

International Union of Pure and Applied Chemistry

# Compendium of Chemical Terminology

## Gold Book

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## chirality axis

**Synonym:** axis of chirality

An axis about which a set of ligands is held so that it results in a spatial arrangement which is not superposable on its mirror image. For example with an allene  $abC=C=Ccd$  the chiral axis is defined by the  $C=C=C$  bonds; and with an *ortho*-substituted biphenyl the atoms C-1, C-1', C-4 and C-4' lie on the chiral axis.

**Source:**

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2203

## chirality centre

**Synonym:** centre of chirality

An atom holding a set of ligands in a spatial arrangement which is not superposable on its mirror image. A chirality centre is thus a generalized extension of the concept of the asymmetric carbon atom to central atoms of any element, for example  $N^+abcd$ ,  $Pabc$  as well as  $Cabcd$ .

**Source:**

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2203

## chirality element

**Synonym:** element of chirality

General name for a chirality axis, chirality centre or chirality plane. Also referred to as an element of chirality.

**Source:**

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2203

## chirality plane

A planar unit connected to an adjacent part of the structure by a bond which results in restricted torsion so that the plane cannot lie in a symmetry plane. For example with (*E*)-cyclooctene the chiral plane includes the double bond carbon atoms and all four atoms attached to the double bond; with a monosubstituted paracyclophane the chiral plane includes the monosubstituted benzene ring with its three hydrogen atoms and the three other atoms linked to the ring (i.e. from the substituent and the two chains linking the two benzene rings).

**Source:**

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2203

## diastereoisomer (diastereoisomeric) excess

**Also contains definition of:** percent diastereoisomer excess

This is defined by analogy with enantiomer excess, as  $D_1 - D_2$  [and the percent diastereoisomer excess as  $100 (D_1 - D_2)$ ], where the mole fractions of two diastereoisomers in a mixture or the fractional yields of two diastereoisomers formed in a reaction are  $D_1$  and  $D_2$  ( $D_1 + D_2 = 1$ ) The term is not applicable if more than two diastereoisomers are present. Frequently this term is abbreviated to d.e.

**See:** stereoselectivity, diastereoisomerism

### **Source:**

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2205

## diastereoisomeric units

*in a polymer*

Two non-superposable configurational units that correspond to the same constitutional unit are considered to be diastereomeric if they are not mirror images.

### **Source:**

Purple Book, p. 27

## diastereoisomerism

**Also contains definitions of:** diastereoisomers, diastereomers

Stereoisomerism other than enantiomerism. Diastereoisomers (or diastereomers) are stereoisomers not related as mirror images. Diastereoisomers are characterized by differences in physical properties, and by some differences in chemical behaviour towards achiral as well as chiral reagents.

### **Source:**

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2205

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1105

## diastereoisomerization

The interconversion of diastereoisomers.

### **Source:**

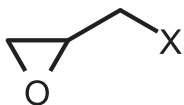
PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2205

**Source:**

PAC, 1992, 64, 143 (*Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992)*) on page 153

## epihalohydrins

Compounds having the (halomethyl)oxirane skeleton:



**Source:**

PAC, 1995, 67, 1307 (*Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995)*) on page 1334

## epimerization

Interconversion of epimers.

**Source:**

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2208

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1114

## epimers

Diastereoisomers that have the opposite configuration at only one of two or more tetrahedral stereogenic centres present in the respective molecular entities.

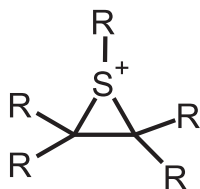
**Source:**

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2208

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1113

## episulfonium ions

Ions derived from thiiranes, in which a trivalent sulfur atom bears a positive charge:



## isomer

One of several species (or molecular entities ) that have the same atomic composition (molecular formula) but different line formulae or different stereochemical formulae and hence different physical and/or chemical properties.

### Source:

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1129

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2210

## isomer shift

*in Mössbauer spectroscopy*

Measure of the energy difference between the source ( $E_s$ ) and the absorber ( $E_a$ ) transition. The measured Doppler velocity shift,  $\delta$ , is related to the energy difference by

$$E_a - E_s = \frac{\delta E_\gamma}{c}$$

where  $E_\gamma$  is the Mössbauer gamma energy and  $c$  is the speed of light in vacuum.

### Source:

PAC, 1976, 45, 211 (*Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data*) on page 214

## isomerases

Enzymes that catalyse intramolecular rearrangements. Isomerases are classified into racemases and epimerases, *cis-trans* isomerases, intramolecular lyases and other isomerases.

### Source:

PAC, 1992, 64, 143 (*Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992)*) on page 158

## isomeric

Adjective derived from isomer.

### Source:

PAC, 1996, 68, 2193 (*Basic terminology of stereochemistry (IUPAC Recommendations 1996)*) on page 2210

## isomeric state

*in nuclear chemistry*

A nuclear state having a mean life long enough to be observed.

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