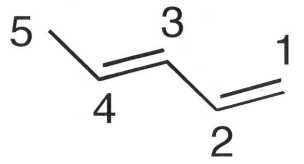
Conjugated Molecules - conjugated systems

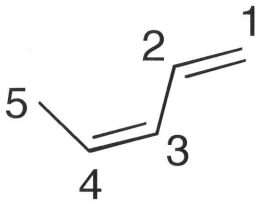
"Separated by a single bond from double bond"

can refer to a double bond, cation, anion or radical

Review of nomenclature and examples



E-1,3-pentadiene

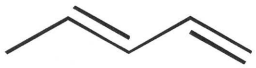


Z-1,3-pentadiene

stereoisomers, both conjugated

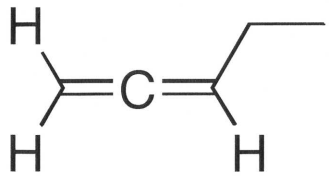
1,4-pentadiene

NOT conjugated



E-1,3-pentadiene

structural (constitutional) isomers, not conjugated



1,2-pentadiene (an allene)

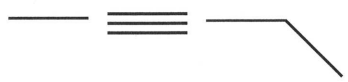
Conjugated Molecules & Systems - Nomenclature

find longest chain with max number double/multiple bonds

number from end to give 1st doubly bonded carbon lowest number

1 double bond = ene : replace “ane” of alkane name

1 triple bond = yne



$CH_3CCCH_2CH_3$

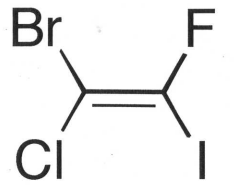
2 double bonds = diene : replace “ne” of alkane name

3 double bonds = triene

4 double bonds = tetraene etc.

E-1,3-pentadiene

Another example for nomenclature : is this E or Z alkene (olefin)?



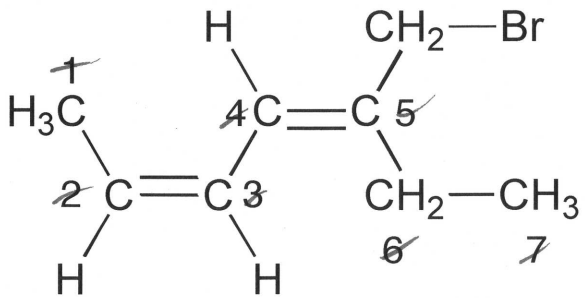
First look at the highest priority
(that is the highest atomic number of the atom directly attached)
on either side of the double bond

I is highest priority relative to F
Br is highest priority relative to Cl

Therefore it is an E double bond
as the high priority groups are on opposite sides of the double bond

its name is (E)-1-bromo-1-chloro-2-fluoro-2-iodoethylene

One more example

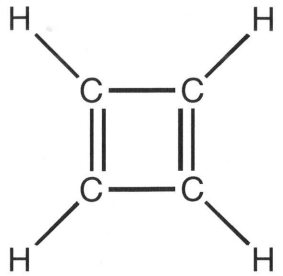


(2*Z*,4*E*)-5-(bromomethyl)-2,4-heptadiene

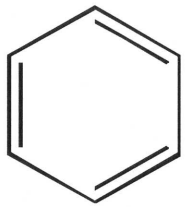
To assign the first double bond between C2 and C3,
methyl group is the larger group compared to H on C2

carbon chain (C4 to C7) is the larger group
compared to H on C3

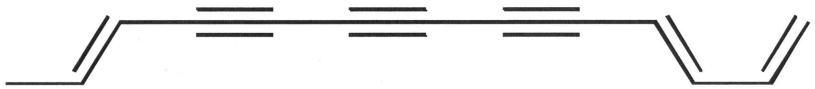
bromomethyl group is the larger group
compared to ethyl group on C5



Cyclobutadiene - formally conjugated



"Cyclohexatriene" = **benzene** special (aromatic system)



(3*E*,11*E*)-trideca-1,3,11-trien-5,7,9-triyne

plant defense mechanism (anti-nematode) from canola kills predatory worms

all double bonds and triple bonds in the above compound are conjugated

derivative of a tridecane (13 carbons). know the names of the first 20 alkanes

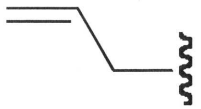
Begin numbering at end of longest chain with maximum number of multiple bonds so as to give the first multiply bonded carbon the lowest number - but name ene-yne

no stereochemistry in the triple bonds because they are linear (180°).

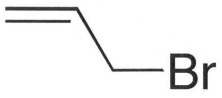
Nomenclature of Allyl and Vinyl Groups

(the squiggly line represents attachment to any group)

Allyl Group

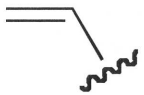


Example

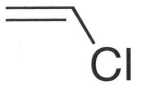


allyl bromide

Vinyl Group

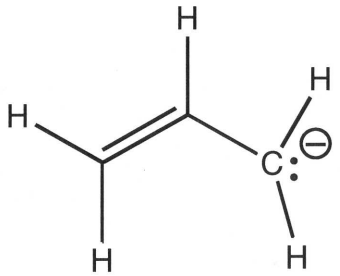


Example

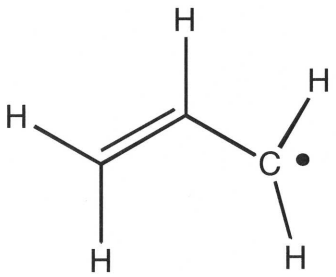


vinyl chloride

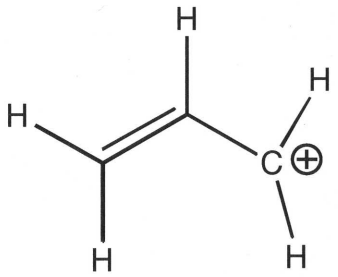
Allyl (Allylic) intermediates include



Allyl anion 8 e^- at C



Allyl radical 7 e^- at C



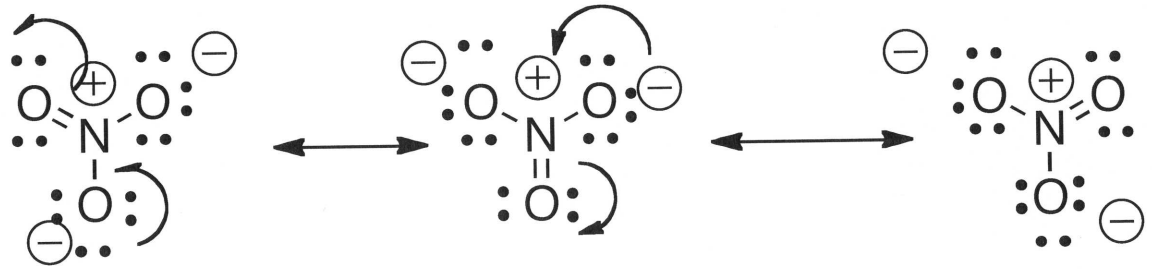
Allyl cation 6 e^- at C

All are conjugated intermediates,
the excess or deficiency of electrons at the carbon atom is stabilized by resonance

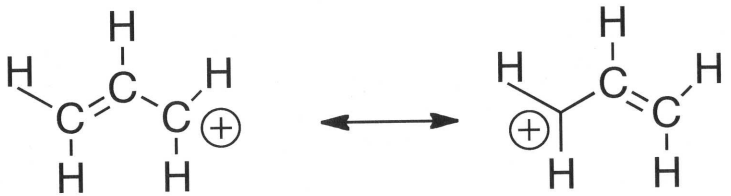
Resonance Forms

Resonance forms (resonance structures) are different pictures of the same molecule obtained by moving electrons without changing the position of the atoms

Shown below are the resonance forms of sodium nitrate ($NaNO_3$).
The anion on oxygen is a conjugated anion.
Resonance forms are connected by a **double headed arrow**



Shown below are the resonance forms of allyl cation (a conjugated cation)



same as