

Flavor Chemicals nomenclature

Stereochemistry of Flavor Chemicals (cis, trans ; E, Z ; d, l, +, - ; R, S ; ortho, meta, para)

Stereochemistry is the study of the three dimensional structure of molecules. Many chemicals can have the same molecular formula but differ on how their atoms are arranged in space.

cis, trans isomers:

The rigidity and lack of rotation about a carbon-carbon double bond allows the possibility of cis-trans isomerism, a form of stereoisomers which which have the same sequence of attachment but differ only in the orientation of the atoms in space.

Two similar groups on the ends of the double bond are considered to be cis or trans to one another when they are respectively on the same or opposite side of a specified reference plane. For example: trans-2-hexenal $\text{CH}_3\text{-CH=CH-CH}_2\text{-CH}_2\text{-CH}_3$ would show the hydrogen atoms (next to the double bond) positioned one on one side, and one on the opposite side of the double bond (visualize the hydrogen atoms above and below the double bond attached to the carbon atom). A cis isomer would contain both hydrogen atoms on the same side of the double bond. Other atoms or groups can participate in cis-trans isomers.

E and Z isomers:

Cis-trans orientation loses its distinction when two of the four groups attached to the double bond are not identical. In this case the steric relations around double bonds can be more precisely described by use of an E or Z designation. This nomenclature system provides a way to rank the substituent atoms or groups in order of preference based on atomic number.

Most flavor chemicals with double bonds have 2 hydrogen atoms attached to the carbon atoms in the double bonds. Some flavor chemical suppliers use the Z and E designation in place of cis and trans respectively. For example: e,z-2,6-Nonadienal is the same as trans, cis-2,6 Nonadienal. "e" is the same as "trans", "z" is the same as "cis" (Remember it as ciz)

Chiral Compounds: (R, S)

Chiral and chirality is derived from Greek meaning "hand". If you compare your left and right hand you will see that they are mirror images of each other, but are not superimposable on each other. Molecules that have left-handed and right-handed forms are chiral and called enantiomers.

The most common chiral molecules are those with one or more (asymmetric) carbon atoms bonded to four different substituents in a tetrahedral configuration. These molecules can exist in two non-superimposable mirror image forms. To differentiate between (chiral) enantiomers, the chiral carbon atom is designated the letter R or S. These designations are determined by 1). Assigning a priority to each group on the chiral carbon atom based on their atomic number; give the group with highest priority the lowest number. 2) With the three groups of highest priority pointing toward you, draw an arrow from the first priority group to the last priority group. If the arrow curves clockwise, the chiral atom is called R (Latin, rectus, "upright"). If the arrow curves counterclockwise, the chiral carbon atom is called S (Latin, sinister, "left").

Optically Active Chemicals: (d, l - +, -)

Mirror-image molecules have similar physical properties, but one way to measure their differences is the direction they rotate the plane of polarized light. Substances that rotate the plane of polarized light are said to be optically active. An instrument that measures the rotation of polarized light is called a polarimeter.

Compounds that rotate the plane of polarized light toward the right (clockwise) are called dextrorotatory from the Greek word dexios meaning toward the right. Compounds that rotate the plane of polarized light toward the left (counterclockwise) are called levorotatory from the Latin word laevus meaning toward the left. These signs are abbreviated by the use of "d" or "l". They are commonly given using the sign of the rotation, positive (+) for dextrorotatory rotations, and negative (-) for levorotatory rotations. Example: d-2-butanol or (+)-2-butanol.

Enzymes in living systems are chiral and are capable of distinguishing between enantiomers. Our nose and taste receptors are also capable of distinguishing between enantiomers...Example: (-)-carvone is spearmint and (+)-carvone is caraway.

(d) and (l) should not be confused with the designation D and L. The latter terms refer to the absolute orientation of the groups in space. (d) and (l) only refer to the direction in which the enantiomers rotate the plane of polarized light. There is no relationship between D and L and (d) and (l).

Ortho, Meta and Para:

Ortho, meta and para are designated positions on a benzene ring. They represent the positions of carbon atoms in the ring relative to the carbon atom bearing the first substituent group. Ortho, meta, para also can be represented by numbers 2,3,4 respectively. para-hydroxybenzaldehyde or 4-hydroxybenzaldehyde are one and the same.

