The graphic representation of chemical formulae in the publications of international nonproprietary names (INN) for pharmaceutical substances

Programme on International Nonproprietary Names (INN)
Division of Drug Management & Policies
World Health Organization
Geneva
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This document is based on the *Guidelines for the graphic representation of chemical formulae*

Compared to the guideline, this document focuses on the styles used within the publication of INNs. All specific styles have been shaded in grey and commented if necessary.

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1. INTRODUCTION

1.1 Chemical names and structures must be portrayed correctly and unambiguously in pharmaco-
poeias and other compendia. For details of nomenclature conventions, readers are referred to
the recommendations of the International Union of Pure and Applied Chemistry (1, 2).

1.2 These guidelines are intended to help scientists draw structural formulae correctly. They are
only recommendations, however, because unwavering adherence to these principles is not
always practicable. Thus, the guidelines should be followed closely wherever possible, but may
be adapted, with certain exceptions, where necessary to produce accurately drawn structural
formulae. Details of the formulae, such as bond lengths, the position of subscripts and super-
scripts, and the closeness of apposition of individual atomic symbols, will depend on the
drawing method used, whether computer-based or manual.

1.3 Where possible, the structures are:
- set out horizontally rather than vertically;
- designed to be read from left to right; the highest-numbered atom in an acyclic structure
  should be on the left, the systematic numbering decreasing from left to right.

1.4 The numbering of rings is consistent with established chemical nomenclature. Where practi-
cable, rings should be numbered in a clockwise direction.

1.5 Links between atoms and/or groups are represented by dashes. The structures should by and
large be shown in full, with the complete rings. However, certain very common groups of atoms
are shown in a more condensed form, as follows:

-CH₃  methyl
-CHO  formyl
-CO₂H  carboxy
-CO₂⁻  carboxylate
-CN  cyano
-NC  isocyano
-OH  hydroxy
-OCH₃  methoxy
-SO₃H  sulfo
-SO₃⁻  sulfonate
-NH₂  amino
-NO₂  nitro
-N₃  azido

1.6 Symbols for groups of this kind such as –Me, –Et, –Pr, –Ph, etc., are often used as a means of
saving space.

Hardly used by the INN Programme, except in polypeptides

1.7 The bulky group tert-butyl (1,1-dimethylethyl) is often shown as -C(CH₃)₃.
Hydroxymethyl and aminomethyl groups can be represented in either expanded or condensed
form:
-CH₂-OH or -CH₂OH
-CH₂-NH₂ or -CH₂NH₂
1.8 A polyatomic group is set out such that the atom that is directly attached to the rest of the structure is shown closest to the connecting dash:

\[
\begin{align*}
\text{HO--CH}_2\text{--CH}_2\text{--CO}_2\text{H} & \quad \text{or} & \quad \text{not} & \quad \text{OH--CH}_2\text{--CH}_2\text{--CO}_2\text{H} \\
\text{HO--CO}_2\text{H} & \quad \text{or} & \quad \text{not} & \quad \text{OH--CO}_2\text{H} \\
\text{HO}_2\text{S--CH--CH}_2\text{--CO}_2\text{H} & \quad \text{or} & \quad \text{not} & \quad \text{SO}_3\text{H--CH--CH}_2\text{--CO}_2\text{H} \\
\text{HO}_2\text{S--CO}_2\text{H} & \quad \text{or} & \quad \text{not} & \quad \text{SO}_3\text{H--CO}_2\text{H} \\
\end{align*}
\]

\[
\begin{align*}
\text{CO}_2\text{H} & \quad \text{not} & \quad \text{not} & \quad \text{CO}_2\text{H} \\
\text{O}_2\text{N} & \quad \text{not} & \quad \text{not} & \quad \text{NO}_2 \\
\end{align*}
\]

1.9 The carbonyl group in ketones is depicted as:

\[
\begin{align*}
\text{C--O--} & \quad \text{or} & \quad \text{C--O} & \quad \text{or} & \quad \text{C--O} \\
\text{O} & \quad \text{not} & \quad \text{not} & \quad \text{not} & \quad \text{not} \\
\text{CH}_2\text{--CH}_2\text{--N(CH}_2\text{CH}_3)_2 & \quad \text{or} & \quad \text{CH}_2\text{--N(CH}_2\text{CH}_3)_2 & \quad \text{or} & \quad \text{CH}_2\text{--N(CH}_2\text{CH}_3)_2 \\
\text{H}_3\text{C--CH}_2\text{--CH}_2\text{--CH} & \quad \text{not} & \quad \text{not} & \quad \text{not} & \quad \text{not} \\
\text{CH}_3 & \quad \text{not} & \quad \text{not} & \quad \text{not} & \quad \text{not} \\
\end{align*}
\]
In aldehydes it is depicted in the condensed rather than expanded form:

\[
\text{not} \quad \text{CH} = \text{O} \quad \text{or} \quad \text{CHO} \quad \text{not} \quad \text{CH} = \text{O} \quad \text{or} \quad \text{CHO}
\]

1.10 The sulfonyl group is depicted as:

\[
\text{or} \quad \text{SO}_2
\]

rather than in the condensed form \( \text{---SO} \). The sulfinyl group is shown as:

\[
\text{or} \quad \text{SO} \quad \text{or} \quad \text{SO}
\]

rather than in the condensed form \( \text{---SO} \); the last representation is useful as a means of recognizing a chiral compound:
2. ACYCLIC STRUCTURES

2.1 In acyclic structures, a single bond is shown as a dash, unless a broken line, a wedge or a wavy line is used to depict stereochemistry,¹ a carbon-carbon or carbon-heteroatom double bond is shown as double dash, and a triple bond is shown as a triple dash:

\[
\begin{align*}
\text{Br–CH}_2–\text{CH}_2–\text{OH} &\quad \text{H}_2\text{C}–\text{CH}–\text{CH}_2–\text{OH} &\quad \text{H}_3\text{C–CH}_2\text{–C}–\text{CO}–\text{CH}_3 \\
\text{OH} &\quad \text{OH} &\quad \text{HO} \\
\text{CH}_3 &\quad \text{CH}_3 &\quad \text{CH}_2\text{NH}_2
\end{align*}
\]

2.2 In computer-aided drawing, because it takes time to insert dashes, a single bonding dash between the atoms of an aliphatic chain need not be used. Nevertheless, in this compact form:

- a dash is used to show a single bond between a substituent and a chain or between a chain and a ring;
- a double dash and a triple dash are used to show a double bond and a triple bond respectively;
- dashes, broken lines or wedges are used to depict stereochemistry.¹

\[
\begin{align*}
\text{BrCH}_2\text{CH}_2\text{OH} &\quad \text{H}_2\text{C}–\text{CH}–\text{CH}_2–\text{OH} &\quad \text{CH}_3\text{C}–\text{C}–\text{C}–\text{C}–\text{C}–\text{CH}_3 &\quad \text{HO}–\text{CH}_2\text{CH}_2\text{N}–\text{CH}_2\text{NH}_2 \\
\text{OH} &\quad \text{OH} &\quad \text{OH} &\quad \text{HO} \\
\text{CH}_3 &\quad \text{CH}_3 &\quad \text{CH}_3 &\quad \text{CH}_3
\end{align*}
\]

Sometimes dashes are replaced by dots, but this practice is not recommended:

\[
\begin{align*}
\text{Br–CH}_2–\text{CH}_2–\text{OH} &\quad \text{H}_2\text{C}–\text{CH}–\text{CH}_2–\text{CN} &\quad \text{H}_3\text{C}–\text{CH}_2\text{–C}–\text{CH}–\text{CH}_3 \\
\text{OH} &\quad \text{OH} &\quad \text{CH}_3
\end{align*}
\]

Not used by the INN Programme

2.3 Acyclic chains can be represented either in linear way or in the form of lines at an angle to one another; the latter option is preferred because it sometimes makes it easier to show an atom next to the atom to which it is linked and offers a better configuration for structures having chiral centres (see section 7):

\[
\begin{align*}
\text{CH}_3\text{CNH}–\text{CH}–\text{CH}_3 &\quad \text{or} &\quad \text{H}_2\text{C}–\text{C}–\text{NH}–\text{CH}–\text{CH}_3 &\quad \text{or} &\quad \text{H}_3\text{C}–\text{C}–\text{N}–\text{CH}–\text{CH}_2–\text{CH}_3
\end{align*}
\]

¹ A bond that lies below the plane of the paper is shown by a broken line, one that lies above that plane by a wedge, and one whose configuration is not known by a wavy line.
The latter representation may be simplified by omitting the letter "C" from the central skeleton and the letter "H" for hydrogen atoms, which can be understood to be present. The carbon chain is then represented by a series of lines at an angle to one another, with all terminal groups set out in full:

\[
\text{H}_3\text{C}-\text{CH}_2-\text{CH}-\text{CH}_2-\text{CH}_3 \quad \text{or} \quad \text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CO}_2\text{H}
\]

This form of representation is particularly useful for drawing long carbon chains and is often used in chemical literature. Moreover, this is the form that computer drawing programs are designed to use.

2.4 The groups at the left-hand end of the formula are always inverted, except in the compact form without dashes.

2.5 Single substituents (whether mono- or polyatomic) are not shown in parentheses and included in the structure, but are linked to it with dashes:

\[
\begin{align*}
\text{H}_3\text{C}-\text{CH}_2-\text{CH}-\text{CH}-\text{CO}_2\text{H} & \quad \text{not} \quad \text{H}_3\text{C}-\text{CH}_2-\text{CH}(\text{CH}_3)-\text{CH}(\text{NH}_2)-\text{CO}_2\text{H} \\
\text{CH}_3\text{CH}_2\text{CH}-\text{CH}-\text{CO}_2\text{H} & \quad \text{not} \quad \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)-\text{CH}(\text{NH}_2)-\text{CO}_2\text{H}
\end{align*}
\]

*Not used by the INN Programme*

2.6 When several identical groups are linked to the same atom, they are often shown in parentheses, a subscript on the right indicating their number; dashes are not used to show bonding in this case:

\[
\begin{align*}
\text{H}_3\text{C}-\text{CH}-\text{CH}-\text{CH}(\text{OCH}_3)_2 & \quad , \quad \text{CH}_3\text{CH}_2\text{CH}-\text{CH}_2-\text{CH}(\text{OCH}_3)_2 \quad \text{or} \quad \text{H}_3\text{C}-\text{CH}(\text{OCH}_3)_2 \\
\text{Ar}-\text{CH}_2-\text{CH}_2-\text{N}^+\text{(CH}_3)_3 & \quad \text{Cl}^- \quad \text{or} \quad \text{Ar}-\text{CH}_2-\text{CH}_2-\text{N}^+\text{(CH}_3)_3 \quad \text{Cl}^-
\end{align*}
\]

\[
\begin{align*}
[(\text{H}_3\text{CO})_2\text{CH}]_2\text{NH} & \quad \text{(HO-CH}_2-\text{CH}_2)_3\text{N} \quad \text{or} \quad \text{(HOCH}_2\text{CH}_2)_3\text{N}
\end{align*}
\]
2.7 In acyclic chains that contain a large number of identical groups, such groups can be placed in square brackets, their number being indicated by a subscript on the right:

\[
\begin{align*}
H_2C-\left[CH_2\right]_4-CO_2H & \quad \text{or} \quad CH_2\left[CH_2\right]_4CO_2H \\
& \quad \left[CH_2\right]_n-\text{CH}_3
\end{align*}
\]

In general, the points of bonding between adjacent repeated groups are not shown, but there are situations in which they may be indicated to avoid ambiguity (see section 15).

2.8 In a polymethylene chain, when one extremity is linked to a heteroatom, the methylene group linked to that heteroatom may be left outside the brackets if a contracted group such as hydroxymethyl, aminomethyl, etc., is to be shown:

\[
\begin{align*}
H_2C-\left[CH_2\right]_5-\text{CH}_2\text{OH} & \quad \text{or} \quad H_2C-\left[CH_2\right]_4-\text{CH}_2\text{NH}_2
\end{align*}
\]
3. CYCLIC STRUCTURES

3.1 Rings are shown in full as polygons. The symbols of the carbon atoms that form the ring are not shown, but are represented by the vertices of the rings. The hydrogen atoms attached to them are not represented unless they are needed to show stereochemistry. The symbols of atoms other than carbon are shown with all the hydrogen atoms attached to them but without linking dashes. Single, double or triple bonds are indicated thus:

![Rings Representation](image)

3.2 In aromatic systems a circle should not be used to depict delocalized electrons; instead, alternating single and double bonds are shown (Kekulé representation):

![Aromatic Systems](image)

In monocyclic aromatic compounds, double bonds should be arranged to have the lowest possible numbering:

![Monocyclic Aromatic Compounds](image)

3.3 In fused polycyclic systems a double bond should form the fusion bond nearest to the right-hand side:

![Fused Polycyclic Systems](image)
3.4 Six-membered rings should be represented with a vertex at the base rather than a horizontal bond when the chains linked to them are represented in the form of lines at an angle to one another (as is preferred for acyclic chains – see section 2.3):

or

3.5 Depiction of the ring with a horizontal bond at the base is, however, preferred when the chains are shown in the compact form:

preferred to

*Not used by the INN Programme*

3.6 Rings are shown as regular polygons when they consist of up to eight atoms:

3.7 Wherever possible, the regularity of the polygons is maintained in the drawing of fused cyclic compounds:

3.8 However, in fused polycyclic systems the polygons may often be distorted in order to maintain the symmetry of the structure:
3.9 Rings with more than eight vertices are often shown with re-entrant angles. It is recommended by Chemical Abstracts Service (CAS) that they should be drawn like amalgamated rings with five, six or seven vertices:

\[ \text{Diagram of rings with 5, 6, or 7 vertices} \]

3.10 These recommendations need not always be followed. In particular, the shape of such large rings as those of macrolide antibiotics is often determined by the presence of more or less bulky substituents and the need to indicate stereochemical conformations:

\[ \text{Diagram of macrolide antibiotics} \]

3.11 When a substituent is attached to an atom occupying a position in a ring (carbon or heteroatom), the direction to be taken by the dash linking it to that atom can be found by extending the line bisecting the cycle:

\[ \text{Diagram showing direction of attachment} \]
3.12 Where two substituents are attached to the same ring atom, they should generally both be at the same angle to the bisector, and preferably at a right angle to the adjacent side:

However, for the graphic representation of certain structures, such as steroids, other considerations may have priority.

3.13 Substituents are normally placed outside rings, except in steroids, terpenes and alkaloids (see sections 9, 10 and 12) and where substituents attached at bridgeheads can only be displayed inside the rings of polycyclic structures:

but

or
3.14 In bridged structures, a non-atomic bridge (direct bond) is represented by a straight line, an atomic bridge by lines at an angle to one another. The symbols for carbon atoms are not shown; however, if the bridge contains one or more heteroatoms, the atomic symbols for those atoms are shown. To give some perspective to the figure or to represent stereochemical features, wedges, thickened lines or broken lines can be used (see p. 19):

![Chemical structures](image)

3.15 Sometimes a three-dimensional approach is possible, if a planar representation is considered not clear enough:

![Chemical structures](image)

*Tridimensional structures are rarely used by the INN Programme*
4. IONIC STRUCTURES

4.1 In general, in ionic structures, the cationic part is placed on the left and the anionic part on the right.

4.2 Ionic charges are not encircled and are shown as superscripts on the right of the charged atom. Multiple charges are indicated by writing \( n^+ \) or \( n^- \) and not by writing the + or - symbol \( n \) times.

4.3 A terminal charge is shown as a superscript on the right of the group concerned, unless the order of atomic symbols in the group is reversed, when the charge is shown as a superscript on the left. In a lateral acyclic chain, if there is no space for a superscript on the right of the atom concerned, the charge can be shown immediately above that atom. When a ring is involved, the charge is usually placed outside the ring. When it is difficult to place the charge without ambiguity, it may be shown inside the ring:

\[
\text{Na}^+ \quad \text{Al}^{3+} \quad \text{Cl}^- \quad \text{SO}_4^{2-}
\]

\[
\text{[H}_3\text{C]}_2\text{C}==\text{CH}==\text{C(CH}_3\text{)}_2]^+
\]

\[
\text{K}^+ \quad \text{[Fe(CO)}_3\text{OH}]^+
\]

\[
\text{[ClO}_4^-\text{]}
\]

4.4 In structures with delocalized charge, the structure is put in square brackets, with the charge sign outside them as a superscript on the right:
4.5 Metal salts of inorganic acids are shown without charges or bonds. If they include several metals, the symbols for the metals are shown in alphabetical order. In acid salts, the metal precedes the hydrogen. Molecules of water of crystallization or of substances of solvation follow the formula of the salt, from which they are separated by a comma:

\[ \text{NaBr} \quad \text{NaHCO}_3 \quad \text{AlK(SO}_4)_2 \cdot 12\text{H}_2\text{O} \quad \text{NaH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O} \quad \text{AlCl}_3 \cdot 4\text{C}_2\text{H}_5\text{OH} \]

For inorganic compounds, centred dots are recommended by the International Union of Pure and Applied Chemistry (2). However, several pharmacopoeias have for a long time been using the comma for both organic and inorganic compounds.

4.6 In the metal salts of organic acids and the metal compounds of alcohols, phenols (and their sulfur, selenium and tellurium analogues), amines and amides, the metal symbol usually replaces the “acid” hydrogen, but neither charges nor bonds are shown:

\[ \text{H}_2\text{C} \cdots \text{ONa} \quad \text{H}_2\text{C} \cdots \text{CH}_2 \cdots \text{OK} \]

\[ \text{SO}_3\text{K} \quad \text{SO}_2\text{NNaH} \quad \text{ONa} \]

\[ \text{CH}_3 \quad \text{CH}_3 \quad \text{CH}_3 \]

Nevertheless, ionic forms may be used when substances contain several “acid” groups to which the various cations cannot easily be attributed:

\[ \text{Na}^+ , 2\text{H}^+ \left[ \begin{array}{c} \text{O}_2\text{C} \cdots \text{CH}\cdots \text{CO}_2^- \\ \text{HO} \cdots \text{CH}\cdots \text{CO}_2^- \end{array} \right] \quad \text{or} \quad \text{Na}^+ , 2\text{H}^+ \left[ \begin{array}{c} \text{O}_2\text{C} \cdots \text{HO} \cdots \text{CO}_2^- \\ \text{CO}_2^- \end{array} \right] \]

\[ \text{Na}^+ , \text{H}^+ \left[ \begin{array}{c} \text{CH}\cdots \text{CO}_2^- \\ \text{CH}_2\cdots \text{CH}\cdots \text{CO}_2^- \end{array} \right] \quad \text{or} \quad \text{Na}^+ , \text{H}^+ \left[ \begin{array}{c} \text{CH}\cdots \text{CO}_2^- \\ \text{CH}_2\cdots \text{CH}\cdots \text{CO}_2^- \end{array} \right] \]
4.7 Amine salts are shown with the structure of the amine on the left and, after a comma, the formula of the acid on the right:

\[(\text{H}_3\text{C})_3\text{N}, \text{HBr}\]

\[\text{N(CH}_3\text{)}_2\text{, HCl}\]

4.8 Quaternary ammonium salts and other compounds with a positive charge on a heteroatom (P, As, Sb, O, S, Se, Te) are shown in ionic form (with + and – charges), the two ions being separated by a space:

\[(\text{H}_3\text{C})_4\text{N}^+ \text{Cl}^-\]

\[(\text{C}_6\text{H}_4\text{CH}_2\text{)}_2\text{S}^+ \text{ClO}_4^-\]

\[\text{N}^+ \text{Br}^-\]

4.9 In inner salts, the positive and negative charges are shown and are normally placed in the structure as recommended above:

\[(\text{H}_3\text{C})_3\text{N}^+ \text{–CH}_2\text{–CO}_2^-\]
5. ISOTOPICALLY MODIFIED COMPOUNDS

5.1 In an isotopically modified compound, the isotope used is indicated by its mass number placed as a superscript on the left of the symbol of the element concerned. Deuterium and tritium are written $^{2}H$ and $^{3}H$ respectively. The carbon atom in a ring or in a simplified angular-chain representation is explicitly designated when its mass number is shown:

\[\text{Na}^{35}\text{I}\quad \text{Na}_2\text{H}^{32}\text{PO}_4\quad ^{99m}\text{Tc}\]

5.2 When atomic symbols in formulae are drawn without square brackets (as above) the compounds are assumed to be isotopically substituted, i.e. the atom concerned is completely replaced by the nuclide shown. To indicate isotopic labelling (partial replacement of the atom by the nuclide shown), atomic symbols in formulae should be in square brackets:

\[\text{H}_2\text{N}[^{14}\text{C}]-\text{CH}_2-\text{CH}-\text{CO}_2\text{H}\]
6. COORDINATION COMPOUNDS

*Non-cyclic linear structures*

6.1 According to current usage (1), in a non-cyclic structure, the symbol of the central atom is placed on the left and is followed by the ionic ligands and then by the neutral ligands. Polyatomic ligands are placed in parentheses, with the atom linked to the central atom on the left. If several identical ligands are attached to the central atom, their number is indicated as a subscript to the right. In each class of ligands, the symbols of the linking atoms, and then of any other atoms, are shown in alphabetical order. The complete formula of the coordination entity (neutral group or complex ion) is placed in square brackets.

6.2 The individual charges usually carried by the central atom and the ligands are not normally shown; they may, however, be shown in structural formulae when it is difficult to show all the coordination links.

6.3 If the entire structure consists of ions, the positive ions are placed on the left and the negative ions on the right, the number of each being indicated as a subscript to the right. No spaces should be left between representations of ionic species within the formula of a coordination compound. If the charge of a coordination entity needs to be specified, it is placed outside the square bracket as a right superscript:

\[
\begin{align*}
\text{Na}_2[\text{Fe(CN)}_6(\text{NO})] & \quad \text{Li}_2[\text{Zn(CH}_3)_6] & \quad [\text{CoCl(NO}_2)(\text{NH}_3)_4]\text{Cl} \\
[\text{CoCl}_2(\text{NH}_3)_4]\text{Br} & \quad [\text{Co(SC[N(CH}_3)_2}_2)_4](\text{NO}_3)_2 & \quad \text{ion } [\text{Fe(CN)}_6]^{3-}
\end{align*}
\]

*Cyclic structures*

6.4 The rings follow the conventions for cyclic compounds. Where possible, the metal atom is placed in the centre of the group. Square brackets are placed round every coordination entity containing one or more rings, even if the charge is zero.

6.5 “Sandwich” structures are shown with the rings connected to the central atom by a line starting from inside the cycle and passing through one side.
6.6 Benzene rings and condensed benzene systems in “sandwich” compounds are drawn with alternating single and double bonds. Pentagonal and heptagonal rings are shown with a circle inside:

\[ \text{[structural formulas]} \]

**Stereochemistry**

6.7 The stereochemistry of mononuclear complexes is expressed by means of special descriptors. The first of these is the “system indicator” formed from an abbreviation for the central atom geometry and the coordination number.

6.8 *T-4: tetrahedral complexes.* Described by the chirality symbol \((R)\) or \((S)\), they are shown in the same way as chiral carbon atoms, a broken line denoting a bond projecting behind the plane of the paper and a filled wedge one projecting in front of that plane:

\[ \text{[diagram]} \]

6.9 *SP-4: square planar complexes.* The four coordination links are shown in the plane of the paper:

\[ \text{[diagram]} \]

lobaplatin
6.10 **TBPY-5: trigonal bipyramidal complexes.** The reference axis is shown in the plane of the paper; of the three other ligands, one is assumed also to be in the plane of the paper, one in front of it and the other behind it:

![Diagram of TBPY-5](image)

6.11 **SPY-5: square pyramidal complexes.** The reference axis with its lone coordinating atom is shown in the plane of the paper and four coordination links are assumed to be in a plane perpendicular to the reference axis, two in front and two behind the plane of the paper:

![Diagram of SPY-5](image)

**technetium**[^99mTc] **bicusate**

6.12 **OC-6: octahedral complexes.** Two coordination links are shown as the axis in the plane of the paper and four are assumed to be in a plane perpendicular to the reference axis, two in front and two behind the plane of the paper:

![Diagram of OC-6](image)

**ormaplatin**

6.13 **PBPy-7: pentagonal bipyramidal complexes.** Two ligands are shown attached to the extremities of an axis in the plane of the paper; the five other coordination links are shown as their projection on to the plane perpendicular to this axis:

![Diagram of PBPy-7](image)
7. STEREOCHEMISTRY

7.1 As already mentioned, a broken line denotes a bond projecting behind the plane of the paper and a filled wedge one projecting in front of that plane. A line of normal thickness denotes a bond lying in the plane of the paper. Hatched lines are sometimes used instead of broken lines. The practice of using a reversed wedge instead of a broken line for a bond projecting behind the plane of the paper is not recommended. In complicated structures, the dashes can be lengthened, shortened or displaced if necessary.

7.2 Hydrogen is represented by its symbol “H” whenever a configuration has to be shown.

*Geometric isomerism*

7.3 For compounds containing double bonds it is customary to draw the formula so that the reference plane of the double bond is perpendicular to that of the paper; the bonds whereby atoms are attached directly to the doubly bonded atoms lie in the plane of the paper and are depicted with lines of normal thickness.

7.4 Isomers are shown with the two sequence-rule-preferred atoms or groups (each attached to one atom of the double bond) placed on the same side of the reference plane for the \( (Z) \)-isomer and on the opposite side of this for the \( (E) \)-isomer:

\[
\begin{align*}
\text{(Z)} & \quad \begin{array}{c}
R_1 \equiv C \equiv C \equiv R_2 \\
H & \equiv C \equiv C \equiv H
\end{array} \\
\text{(E)} & \quad \begin{array}{c}
H \equiv C \equiv C \equiv R_2 \\
R_1 & \equiv C \equiv C \equiv H
\end{array}
\end{align*}
\]

7.5 In simplified carbon chains depicted by lines at an angle to one another, the hydrogen, if any, may be omitted (see sections 10 and 11):
Examples of (Z)-compounds:

or

zimeldine

or

zuclopenthixol

Examples of (E)-compounds:

or

baxitozine

or

terbinafine

(Note that the two bonds attached to the carbons of the triple bond are drawn in a straight line.)
7.6 The same conventions are used for the isomers of oximes:

![Diagram of oxime structure]

or

![Diagram of another oxime structure]

cefdaloxime (Z)

7.7 If the stereochemistry relative to the double bond is not specified a linear representation may be useful:

![Diagram of ethchlorvynol]

ethchlorvynol

7.8 The same conventions are used for compounds with several double bonds:

![Diagram of sorbic acid structure]

or

sorbic acid (E,E)
Compounds with one centre of asymmetry

7.9 In acyclic compounds with one centre of asymmetry, the general conventions can be used to represent each isomer either as a linear structure or with lines at an angle to each other (if possible, the larger "condensed" groups should be on the right, for aesthetic reasons).

\[
\begin{align*}
\text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} \\
\text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} & \text{or} & \text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} & \text{or} & \text{H}_3\text{N} & \text{H} & \text{CO}_2\text{H} \\
\text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} & \text{preferred to} & \text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} \\
\end{align*}
\]

\[d\text{-alanine \( (R)\)}\]

\[
\begin{align*}
\text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} \\
\text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} & \text{or} & \text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} & \text{preferred to} & \text{H}_3\text{N} & \text{H} & \text{CO}_2\text{H} \\
\end{align*}
\]

\[\text{L\text{-alanine \( (S)\)}}\]

(International Nonproprietary Names apply, by definition, to the \(L\)-form.)

7.10 The racemate can be represented by showing both isomers side by side or, more simply, showing only the \((R)\)-isomer followed by the legend “and enantiomer”.

\[
\begin{align*}
\text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} & \text{and} & \text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} & \text{or} & \text{H}_3\text{C} & \text{C} & \text{NH}_2 & \text{CO}_2\text{H} & \text{and enantiomer} \\
\text{DL\text{-alanine \( (RS)\)}}
\end{align*}
\]

and enantiomer

or

and enantiomer

ibuprofen
7.11 Similar representations are used for cyclic compounds with one centre of asymmetry:

\[
\begin{align*}
\text{d-proline (R)} & \quad \text{L-proline (S)} & \quad \text{dl-proline (RS)}
\end{align*}
\]

(International Nonproprietary Names apply, by definition, to the L-form.)

7.12 If the chirality of the centre is unknown or not specified, the bonds joining atoms or groups to the chiral atom are shown as lines of "normal" thickness. The use of a star or asterisk to identify the chiral centre may be useful:

ethoheptazine (non specified)

Compounds with several chiral centres

7.13 In compounds containing several centres of asymmetry, the same conventions apply to each of these centres:

ephedrine (1R,2S) or levomenthol
7.14 The racemates (racedehrine and racemethol respectively) are depicted by the same structures followed by the legend "and enantiomer", rather than by showing the two isomers side by side.

7.15 The same conventions are used for cis-trans isomerism relative to a planar (or approximately planar) ring:

![Chemical Structure of Pemadolc (±)-cis](image)

and enantiomer

**pemadolc (±)-cis**

![Chemical Structure of Spiradoline (±)-(5R*,7S*,8S*)](image)

and enantiomer

**spiradoline (±)-(5R*,7S*,8S*)**

7.16 Mixtures of epimers are often shown by using the "normal" dashes at the epimeric centre (see also section 11):

![Chemical Structure of Enlazone](image)

**englazone**

However, the substance is preferably represented by showing the (R)-isomer at the epimeric centre, placing an asterisk near this C atom and adding the legend "and epimer at C*":

![Chemical Structure of Enlazone Epimer](image)

and epimer at C*
7.17 In more complicated cases, it is better to draw each component of the mixture so as to show all the peculiarities of the structure:

\[
\text{crilvastatin : } [(\pm)-\text{cis-}] \text{ only for the cyclohexane ring}
\]

**Isomerism of fused rings**

7.18 In polycyclic compounds, the atoms or groups attached at saturated bridgeheads common to two rings are shown by their symbols so as to indicate the stereochemistry resulting from the way that the cycles are fused.

The cis-isomer is depicted with the bonds shown either both as wedges or both as broken lines:

\[
\text{tandospirone}
\]

The trans-isomer is depicted with one of the bonds as a wedge and the other as a broken line:

\[
\text{and enantiomer}
\]

\[
\text{isomolpan}
\]
8. CARBOHYDRATES

8.1 The Fischer projection is used to depict the acyclic forms of monosaccharides: the chain is shown vertically with carbon-1 on top and the horizontal bonds from carbon-2 to the penultimate carbon atom are assumed to be oriented towards the observer. This representation may be simplified by omitting the letter "C" in the central chain. The formulae are sometimes set out horizontally: they are then turned 90° clockwise, so that carbon-1 is on the right. Since such a representation is no longer a true Fischer projection, the vertical bonds should be shown as wedges to avoid any ambiguity:

8.2 The Haworth representation is preferably used to show the cyclic forms of monosaccharides, and not those with “chair-shaped” rings. In a pyranose ring, the oxygen is in the upper right-hand corner; in a furanose ring, the oxygen is at the top in the centre. If the configuration of the anomeric carbon is not specified, a wavy line is used. In practice, the conventional Haworth representation is simplified; the lower side of the ring, assumed to be nearer to the observer, is not thickened, and the hydrogen atoms linked to the carbon atoms in the ring are not shown:

conventional

Haworth representation of

α-D-glucopyranose
8.3 The non-cyclic part of a saccharide is shown as a Fischer projection (wedges are not necessary):

\[ \alpha\text{-d-glucofuranose} \]

\[ \text{lactitol} \]

8.4 The standard conventions are used to show the oligo- and polysaccharides:

\[ \text{saccharose} \]

\[ \text{sizefiran} \]
8.5 In structures that are only partly saccharide, that part is shown in accordance with the standard provisions for carbohydrates, and the rest of the structure according to the conventions for acyclic or cyclic chemical compounds, or for compounds such as steroids, polypeptides, etc.:

- Rutoside
- Cytarabine
- Adenosine
- Ouabain
- $\alpha$-xylopyranosyl-\(\text{L}\)-serine
9. STEROIDS

9.1 The rings of a steroid are depicted as a projection on to the plane of the paper. The projection should normally be oriented so that position 3 is at the bottom left and the regular pentagonal ring D at the top right, with position 17 uppermost.

9.2 A bond that lies below the plane of the paper is given the designation $\alpha$ and shown by a broken line; a bond that lies above the plane of the paper is designated as $\beta$ and shown by a wedge, while a bond whose configuration is not known is designated as $\xi$ and denoted by a wavy line. All the hydrogen atoms attached to centres of asymmetry are shown.

9.3 The backbone of a side-chain at C-17 is best shown as in the plane of the paper (lines of ordinary thickness), the bond between C-17 and C-20 being similarly shown. Side-chains are usually represented by lines at an angle to one another, the terminal groups being set out in full, as shown below. Stereochemistry due to substituents in the chain is indicated by the customary wedges and broken lines:

- Dexamethasone
- $(23E)$-$5\xi$-cholest-23-en-3$\beta$-ol
- Ethinylestradiol
Cardenolides (see also section 8.5), bufanolides and derivatives of calciferol are depicted as shown below:

digitoxigenin

scillarenin

calcitriol
10. TERPENOIDS

10.1 Terpenes and the compounds that can be related to them are depicted in a similar way to steroids, using the same conventions. Long chains are shown as angular lines with all terminal groups drawn in full:

- enoxolone
- labdane
- colforsin
- acitretin
11. PROSTANOIDS

11.1 Prostaglandins and their derivatives are depicted using the same conventions as those applicable to steroids and terpenes. Long chains are shown as lines at an angle to one another, all terminal groups being shown in full:

- alprostadil
- ciprostene
- enisoprost
- doxaprost

The last two are mixtures of epimers in the carbon chain, which can be shown in the manner indicated in section 7.16:

- and epimer at C*

This structure is preferred for epimers by the INN Programme
12. ALKALOIDS

12.1 There are no general rules for depicting alkaloids, though many are depicted with a preferred conventional skeleton that can be used for a family of similar products:

- Hyoscyamine

- Morphine

- Quinine

- Ergotamine
13. ANTIBIOTICS

13.1 Some antibiotics can be depicted by means of conventional diagrams that can be used for a family of similar products.

13.2 β-Lactams (penicillins and cefalosporins) are shown as below:

![Diagram of amoxicillin]

amoxicillin

![Diagram of cefotaxime]

cefotaxime

13.3 Aminosides are related to 2-deoxy-α-streptamine according to the conventions used for carbohydrates:

![Diagram of 2-deoxy-α-streptamine]

2-deoxy-α-streptamine

![Diagram of kanamycin]

kanamycin
13.4 Tetracyclines and rubicins are depicted as follows:

- **Tetracycline**
- **Daunorubicin**

13.5 The representation of the large rings of macrolides is variable. For example:

- **Tylosin**
13.6 The depiction of derivatives of rifamycin is based on that of the parent structure, which is shown as below:
14. POLYPEPTIDES

14.1 In polypeptides, the linear sequence of amino acid residues is shown with the amino-terminal residue on the left and the carboxy-terminal residue on the right (followed by "-NH2" if it is carboxamide).

14.2 Oligopeptides produced by the condensation of fewer than about five amino acids are often depicted in their full form. Since several polypeptides of this type are used as drugs, the full structure may be useful for showing any chemical modifications present:

\[
\text{H}_3\text{N} - \text{C} - \text{C} - \text{N} - \text{C} - \text{N} - \text{C} - \text{O} - \text{H} - \text{CH}_2 - \text{OH} - \text{CO}_2\text{H} \quad \text{or} \quad \text{H}_3\text{N} - \text{C} - \text{C} - \text{N} - \text{C} - \text{N} - \text{C} - \text{N} - \text{C} - \text{N} - \text{C} - \text{CO}_2\text{H}
\]

pentigetide

14.3 In the representation of polypeptides, amino acids are shown by means of the standard three-letter codes, peptide bonds being assumed to exist between C-1 and N-2 of adjacent residues. A code given without further qualification means that the amino acid concerned belongs to the L-series. If an amino acid belongs to the D-series, the letter "D" precedes the three-letter code and is joined to it by a hyphen. Unusual residues are shown in full. If a polypeptide occupies more than one line, a hyphen is placed at the end of each successive line until the formula has been completed.
14.4 Disulfide bridges are drawn as lines attaching the S atoms to the “Cys” units but without showing those atoms. The lines must be drawn vertically and appear to pass through the letter “y”. They may be placed above or below the unit chain, according to requirements. Either of the forms shown below is acceptable:

\[
\text{Cys—Tyr—Ile—Gln—Asn—Cys—Pro—Leu—Gly—NH}_2
\]

**oxytocin**

Ser-Leu-Arg-Arg-Ser-Ser-Cys-Phe-Gly-Gly-Arg-Met-Asp-Arg-Ile-
1 5 10 15
Gly-Ala-Gln-Ser-Gly-Leu-Gly-Cys-Asn-Ser-Phe-Arg-Tyr
20 25 28

or

Ser-Leu-Arg-Arg-Ser-Ser-Cys-Phe-Gly-Gly-Arg-Met-Asp-Arg-Ile-
1 5 10 15
Gly-Ala-Gln-Ser-Gly-Leu-Gly-Cys-Asn-Ser-Phe-Arg-Tyr
20 25 28

**carperitide**

Sometimes a mixture of the two styles will be needed so as to ensure that the bridges do not cross over one another.

14.5 If an amino acid residue is substituted on the N-2 atom, the symbol for the substituent is placed before the three-letter code. If a side-chain modification occurs, the substituent may be depicted either in full or by means of its conventional symbol placed above or below the three-letter code and joined to it by a vertical line passing through the central letter. If necessary, a locant is placed beside the vertical line that represents side-chain substitution:

\[
\text{Ac—D-Ala—D-Phe—D-Ala—Ser—Tyr—D-Lys—Leu—Lys—Pro—D-Ala—NH}_2
\]

**ganirelix**
14.6 In cyclic peptides, the amino acid sequence is formulated in the usual manner but the residues at each end of the line are joined by a lengthened bond. If the residues are written on two lines, the sequence is reversed on one of them; hence the CO to NH direction within the peptide bond must be indicated by arrows:

\[
\begin{align*}
\text{Leu} & \text{ d-Phe} \text{ Pro} \text{ Val} \text{ Orn} \text{ Leu} \text{ d-Phe} \text{ Pro} \text{ Val} \text{ Orn} \\
\text{Leu} & \text{ d-Phe} \text{ Pro} \text{ Val} \text{ Orn} \text{ Leu} \text{ d-Phe} \text{ Pro} \text{ Val} \text{ Orn}
\end{align*}
\]

or

\[
\begin{align*}
\text{Leu} & \text{ d-Phe} \text{ Pro} \text{ Val} \text{ Orn} \\
\text{Orn} & \text{ Val} \text{ Pro} \text{ d-Phe} \text{ Leu}
\end{align*}
\]

gramicidin S

\[
\begin{align*}
\text{H}_3\text{C} & \text{CH}_3 \\
\text{H} & \text{CH}_3
\end{align*}
\]

\[
\begin{align*}
\text{Ala} & \text{ d-Ala} \text{ MeLeu} \text{ MeLeu} \text{ MeVal} \text{ N} \text{ C} \text{ C} \text{ Abu} \text{ MeGly} \text{ MeLeu} \text{ Val} \text{ MeLeu} \\
\text{CH}_3 & \text{H} & \text{O}
\end{align*}
\]

ciclosporin

14.7 Cyclic esters are shown by means of a lengthened bond starting from the carbonyl end of the sequence and ending at the symbol of the hydroxy amino acid:

\[
\begin{align*}
\text{Thr} & \text{ Gly} \text{ Gly} \text{ Gly}
\end{align*}
\]

14.8. If part of the molecule is not polypeptide, it can be represented in accordance with the rules for acyclic or cyclic compounds:

\[
\begin{align*}
\text{H}_3\text{C} & \text{ C} \text{ Thr} \text{ d-Val} \text{ Pro} \text{ MeGly} \text{ MeVal} \\
\text{O} & \text{ N} & \text{C} & \text{O} & \text{NH}_2 \\
\text{H}_3\text{C} & \text{ C} \text{ Thr} \text{ d-Val} \text{ Pro} \text{ MeGly} \text{ MeVal}
\end{align*}
\]

dactinomycin
14.9 In showing polypeptides produced by the condensation of a large number of amino acids, one-letter codes rather than three-letter codes can be used to save space and facilitate computer processing. The one-letter codes are arranged in sets of ten letters separated by a space. For purposes of sequential numbering, the numbers of individual amino acids are generally placed below the codes. As an example, the polypeptide sequence of epoetin alfa:

```
Ala-Pro-Pro-Arg-Leu-Ile-Cys-Asp-Ser-Arg-Val-Leu-Glu-Arg-Tyr
Leu-Leu-Glu-Ala-Lys-Glu-Ala-Glu-Asn-Ile-Thr-Thr-Gly-Cys-Ala
Glu-His-Cys-Ser-Leu-Asn-Glu-Asn-Ile-Thr-Val-Pro-Asp-Thr-Lys
Val-Asp-Phe-Tyr-Ala-Trp-Lys-Arg-Met-Glu-Val-Gly-Gln-Gln-Ala
Val-Glu-Val-Trp-Gln-Gly-Leu-Ala-Leu-Leu-Ser-Glu-Ala-Val-Leu
Arg-Gly-Gln-Ala-Leu-Leu-Val-Asn-Ser-Ser-Gln-Pro-Trp-Glu-Pro
Leu-Gln-Leu-His-Val-Asp-Lys-Ala-Val-Asp-Gly-Leu-Arg-Ser-Leu
Thr-Thr-Leu-Leu-Arg-Ala-Leu-Gly-Ala-Gln-Glu-Ala-Ile-Ser
Pro-Pro-Asp-Ala-Ala-Asp-Ala-Pro-Leu-Arg-Thr-Ile-Thr-Ala
Asp-Thr-Phe-Arg-Lys-Leu-Phe-Arg-Val-Tyr-Ser-Asn-Phe-Leu-Arg
Gly-Lys-Leu-Lys-Leu-Tyr-Thr-Gly-Glu-Ala-Cys-Arg-Arg-Thr-Gly-Asp
```

becomes in abbreviated form:

```
APPRLICDSR  VLERYLLEAK  EAENITGCA  EHCSLNNIT  VPDTKVNPYA
WRKMEVQQA  VEVWQGLALL  SEAVLRGQAL  LVNSSQWEP  LQLHVNKAVS
GLRSLTTLR  ALGAQKEAIS  PPNAASAAPL  RTITADTFRK  LFRVYSGNFLR
GKLKLYTGEA  CRTGD
```
15. POLYMERS

15.1 The representation of polymers is based on the use of "repeated groups", i.e. sequences of identical groups. These groups are abbreviated $[X]_n$ in square brackets, where $n$ is the number of times that they appear.

15.2 Repeated groups are either "monomers", i.e. "normal" structural formulae, or "repeated structural units", which are relatively complex multivalent radicals.

15.3 The normal formulae, i.e. those of the relevant monomers, are used when it is difficult to specify how the monomers are bonded, or in order to show simple oligomers with a maximum of eight repeated groups:

\[
\begin{align*}
\text{H}_3\text{C}-\text{C}=\text{NH} & - \text{Sb(OH)}_2 \\
\text{O} & \\
\end{align*}
\]\n
\[
\left[\text{H}_3\text{C}-\text{CH}=\text{CH}_2\right]_4
\]

15.4 By and large, polymers are depicted as repeated structural units in which terminal bonds are shown. In linear polymers, such units are bivalent radicals:

poly(alkene)

poly(alkene)
This also applies to polymers when the terminal groups are shown:

\[
\text{H}_3\text{C}-(\text{CH}_2)_n\{\text{O}-(\text{CH}_2-\text{CH}_2)_m\text{OH}
\]

\[
\text{H}_3\text{C}-(\text{CH}_2)_n\{\text{O}-(\text{CH}_2-\text{CH}_2)_m\text{OH}
\]

lauromacrogol

\[
\text{H}_3\text{C}-\text{SiO}_{\overline{\text{Si}}}-\text{CH}_3
\]

\[
\text{H}_3\text{C}-\text{SiO}_{\overline{\text{Si}}}-\text{CH}_3
\]

dimeticone

15.5 Network polymers can be shown by multivalent repeated structural units:

\[
\begin{array}{c}
\text{R}=	ext{CH}_2-\text{CH}_2-\text{CO}_2\text{H}
\end{array}
\]

repagermanium

15.6 The representation of copolymers depends on what is known about the bonding of the constituent monomers. Thus normal formulae are used when it is difficult to specify the way in which the monomers are bonded:

\[
\begin{array}{c}
\text{H}_3\text{C}-\text{CH}-\text{CH}_2-\text{C}=\text{CO}_2\text{H}
\end{array}
\]

\[
\begin{array}{c}
\text{H}_3\text{C}-\text{CH}-\text{CH}_2-\text{C}=\text{CO}_2\text{H}
\end{array}
\]

\[
\begin{array}{c}
\text{NH}_2
\end{array}
\]

\[
\begin{array}{c}
\text{NH}_2
\end{array}
\]

\[
\begin{array}{c}
\text{H}_3\text{C}-\text{CH}-\text{CH}_2-\text{C}=\text{CO}_2\text{H}
\end{array}
\]

\[
\begin{array}{c}
\text{H}_3\text{C}-\text{CH}-\text{CH}_2-\text{C}=\text{CO}_2\text{H}
\end{array}
\]

\[
\begin{array}{c}
\text{NH}_2
\end{array}
\]

\[
\begin{array}{c}
\text{NH}_2
\end{array}
\]

or

\[
\begin{array}{c}
\text{H}_3\text{C}-\text{CH}-\text{CH}_2-\text{C}=\text{CO}_2\text{H}
\end{array}
\]

\[
\begin{array}{c}
\text{H}_3\text{C}-\text{CH}-\text{CH}_2-\text{C}=\text{CO}_2\text{H}
\end{array}
\]

\[
\begin{array}{c}
\text{NH}_2
\end{array}
\]

\[
\begin{array}{c}
\text{NH}_2
\end{array}
\]

leuciglumer
Repeated structural units are used when the atoms involved in bonding are defined. The bonds are represented as unbroken lines between the monomers when their positions are known, but they are shown as unattached when the way in which the monomers are linked has not been precisely determined:

**polietadene**

**poliglecaprone**

Copolymers of ethene and vinyl ethanoate (acetate) (EVA)

**polacrilin**

15.7 Sequences of polymers are shown in a similar way:

**poloxamer**

******
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Acknowledgements

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References
