that the common organic elements carbon and nitrogen are virtually never found as the central atom in a T-shaped configuration. Even if a diagram is drawn in one of the recommended depiction styles below, it should not be considered to represent a T-shaped configuration if the central atom is a carbon or a nitrogen.

Because the recommended depiction style lacks any solid wedged or hashed wedged bonds, there is no way to distinguish visually a T-shaped structure of known configuration from one of unknown configuration. T-shaped structures of unknown axial/equatorial configuration should be described textually by using the (TS-3) prefix before the systematic name or formula, but no attempt should be made to draw them graphically.

In the recommended depictions, three plain bonds extend from the center exactly horizontally or exactly vertically.

```
Preferred Preferred Preferred Preferred
```

The T-shaped configuration is inherently planar. Depictions that involve solid wedged or hashed wedged bonds, even though formally correct, are discouraged.

```
Not acceptable Not acceptable Not acceptable Not acceptable
```

Sample depiction of a compound known to exist in T-shaped configuration:

```
F
\(\text{Br} - F\)
F
```

Preferred
ST-2.4 Trigonal planar  Polyhedral symbol: TP  Number of ligands: 3

Trigonal planar configurations also have three ligands, and share many of the concerns seen with T-shaped configurations. They must be clearly differentiated not only from T-shaped and trigonal pyramidal configurations, but also from tetrahedral configurations that are drawn with an implicit hydrogen on the central atom. Although this configuration does not technically need a depiction style of its own since all atoms are coplanar, it is useful to specify a recommended style to distinguish it from the other three-coordinate configurations. In other words, the recommended styles for a trigonal planar configuration are not recommended for any of the other configurations.

Because they may also be mistakenly viewed as representing a tetrahedral configuration with one missing ligand, depictions of trigonal planar configurations must clearly distinguish themselves from tetrahedral depictions with, for example, an implicit hydrogen on the central atom. Accordingly, these configurations must never be drawn with implicit ligands. All three ligands must be drawn so that they are connected to the central atom by explicit bonds, and the central atom must clearly be labeled as a single atom (that is, as “B” versus “BF”, for example).

In the recommended depictions, three plain bonds extend from the center with equal angular spacing between them.

Preferred  Preferred  Preferred  Preferred

It is worth noting that sp² carbons are amongst the more common examples of trigonal planar configurations. In the case of an sp² carbon, the central atom does not need to be labeled. Further information about depiction of sp² carbons and related compounds may be found in the double-bond configuration recommendations in ST-0.4.

Preferred  Preferred  Preferred

Unfortunately, although the simplest and most accurate way to represent trigonal planar configurations is using three plain bonds as above, that leaves no way to distinguish a configuration that is explicitly known to be trigonal planar from an arbitrary three-coordinate center of unknown configuration, which might also be depicted with three plain bonds. When it is necessary to emphasize that a three-coordinate system definitely is in a trigonal planar configuration, it should be depicted with one plain bond, one solid wedged bond, and one hashed wedged bond. The solid wedged bond and the hashed wedged bond should be separated by an angle that is significantly less than 120°, and ideally close to 60° as shown here. The bisector of the angle between the solid wedged bond and the hashed wedged bond must be collinear with the plain bond. If the plain bond is oriented horizontally, the solid wedged bond should be positioned below the hashed wedged bond.

Preferred  Acceptable  Acceptable  Not acceptable  Not acceptable
Sample depiction of a compound known to exist in trigonal planar configuration:

```
F
\(\text{F} \ - \ B \ - \ F\)
```

**Preferred**

**ST-2.5 Trigonal pyramidal Polyhedral symbol: TPY -3 Number of ligands: 3**

Trigonal pyramidal configurations have three ligands, but are perhaps the most difficult configurations to depict unambiguously. Because they may also be viewed as representing a tetrahedral configuration with one missing ligand, depictions of trigonal pyramidal configurations must clearly distinguish themselves from tetrahedral depictions with, for example, an implicit hydrogen on the central atom. Accordingly, as with T-shaped configurations, trigonal pyramidal configurations must never be drawn with implicit ligands. All three ligands must be drawn so that they are connected to the central atom by explicit bonds, and the central atom must clearly be labeled as a single atom (that is, as “N” versus “NH”, for example).

In the first recommended depiction, a plain bond and a hashed wedged bond form an angle between them of greater than 90° but less than 180°. The third bond is drawn as a solid wedged bond between the first two, but separated from the plain bond by greater than 90°.

```
\(\text{M} \ \ M \ \ M\)
```

Preferred Not acceptable

In the second recommended depiction, two bonds are drawn as plain bonds, separated by an angle less than 180°. The third bond is drawn as a solid wedged bond or a hashed wedged bond, positioned at any angle. The third bond will traditionally bisect the angle formed by the plain bond, positioned either between them or opposite them, but such positioning is not mandatory.

This depiction style is very similar to depiction styles recommended for tetrahedral configurations. That is appropriate, since a trigonal pyramidal configuration does correspond to a tetrahedral configuration with one fewer ligand. This depiction style must therefore not be used in cases where the central atom might incorrectly be interpreted as having a fourth ligand.

```
\(\text{M} \ \ M\)
\(\text{M} \ \ M\)
```

Preferred Acceptable Preferred Acceptable Acceptable

A third depiction consists of one plain bond and two other bonds that are drawn both as solid wedged bonds or both as hashed wedged bonds, with each adjacent pair of atoms separated by less than 180°. This style, while formally correct, is discouraged because it has many stereobonds and may be confusing to the reader.

```
\(\text{M} \ \text{M}\)
```

Not acceptable Not acceptable

A related depiction consists of a plain bond, a solid wedged bond, and a hashed wedged bond,
where the bisector of the angle formed by the solid and hashed wedged bonds is collinear with the plain bond. This should be avoided, as it actually describes a planar rather than a pyramidal configuration.

\[
\begin{array}{c}
\text{Not acceptable} \\
\end{array}
\]

A final depiction style consists of a three solid wedged bonds or three hashed wedged bonds. This style, while formally correct, is discouraged because it has so many stereobonds as to be confusing to the reader.

\[
\begin{array}{c}
\text{Not acceptable} \\
\text{Not acceptable} \\
\end{array}
\]

Trigonal pyramidal atoms should never be drawn with an explicit lone pair at the end of a bond because that bond could be misinterpreted as an additional methyl group.

\[
\begin{array}{c}
\text{Preferred} \\
\text{Acceptable} \\
\text{Not acceptable} \\
\end{array}
\]

In rare cases, a trigonal pyramidal atom with at least one double bond may be flanked by other stereocenters at the other ends of all of its single bonds. In such cases, one of the plain bonds should be changed to a wedged bond even though it joins two stereocenters. It is also acceptable to use a solid wedged or hashed wedged double bond, but that would not be preferred because wedged double bonds are so rarely seen in the literature.

\[
\begin{array}{c}
\text{Preferred} \\
\text{Acceptable} \\
\end{array}
\]

Sample depictions of some compounds known to exist in trigonal pyramidal configuration:
ST-2.6 Square planar  Polyhedral symbol: SP-4  Number of ligands: 4

Square planar configurations have four ligands, the same as tetrahedral ones. One of the key issues in depicting these configurations is in making clear that a square planar configuration really is intended, and not a tetrahedral one. The recommended depictions are explicitly recommended not to be used for tetrahedral configurations.

The first recommended depiction should be drawn with two solid wedged bonds and two hashed wedged bonds. The two solid wedged bonds should be positioned below the central atom, while the two hashed wedged bonds should be positioned above. The angle between the solid wedged bonds should be equal to the angle between the hashed wedged bonds, and the bisectors of both angles should be coincident with the $y$-axis. Additionally, the angle between the solid wedged bonds should be greater than 90°, which implies that the angle between either solid wedged bond and its adjacent hashed wedged bond should be less than 90°.

It is also acceptable to draw similar structures with plain bonds. There are some cases where this drawing style would even be preferred, particularly when all four bonds are required to be in the plane of the paper by virtue of other aspects of the structural diagram (such as with the central atom of metalloporphyrins). When square planar configurations are drawn with plain bonds, it is preferable to have the angle between the bonds to be exactly 90°, and, as previously, the bisectors of angles formed by adjacent bonds should be coincident with the $x$- and $y$-axes. The similar depiction with the bonds themselves positioned along the axes is acceptable but should be avoided as it is extremely commonly used to represent tetrahedral centers, either if the tetrahedral configuration is nonstereogenic (carbon tetrachloride) or in Fischer projections.

Four other depictions are formally correct, but are often used as (incorrect) depictions of tetrahedral configuration, particularly in bridged ring systems.

Sample depictions of some compounds known to exist in square planar configuration:
ST-2.7 Square pyramidal  Polyhedral symbol: SPY-4  Number of ligands: 4

Square pyramidal configurations represent yet another type that has four ligands, the same as tetrahedral ones. Again, one of the key issues in depicting these configurations is in making clear that a square pyramidal configuration really is intended, and again the recommended depictions are explicitly recommended not to be used for tetrahedral configurations.

Furthermore, it is understood that the common organic element carbon is virtually never found in a square pyramidal configuration. Even if a diagram is drawn in one of the recommended depiction styles below, it should not be considered to represent a square pyramidal configuration if the central atom is isoelectronic with any member of the carbon group. Central atoms of that group are almost always found in tetrahedral configurations rather than square pyramidal configurations.

The first recommended depiction should be drawn with two solid wedged bonds and two hashed wedged bonds. The two solid wedged bonds should be positioned below the central atom, and the two hashed wedged bonds should also be positioned below the central atom. The angle between the solid wedged bonds should be less than to the angle between the hashed wedged bonds, and the bisectors of both angles should be coincident with the y-axis.

Preferred  Preferred  Not acceptable

To further emphasize the perspective implied by the solid wedged and hashed wedged bonds, the two solid wedged bonds may be adjusted so that they are slightly longer than but less than 150% of the length of the hashed wedged bonds.

Preferred

It is also acceptable to draw similar structures with plain bonds.

Preferred

Sample depiction of compound known to exist in square pyramidal configuration:
ST-2.8 See-saw

Polyhedral symbol: SS -4 Number of ligands: 4

See-saw configurations, like square pyramidal ones, can be very difficult to distinguish from tetrahedral configurations. Yet again, one of the key issues in depicting these configurations is in making clear that a see-saw configuration really is intended, and again the recommended depictions are explicitly recommended not to be used for tetrahedral configurations.

Furthermore, it is understood that the common organic element carbon is virtually never found in a see-saw configuration. Even if a diagram is drawn in one of the recommended depiction styles below, it should not be considered to represent a see-saw configuration if the central atom is isoelectronic with any member of the carbon group. Central atoms of that group are almost always found in tetrahedral configurations rather than see-saw configurations.

The first recommended depiction should be drawn with two plain bonds extending exactly vertically above and below the center. A solid wedged bond should extend downward from the center, and a hashed wedged bond should similarly extend upward so that the bisector of the angle formed by the solid and hashed wedged bonds is coincident with the \( x \)-axis.

\[
\begin{array}{cccc}
\text{Preferred} & \text{Preferred} & \text{Not acceptable} & \text{Not acceptable} \\
\end{array}
\]

An acceptable variant on this preferred depiction would be to slant the plain bonds a small but equal amount from the vertical, so that they lean towards the solid and hashed wedged bonds. The plain bonds should remain closer to the \( y \)-axis than they are to the solid and hashed wedged bonds.

The third preferred depiction should be drawn with two plain bonds extending exactly horizontally to the left and the right of the center. A solid wedged bond and a hashed wedged bond should extend downward from the center so that the bisector of the angle formed by the solid and hashed wedged bonds is coincident with the \( y \)-axis.

\[
\begin{array}{cccc}
\text{Preferred} & \text{Preferred} & \text{Preferred} & \text{Preferred} \\
\end{array}
\]

An acceptable variant on this preferred depiction would be to slant the plain bonds a small but equal amount from the horizontal, so that they lean towards the solid and hashed wedged bonds. The plain bonds should remain closer to the \( x \)-axis than they are to the solid and hashed wedged bonds.
bonds.

It is also acceptable to draw similar structures with plain bonds, particularly when at least one of the equatorial bonds is a double or triple bond. In this case, however, the axial bonds must be collinear, to distinguish this configuration from a square pyramidal one. Four plain bonds may be used only if the see-saw center is not itself chiral. Chiral see-saw configurations must be drawn with solid wedged bonds and hashed wedged bonds in order to confirm the specific chirality of the central atom.

Six other depictions are formally correct, but are often used as depictions of tetrahedral configuration, and should be avoided as to reduce confusion.

Sample depictions of some compounds known to exist in see-saw configuration:

**ST-2.9 Trigonal bipyramidal**  **Polyhedral symbol: TBPY-5  Number of ligands: 5**

Trigonal bipyramidal configurations have five ligands, and offer fewer problems of interpretation than configurations with three or four ligands.

The preferred depiction views the bipyramid axis from the side. In this case, the two axial bonds are drawn as plain bonds oriented vertically and a third bond is also drawn as a plain bond, oriented exactly at right angles to the two axial bonds and extending to either the left or the right. The fourth bond is drawn as a solid wedged bond extending opposite the third bond and downward from the center, while the fifth bond is drawn as a hashed wedged bond opposite the
third bond and extending upwards from the center. The bisector of the angle formed by the fourth and fifth bonds is coincident with the $x$-axis.

```
Preferred | Preferred | Not acceptable | Not acceptable
```

It is also acceptable to draw similar configurations with plain bonds if the trigonal bipyramidal center is not itself chiral. Chiral trigonal bipyramidal configurations must be drawn with solid wedged bonds and hashed wedged bonds in order to confirm the specific chirality of the central atom.

```
Acceptable | Acceptable
```

A third depiction shows the bipyramid axis viewed from above. In this case, the three equatorial bonds are drawn as plain bonds with equal separation. The fourth bond is drawn as a solid wedged bond extending downward from the center. The fifth bond is drawn as a hashed wedged bond that is collinear with the fourth bond, and hence extending upward. This depiction is acceptable but not preferred. It is used primarily in cases where it is useful to emphasize the coplanarity of the equatorial ligands.

```
Acceptable | Acceptable | Not acceptable | Not acceptable
```

A fourth case, also viewed “from the side”, is considered not acceptable. In this case, the third and fourth bonds are drawn as solid wedged bonds, both extending downward from the center, with the bisector of the angle formed by those bonds coincident with the $y$-axis. The fifth bond is drawn as a hashed wedged bond extending upwards from the center. A variation of this case has hashed wedged bonds drawn instead of solid wedged bonds and solid wedged bonds drawn instead of hashed wedged bonds; it is also considered not acceptable.

```
Not acceptable | Not acceptable | Not acceptable | Not acceptable
```

A fifth case, also viewed “from the side” is also considered not acceptable. In this case, the third and fourth bonds are drawn as hashed wedged bonds, both extending upwards from the center, with the bisector of the angle formed by those bonds coincident with the $y$-axis. The fifth bond is drawn as a solid wedged bond extending downwards from the center. A variation of this case has hashed wedged bonds drawn instead of solid wedged bonds and solid wedged bonds drawn instead of hashed wedged bonds; it is also considered not acceptable.
Sample depictions of some compounds known to exist in trigonal bipyramidal configuration:

**ST-2.10 Square pyramidal**

Square pyramidal configurations have five ligands, like trigonal bipyramidal configurations, but the configurations themselves are different enough that confusion is rare.

The first recommended depiction views the pyramid from the front. This depiction should be drawn with two solid wedged bonds and two hashed wedged bonds. The two solid wedged bonds should be positioned below the central atom, while the two hashed wedged bonds should also be positioned below, but above the two solid bonds. The bisectors of both angles should be coincident with the y-axis. The fifth bond is drawn as a plain bond extending exactly upwards from the center. This depiction emphasizes the noncoplanarity of the central atom with the four equatorial ligands and should not be used when it is known that the central atom is coplanar with them.

The second recommended depiction also views the pyramid from the front. This depiction should be drawn with two solid wedged bonds and two hashed wedged bonds. The two hashed wedged bonds should be positioned above the central atom, while the two solid wedged bonds should also be positioned above, but below the two solid bonds. The bisectors of both angles should be coincident with the y-axis. The fifth bond is drawn as a plain bond extending exactly downwards from the center. This depiction emphasizes the noncoplanarity of the central atom with the four equatorial ligands and should not be used when it is known that the central atom is coplanar with them.

The next two recommended depictions view the pyramid from the front. These depictions should be drawn with two solid wedged bonds and two hashed wedged bonds. The two solid
wedged bonds should be positioned below the central atom, while the two hashed wedged bonds should be positioned above. The angle between the solid wedged bonds should be equal to the angle between the hashed wedged bonds, and the bisectors of both angles should be coincident with the $y$-axis. The fifth bond is drawn as a plain bond extending exactly upwards or exactly downwards from the center. These depictions (and all of the subsequent ones) emphasize the coplanarity of the central atom with the four equatorial ligands and should not be used when it is known that the central atom is not coplanar with them.

\[
\begin{array}{cccc}
\text{Preferred} & \text{Preferred} & \text{Not acceptable} & \text{Not acceptable} \\
\end{array}
\]

A fifth depiction views the pyramid from the top. Four bonds are drawn as plain bonds, with equal angular spacing between them. The fifth bond is drawn as a solid wedged bond that may be positioned at any angle. This depiction is acceptable but not preferred for most cases. It is used primarily in cases where it is useful to emphasize the coplanarity of the equatorial ligands, and would be preferred primarily when all four bonds are required to be in the plane of the paper by virtue of other aspects of the structural diagram (such as with the central atom of metalloporphyrins). When square pyramidal configurations are drawn in this configuration, it is preferable for the bisectors of angles formed by adjacent bonds to be coincident with the $x$- and $y$-axes. The similar depiction with the bonds themselves positioned along the axes is acceptable but should be avoided.

\[
\begin{array}{cccc}
\text{Preferred} & \text{Acceptable} & \text{Not acceptable} & \text{Not acceptable} \\
\end{array}
\]

The sixth acceptable depiction views the pyramid from a corner. Two bonds are drawn as plain bonds, extending exactly horizontally in either direction from the center. The third bond is drawn as a solid wedged bond extending downward from the center. The fourth bond is drawn as a hashed wedged bond that is collinear with the third bond, and therefore extending upwards from the center. The fifth bond is drawn as a plain bond extending exactly vertically upwards or from the center. As in the previous depiction, this would most commonly be used when all the axial and two equatorial bonds are required to be in the plane of the paper by virtue of other aspects of the structural diagram (such as with the central atom of metalloporphyrins).

\[
\begin{array}{cccc}
\text{Acceptable} & \text{Acceptable} & \text{Not acceptable} & \text{Not acceptable} \\
\end{array}
\]

Sample depictions of some compounds known to exist in square pyramidal configuration:
ST-2.11 Octahedral Polyhedral symbol: OC-6 Number of ligands: 6

Octahedral configurations are by far the most common for six ligands.

The first recommended depiction should be drawn with two solid wedged bonds positioned below the central atom, while two hashed wedged bonds should be positioned above. The angle between the solid wedged bonds should be equal to the angle between the hashed wedged bonds, and the bisectors of both angles should be coincident with the $y$-axis. Finally, two plain bonds should extend exactly vertically, upwards and downwards from the center.

It is also acceptable to draw similar configurations with plain bonds if the octahedral center is not itself chiral. Chiral octahedral configurations must be drawn with solid wedged bonds and hashed wedged bonds in order to confirm the specific chirality of the central atom.

A third depiction is formally correct, but is not preferred because it has so many stereobonds as to be confusing to the reader. This depiction is used primarily to emphasize the $C_3$ symmetry of a configuration, or to emphasize that a configuration is explicitly not trigonal prismatic. In this configuration, three solid wedged bonds and three hashed wedged bonds are separated by equal angular spacing with the solid wedged bonds and hashed wedged bonds alternating.

A fourth depiction should be drawn with four plain bonds. Two of those should extend exactly vertically, one each above and below the center. Two others should extend exactly horizontally, one each to the left and to the right of the center. A fifth bond should be drawn as a solid wedged bond, extending downward from the center either to the left or the right. The sixth bond should be drawn as a hashed wedged bond, positioned collinear with the fifth, and therefore extending upwards from the center. It is also acceptable for the plain bonds to be rotated 45°, so that the bisectors of angles formed by adjacent plain bonds are coincident with the $x$- and $y$-axes.

Sample depictions of some compounds known to exist in octahedral configuration:
ST-2.12 Trigonal prismatic Polyhedral symbol: TPR -6 Number of ligands: 6

Trigonal prismatic configurations are rather uncommon, and can be distinguished from octahedral configurations without much problem.

The recommended depiction should be drawn with two solid wedged bonds, two hashed wedged bonds, and two plain bonds. The two solid wedged bonds should be positioned to the right of the central atom, and the bisectors of the angle formed by these bonds should be coincident with the x-axis. The two hashed wedged bonds should be placed similarly, with the angle between them sufficiently larger or smaller than the angle between the solid wedged bonds so as to avoid overlap. The two plain bonds should be placed collinear with the two hashed or solid wedged bonds that form the smaller angle, and hence should extend to the left of the center. Similar depictions with the left and right sides reversed are also acceptable.

To further emphasize the perspective implied by the solid and hashed wedged bonds, the two solid wedged bonds may be adjusted so that they are slightly longer than but less than 150% of the length of the hashed wedged bonds.

Two other depictions are formally correct, but are discouraged because they have so many stereobonds as to be confusing to the reader.

The two depictions shown below should be strongly avoided because they imply that the central atom is coplanar with four of its ligands.
Additionally, this is the first configuration that is commonly depicted as the polyhedral solid, showing lines between ligands and not showing the central atom.

Sample depictions of compounds known to exist in trigonal prismatic configuration:

**ST-2.13 Higher configurations**

Many compounds exist in configurations with more than six ligands, but such configurations quickly become difficult to depict accurately in two dimensions. Configurations with 7 or more ligands are most commonly depicted as polyhedral solids, showing lines between ligands and not showing the central atoms.

A fuller discussion of polyhedral solids may be found in the recommendations on the nomenclature of inorganic chemistry [10].

**ST-3. USE OF PERSPECTIVE TO INDICATE CONFIGURATION**

Most often, the three-dimensionality of chemical structures can simply be ignored when creating chemical diagrams. Thus, cyclohexane is traditionally drawn as a regular hexagon even though its prevailing chair configuration is far from planar. Sometimes, however, the precise three-dimensional configuration of a structure is critical to understanding its properties or behavior. Perspective drawings are most often used in bridged ring systems. There are many cases where perspective drawings are highly appropriate (bicyclo[2.2.1]heptane) or unavoidable without significant distortion of the parent structure (cubane, pagodane, buckminsterfullerene).
The biggest caveat with regard to perspective drawings is straightforward: perspective is a difficult concept. The artwork of M. C. Escher [11] famously demonstrates the ambiguities that can easily arise from the use and misuse of perspective. Even when used completely properly, perspective diagrams of chemical structures rely on subtle visual cues to impart significant changes of meaning in portions of the diagram that are far removed from those cues. In the first depiction of adamantane above, for example, the single bond crossing implies the configuration of all four bridgehead atoms.

Human researchers, for the most part, are trained to understand perspective diagrams and can usually interpret them properly. Unfortunately, computer interpretation of chemical structures is not as advanced. At the current time, few computer-based software packages will recognize perspective at all, let alone recognize it accurately and completely. For this reason, although perspective-based diagrams can be quite useful for humans, they should still be avoided in situations where accurate computer interpretation is important.

**ST-3.1 Restrictions on perspective drawings**

Except where the author specifically wants to convey a three-dimensional concept, the use of perspective drawings should be limited to ring systems, and should usually be further limited to bridged ring systems.

Perspective drawings of ring systems should always be drawn “from above and to the right”, so that the nearer atoms of a mostly-horizontal ring are positioned lower in the drawing than those that are further away. As a guide to the viewer, the front-to-back ordering of crossing bonds must be indicated. That ordering is depicted with a small discontinuity in the backmost bond.

The similar style drawn “from above and to the left” is acceptable, but not preferred because the “from above and to the right” style is much more prevalent in common usage.
In cases where the depicted front-to-back ordering (as indicated by such a discontinuity) conflicts with the notion that the lower atoms be nearer to the viewer, the depicted front-to-back ordering should take precedence and the diagram should be interpreted as being drawn “from below”. These situations should be strongly avoided.

When considering perspective drawings — as when considering all types of drawings — the diagram must be unambiguous, and it is the author’s responsibility to use whatever techniques are practical to remove ambiguity. In the specific case of perspective drawings, the proper indication of front-to-back ordering (by use of a discontinuity in the backmost bond) is especially important. Without the use of such a discontinuity, the point of intersection might reasonably be interpreted as an additional quaternary carbon in its own right. It is often possible to depict such structures with no ambiguity or overlap whatsoever if a non-perspective depiction style is used.

When present, the discontinuity should always be clear and unambiguous. For printed materials, that will generally mean that the discontinuity should be at least twice as wide as the width of a single bond. In low-resolution usages (for example, in GIF or JPEG files on the web or in documents that are expected to be faxed), the discontinuity may need to be larger so that it doesn’t risk disappearing due to blurring of the drawing.

**ST-3.2 Configuration in perspective drawings**

At a basic level, a perspective drawing is a simple projection of a three-dimensional structure into a two-dimensional plane. Accordingly, a well-drawn projection always can be interpreted as implying the absolute configuration specified by the original three-dimensional structure. A disubstituted bicyclo[2.2.1]hept-2-ene may be depicted as shown as with a bond crossing shown explicitly.
In this case, the proper interpretation of the bicyclic system implies that the hydrogens at each bridgehead must be directed outwards relative to the small cyclic system. The hydrogen connected to the lower bridgehead is projecting toward the viewer, while the hydrogen connected to the other bridgehead is projecting away from the viewer.

Unfortunately, there is a significant limitation in this common approach. If the original drawing — with no hashes or wedges — is taken to imply an absolute configuration, then there is no way to depict the similar structure where no absolute configuration is implied. Taken a step further, even the second structure with explicit bridgehead hydrogens leads to further problems. With the presence of the wedged and hashed bond, it is clear that the author intended the two bridgehead atoms to have the absolute configurations shown. However, what is intended by the bridging atom, with the A and B substituents? By perspective, the viewer must assume that it also represents an absolute configuration, but that leads to the same quandary: how would the similar structure be drawn if the absolute configuration at the bridging atom is not known?

Accordingly, perspective drawings must always be interpreted as having fully-specific absolute configuration at all stereogenic atoms (in the absence of other textual description — see ST-6 for examples). It is acceptable to further emphasize those stereocenters with additional solid wedged or hashed wedged bonds, but it is not necessary to do so.

When solid wedged or hashed wedged bonds are used, however, they must be used in agreement with other configurational details implied by the perspectivity.
If the absolute stereochemistry of a structure is not known, a perspective drawing should not be used, and a flat depiction style should be used instead.

\[ \text{Preferred} \]

**ST-3.3 Use of bold bonds to emphasize perspective**

Since perspective diagrams imply a single absolute configuration, it is not necessary to use solid wedged or bold bonds to emphasize that configuration further. Although such bonds may in some cases make the diagram slightly easier for an inexperienced viewer to understand the perspective used, such benefits are counterbalanced by the ambiguities introduced by depictions that incorporate stereobonds that connect two stereocenters.

![Acceptable](image1)

![Acceptable](image2)

![Acceptable](image3)

![Acceptable](image4)

Only solid wedged and bold bonds should be used for the purpose of emphasizing perspective. Hashed wedged bonds and hashed unwedged bonds should not be used, either in isolation or in combination with bold bonds.

![Not acceptable](image5)

![Not acceptable](image6)

It is, of course, always appropriate to depict such a structure in a non-perspective form, in which case solid wedged and hashed wedged bonds would be used normally to indicate stereochemical configuration.
**ST-4. DOUBLE-BOND CONFIGURATIONS**

Unlike all of the other types of stereochemistry discussed here, stereochemistry associated with a double bond is invariant with regard to a mirror plane. Instead, double-bond stereochemistry is directly related to the positioning of substituents relative to the double bond itself. Double bonds (and related systems) have a maximum of four substituents, a maximum of two on each end of the double bond. Compared to a substituent on the other end of the double bond, a substituent on one end may be on the same (cis) or the opposite (trans) side. This description implies that rotation around the double bond is hindered, and that the positions of the two substituents on one end are indeed fixed relative to the other end. Determination of whether a given double bond really does have hindered rotation is beyond the scope of this document; if the double bond does not have hindered rotation, it does not have double-bond stereochemistry and the depiction recommendations discussed here would not apply.

**ST-4.1 Positioning of substituents on double bonds**

Double bonds (and related systems) have a maximum of four substituents, a maximum of two on each end of the double bond. Double bonds are planar, and so should be preferably be depicted with plain bonds at all four substituents.

Substituents consisting of a hydrogen atom may be omitted according to standard conventions regarding the use of implicit hydrogens. Substituents consisting of a lone pair will also generally be omitted. When a substituent is omitted from the drawing, it is assumed to be positioned on the side of the double bond opposite to an existing substituent on the same atom.

For sterically unstrained, acyclic double bonds, the angle between substituents should generally be close to 120° as shown. Double bonds with highly congested substituents and double bonds in rings other than six-membered rings will commonly have angles other than 120°. In no case, however, should two substituents on the same atom of a double bond be positioned on the same side of the bond.
ST-4.2 Double bonds with implicit substituents

Asymmetric double bonds should never be drawn with implicit substituents, that is, where one or more substituents are “contracted” into an atom label at one end of the bond or the other. The substituents should always be drawn explicitly. This is particularly true when the double bond is oriented vertically, since the horizontal nature of atom labels may imply a cis/trans relationship where one was not intended.

Preferred | Preferred | Preferred | Not acceptable | Not acceptable

ST-4.3 Extended double-bond-like systems

Double-bond-like systems are not restricted to isolated double bonds. The same issues apply to any systems containing four coplanar substituents with two on each end of a central axis. Extended cumulenic systems with an odd number of bonds describe one such family (similar systems with an even number of double bonds have tetrahedral stereochemistry instead).

Preferred

ST-4.4 Double bonds in rings

In some cases, particularly in perspective drawings and in other bridged ring systems, it may be necessary to draw a double bond viewed from a non-standard orientation. Whenever possible in such cases, the local configuration of the double bond as drawn should match the actual configuration intended. That is, a cis double bond with two substituents should always be drawn with both of those substituents on the same side of the bond, regardless of the orientation of the bond itself.

Preferred | Not acceptable

That said, a viewer should generally expect that any double bond within a ring containing six or fewer atoms will be in a cis configuration relative to the ring. In small rings of this type, the
depiction of a trans bond when it could otherwise be drawn as cis only adds extra confusion for the viewer. Interpretation is much more of an issue in slightly larger ring systems where both cis and trans orientations are possible. 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 four or more bonds oriented trans rather than cis. Double bonds in large rings must always be drawn in the configuration that is intended, even if that requires that the ring system itself be depicted in a different shape.

Prefered Not acceptable

ST-4.5 Double bonds of unspecified configuration

It is often useful to be able to depict a double bond of unspecified configuration, such as the structure of “but-2-ene” as distinct from “cis-but-2-ene” and “trans-but-2-ene”. There are at least three different conventions that have been used to depict these configurations.

The simplest option is to draw the double bond and its substituents linearly. This depiction style should only be used when the double bond has exactly two substituents, one on each end. When possible, the double bond itself should be arranged horizontally. If the entire structure is linear, it may be represented in textual form instead, without any explicit bonds. In practice, linear styles are primarily used for small compound, although they are acceptable for compounds of any size.

Preferred Preferred Not acceptable Not acceptable

The most common convention for depicting unspecified double bonds in compounds of all sizes uses a wavy bond adjacent to the double bond. Under no circumstances, however, should the wavy bond join the double bond to another stereogenic center.
This style is usually used only in cases where the double bond has a single substituent one or both ends; the wavy bond would preferably be positioned on that substituent.

If that single substituent connects the bond to another stereogenic center, however, the wavy bond must not be positioned there, and instead should be placed on the other end of the double bond.

If a wavy bond is used on the end of a double bond that has two substituents, both substituents should preferably be depicted with a wavy bond unless one of the substituents connects the double bond to another stereogenic center.
In rare cases, it is impossible to depict an unspecified double bond either by drawing the substituents linearly or by using wavy bonds. In those cases, it is clearest to depict the two configurations as separate structures separated by the word “or”.

\[
\text{Preferred}
\]

A crossed double bond has in the past been used to indicate unspecified double bond configurations. This type of bond is no longer considered acceptable for general use, although it may still be required by some computer software.

\[
\text{Not acceptable}
\]

ST-5. OTHER CONFIGURATIONS

Beyond stereochemistry associated with a central atom or bond, there are some types of stereochemistry that are dependent on the relationships between larger portions of a structure. These are fairly uncommon, and tend to be explained clearly in associated text when they are used, simply because they are so unusual.

**ST-5.1 Planar chirality**

Compounds with planar chirality have some portion of their structure that is planar or nearly so, where that portion is not symmetric with respect to rotation within its plane, and some other portion of the compound with fixed orientation relative to that plane. Most commonly that is accomplished by some sort of bridging configuration over the planar system in a way that prevents further rotation.

Compounds with planar chirality should be depicted in accordance with the earlier recommendations for the depiction of perspective structures. In planar chirality, the most important information is to distinguish the portions of the structure that are in the plane from those that are out of it. Typically, the planar portions are depicted as perpendicular to the plane of the paper, in which case they would include solid wedged bonds to indicate perspective. Alternatively, the planar portions may be depicted within the plane of the paper, in which case the portions connected directly to the planar parts would be indicated with solid wedged bonds.
ST-5.2 Helicenes

Helicenes are extended fused systems that are forced out of planarity when the fused system “loops back” on itself, forming a helical or screw-shaped figure in three dimensions. The non-planarity should be indicated by a pair of solid wedged bonds on one end of the helix separated, in even-membered rings, by another that is preferably depicted as bold and unwedged. It is additionally acceptable to display a corresponding pair of hashed wedged bonds on the other end of the helix. In no cases should solid wedged or hashed wedged bonds be present anywhere but at the termini of the helix.

ST-5.3 Molecular propellers

Molecular propellers consist of three or more rigid planar or mostly-planar systems connected to a central atom. In terms of depiction, they should be considered as extended analogs of hindered biaryls. The same recommendations made for biaryls would apply to propellers. Propellers should always be drawn with solid wedged and hashed wedged bonds within the rings and directly connected to the bonds about which they rotate. When one such bond in a ring is drawn as a solid wedged bond, it is preferable for the opposite bond also to be drawn as a solid wedged bond, and for any bonds between them to be drawn as bold unwedged bonds, but it is acceptable to leave those bonds as plain. The configuration of the propeller system should not solely be represented by solid wedged and hashed wedged bonds to other ring substituents that are distant from the rotatable bond.

ST-6. RELATIVE STEREOCONFIGURATION

Many compounds — and in particular, many compounds of biological interest — contain more than one stereogenic center. It can be very useful to be able to talk about the relative configuration of various asymmetric centers even in cases where the absolute configuration is not known. Consider the case of tartaric acid:
A known, specific, single configuration could be depicted using diagram A, B, or C. Diagram D should be used when nothing is known about the absolute configuration of the two stereogenic centers; a substance represented by D might, on further analysis, prove in fact to be A, B, or C, but it might also prove to be any combination or mixture of the three.

Those diagrams can depict many common situations, but not all. For example, it is common to have a substance containing a racemate of the (R,R)-form A and its (S,S)-enantiomer B, but definitely not containing any of the meso-diastereoisomer C. In that case, the relative configuration of the two stereocenters is known (both “same” according to CIP rules, or both “different” according to the specific use of hashes and wedges above), but the racemic quality cannot easily be depicted without additional descriptive text.

That racemic mixture might be further characterized, and the two enantiomeric forms crystallized separately. At that point, each separate enantiomer has a known relative configuration, but it still might not be known which crystal actually contains the (R,R)-form and which contains the (S,S)-form. There is no easy way to depict this situation either.

Tartaric acid is a very simple example, with only two stereogenic centers. The same problems are only multiplied in structures that contain more than two. As a still-simple example, a structure with four asymmetric centers might be known to have a specific relative configuration between the first two centers, a different relative configuration between the last two centers, but have nothing known about the relation between the first two and the last two.

It can be useful to discuss relative configurations even in a compound with a single stereogenic center; in that case, the relative stereochemistry would be in relation to some quantity that might contain many moles of individual molecules. Relative configurations of this sort play an important role in chemical syntheses, where a starting material and its reactive transformations are known. Reduction of an asymmetric carbonyl such as butan-2-one will produce a sample that is (probably) racemic. That racemate can be resolved, for example by chiral phase chromatography, into two fractions of known relative configuration, but unknown absolute configuration. One of those samples may be further analyzed, possibly via X-ray crystallography, to determine its absolute configuration. In such a sequence, the carbonyl moiety may itself be part of a larger structure that has other stereocenters, and each of those other stereocenters may be identified in racemic, relative, or absolute terms. This procedure can quickly become very complex.

**ST-6.1 Historical approaches**

There are a variety of obscure conventions for indicating relative configuration. The most common (but still obscure) of these conventions says that bold and hashed wedges should be used for absolute configuration, unwedged bold and unwedged hashed lines represent relative configuration and racemic character, while hollow wedges and dashed lines represent relative configuration only [12,13]. In 2002, Elsevier MDL added extensive support for relative tetrahedral configurations to their ISIS system [14]. Other conventions have been used by various other authors and by various chemical software applications. Yet other conventions have been used to describe relative configuration in nomenclature [15], although generally with little direct
application to depiction styles. At this point, there does not seem to be any consensus for a preferred depiction style. This is an unresolved area. Given the lack of consensus among different systems and the poor general acceptance of any given one, the safest approach currently is to depict multiple structures explicitly, optionally accompanied by additional descriptive text as discussed below.

**ST-6.2 Representation goals**

The goals of structure representation here are the same as elsewhere: it is important to indicate clearly what chemical substances are intended by the authors. In the case of relative configuration, it is critical not to conflate unknown, unspecified, and racemic in any way. For a given center there are at least the following values:

- Known absolute
- Unknown absolute (i.e. a single stereoisomer)
- Racemic (known to be 50/50, at least at some stage in the experiment)
- Scalemic (mixed, but not necessarily 50/50)
- Unknown (no information known experimentally)
- Unspecified (no knowledge whatever)
- Known relative (there is a known relationship to some/all of the other centers, but the absolute value in the relationship is unknown)
- Unknown relative (it is known that the configuration depends on another center, but it is not known what the relationship is. For example, a new reagent is known to provide stereospecificity, but the nature of that (cis or trans, for example) has not yet been determined)

Unfortunately, it is extremely difficult to represent all of these different possibilities in a legible manner simply by using variations of bond types (the Maehr proposal) or atom-based indicators (the Elsevier MDL approach).

**ST-6.3 Absence of indicators indicates configuration as drawn**

In the absence of any other sort of indicators, a structural diagram is expected to represent the specific substance drawn. If stereochemical hashed wedged and/or solid wedged bonds are present in the diagram, it will represent a single stereoisomer. If no stereochemical information is present in the diagram, it represents a substance with unknown configuration.

This recommendation is at odds with the historic (last 20-25 years) behavior of the MDL family of software (ChemBase, MACCS, ISIS/Draw, ISIS/Base, etc.). In MDL software, diagrams were assumed to represent a racemate of the absolute configuration drawn and its enantiomer unless an additional “chiral flag” was added explicitly. The present recommendations, however, correspond to prevailing usage within printed chemical communications such as journal articles, books, patents, and so on. More recent software from MDL has also moved in the same direction.

**ST-6.4 Mixtures should be represented with additional explanatory text**

Other types of relative configuration should be represented with a more verbose description than a single structure. In some situations, it might be acceptable to list separate depictions for all stereoisomers present. In printed materials, it would usually be appropriate to have some additional text, such as the word “and” present, to indicate that the two structures were both intended. It is also permissible to depict a single stereoisomer with a longer piece of descriptive text, such as “and enantiomer”, or “(±)-form”.

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Non-alphabetic symbols should not be used to separate multiple depictions. In particular, a plus sign should not be used to replace the word “and” since the plus sign already has several other meanings (as a charge, or as a separator of multiple reactants or products in a reaction) that could cause further confusion.
The explanatory text should be positioned no further from the structural diagram than a distance equal to the median bond length used in the diagram. In no case should it be positioned closer to some other diagram than the one to which it applies. Positioning of the explanatory text below or to the right of the structure is preferred, but such positioning may conflict with other symbols including reaction arrows and compound numbers in journal articles. If such positioning would possibly create any ambiguity or confusion, any other positioning is also acceptable.

The recommendations presented here are primarily focused on the depiction of substances that can be represented with a single structure; a comprehensive discussion of arbitrary mixtures of substances is outside the scope of this document.

**ST-6.5 Avoid use of “racemate” and “relative” as structural labels**

The use of the terms “racemate” and “rac” should be avoided because it has historically had several different meanings. The most common historical meanings appear to be “a 50:50 mixture of enantiomers” and, colloquially, “an equilibrium mixture of enantiomers”]. To ensure understanding, the clearest and most accurate description should always be used.

The terms “relative” and “rel” should similarly be avoided unless accompanied with a clear explanation of what the structure is relative to. It remains acceptable to use the term “relative” in a generic sense, as it has been used in these recommendations.

**REFERENCES**