ChemFactsheet

www.curriculum-press.co.uk Number 207

E-Z Isomerism

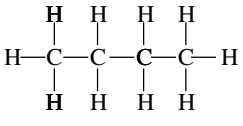
Reminders

Isomers are molecules with the same molecular formula but different structural formulas.

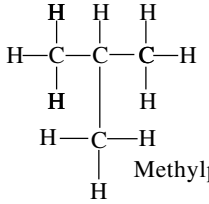
Structural isomers differ in the sequence in which the atoms are bonded together.

Structural isomers are of three types:

(a) **Chain isomers** : (also called **skeletal isomers**) where the carbon backbone of the molecule is re-ordered to create different structures. For example, butane and methylpropane.

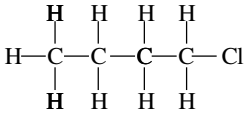


Butane

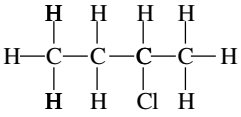


Methylpropane

(b) **Positional isomers :** where a functional group changes its position on the basic carbon structure. For example, 1-chlorobutane and 2-chlorobutane.

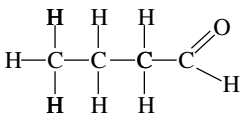


1-chlorobutane

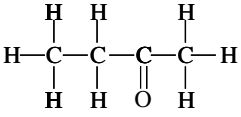


2-chlorobutane

(c) **Functional group isomers :** where the atoms are arranged differently to form different functional groups. For example, butanal and butanone.



Butanal

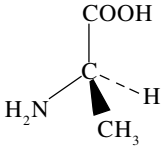


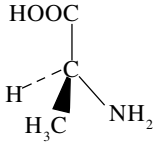
Butanone

Stereoisomers are molecules with the same sequence of bonded atoms but different three-dimensional arrangements of their atoms/ groups in space.

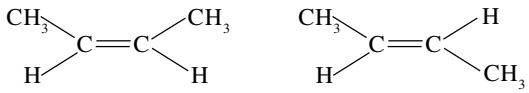
Stereoisomers are of two types:

(a) **Optical isomers**: (also called enantiomers) where the same functional groups are arranged differently in space such that one structure is the non-identical mirror image of the other. For example, the two optical isomers of 2-aminopropanoic acid ("alanine").



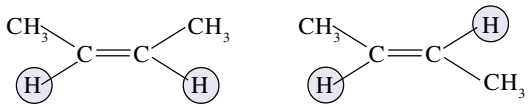


(b) **Geometric isomers**: (also called cis-trans or EZ isomers) where the same functional groups are arranged differently in space around a non-rotatable region (usually a C=C double bond) of a molecule. For example, the two geometric isomers of but-2-ene.



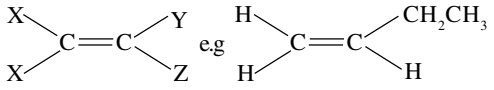
Having reviewed the general topic of isomerism, this FactSheet will now concentrate on the nature and naming of geometric isomers with particular emphasis on the EZ classification system.

In "simple" cases, such as the isomers of but-2-ene shown above, it is sufficient to distinguish them from each other using the fact that in one, both H atoms are on the **same side of the molecule** whereas in the other, they are positioned **"across" the molecule from each other** as shown below.



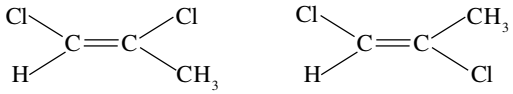
The prefix "cis" is used since it is Latin for "*on this side*" whereas "trans" is used for the other isomer because it means "*across*" in Latin.

These are different structures because the C=C double bond is not able to rotate about its axis.
Geometrical isomers CANNOT exist if either C atom of C=C bond has two identical groups bonded to it.



But-1-ene

But what about cases such as the geometric isomers of 1,2-dichloropropene?



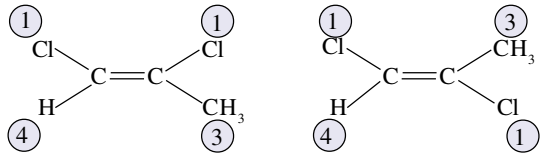
The "cis-trans" system of naming is inadequate in cases like this. Instead, the EZ system is applied using a set of rules to assign an order of priority to the groups attached to the C=C bond (ie Cl, Cl, H and CH_3) and then an allocation of E or Z according to the arrangements of the groups relative to this order of priority.

The rules for assigning an order of priority to the groups are called the Cahn-Ingold-Prelog (CIP) rules and are now adopted by I.U.P.A.C. for naming any geometric isomers – the cis-trans system is now redundant!

RULE 1: The atoms bonded directly to the C=C bond are given an **increasing order of priority in order of increasing atomic *number*** - the higher atomic number, the higher priority!

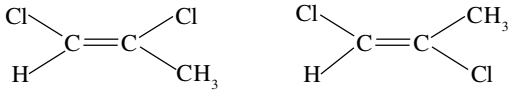
Hence, in the 1,2-dichloropropene example (above):

Atom bonded to C=C	Cl	Cl	H	C
Atomic number	17	17	1	6
Priority (1 most important)	1	1	4	3



RULE 2: The isomer with the **two highest priority groups** (here 1 and 1) **on the *same* side of the C=C bond** is called the **Z isomer**. Otherwise (ie they are on opposite sides of the C=C bond) it is called the **E isomer**.

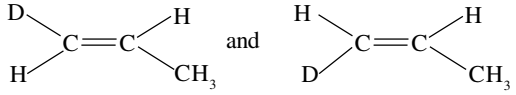
Hence the final names are:



Z - 1,2 dichloropropene E - 1,2 dichloropropene

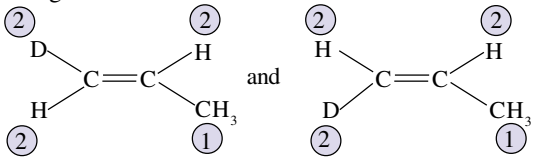
What about isotopes?

Deuterated (i.e. H atoms substituted by the isotope deuterium, D) molecules are often used in n.m.r. studies and it is important to differentiate molecules such as:



Atom bonded to C=C	D	H	H	C
Atomic number	1	1	1	6
Priority (1 most important)	2	2	2	1

Hence we get



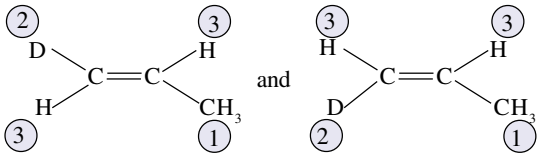
This will not differentiate the structures because both have a 1,2-priority on the same side of the molecule.

An additional rule is needed!

RULE 3: Where necessary, atoms with the same atomic number but different mass numbers (i.e. isotopes) are assigned a secondary **priority in order of increasing mass number** – the higher mass number being given the higher priority.

Hence the prioritisation changes to:

Atom bonded to C=C	D	H	H	C
Atomic number	1	1	1	6
Priority 1 (1 most important)	2	2	2	1
Mass number	2	1	1	12
Priority 2 (1 most important)	2	3	3	1



Now, looking at the new priorities, rule 2 can be applied and the names assigned unambiguously. The first isomer is **Z**-(1-^{2}H)-propene and the second is **E**-(1-^{2}H)-propene.

Note: -(1-^{2}H)- shows the ^{2}H atom (i.e. D) is bonded to Carbon-1 of the molecule.

This gives you enough information to name any examples you might encounter at A-level. However, after trying the following examples for yourself, you might want to work through the extension work that follows to see how the EZ system is applied to more complex cases.

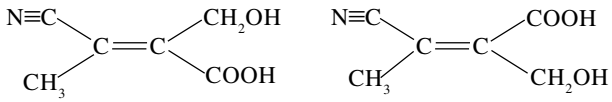
Examples

Consider each of the following molecules and decide whether geometric isomers exist or not. If they do, draw their structures and name them.

1. 2-bromobut-2-ene
2. 2-methybut-2-ene
3. 1-bromo-2-chloro-1-fluoropropene
4. 1,1-dichloroethene
5. 1-chloro-2-fluoroethene.

Extension work

But what about more complex cases such as the following geometric isomers?



The atoms bonded directly to the C atoms of the C=C bond are all C atoms. Hence, these cannot differentiate the two isomers.

The system is extended, first of all, to look at the ***combined*** *priorities* of the **other** atoms bonded directly to these four C atoms.

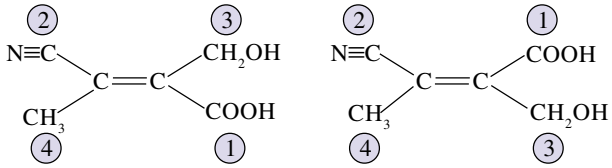
There will be three other bonds in every case. Double bonds count twice and triple bonds count three times when working out the priorities.

e.g. $-CH_3$ scores 1+1+1 = 3 for the 3 H atoms.
$-CH_2Cl$ scores 1+1+17 = 19 for the 2 H atoms and one Cl atom.
–CHO scores 1+8+8 = 17 for the 1 H atom and 2 × 8 for the doubly bonded O atom etc.

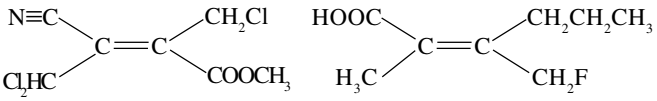
Hence, for the example above:

Atom bonded to C=C	C	C	C	C
Atomic number	6	6	6	6
Priority 1 (1 most important)	1	1	1	1
Atoms bonded to C's	≡N	–H –H –H	–H –H –O	=O –O
Combined priority	3×7=21	3×1=3	2+8=10	2(8)+8=24
Priority 2 (1 most important)	2	4	3	1

Hence the isomers can be assigned as follows:



Now try some examples for yourself. Assign E or Z to the following.

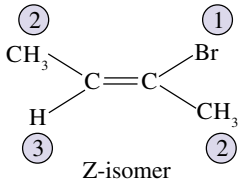


If the priorities are not resolved after this ananysis, the same ideas can be extended to the next atoms along any chain.

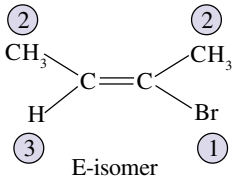
Answers

1. 2-bromobut-2-ene = $CH_3CH{=}CBrCH_3$
   → **EZ isomers possible** - see below.
2. 2-methybut-2-ene = $CH_3CH{=}C(CH_3)_2$
   → **EZ isomers not possible** because $2CH_3$ groups on same C of C=C bond.
3. 1-bromo-2-chloro-1-fluoropropene = FBrC=CHCl
   → **EZ isomers possible** - see below.
4. 1,1-dichloroethene = $Cl_2C{=}CH_2$
   → **EZ isomers not possible** because 2Cl atoms (or 2H atoms) on same C of C=C bond.
5. 1-chloro-2-fluoroethene = HClC=CHF
   → **EZ isomers possible** - see below.

1.

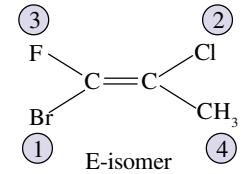


Z-isomer

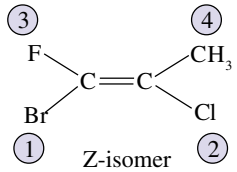


E-isomer

3.

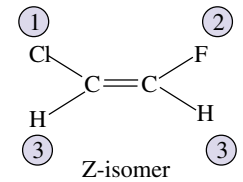


E-isomer

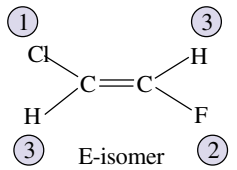


Z-isomer

5.



Z-isomer



E-isomer

Answers to extension questions

1. Z isomer – CN = 21 ; CH_2Cl = 19 ; $CHCl_2$ = 35 ; $COOCH_3$ = 24.
2. E isomer – COOH = 24 ; $CH_2CH_2CH_3$ = 8 ; CH_3 = 3 ; CH_2F = 9.

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