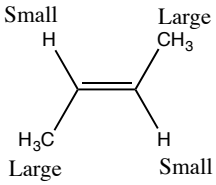
Conjugated Molecules and Intermediates

Conjugated means "Separated by one single bond from a double bond"

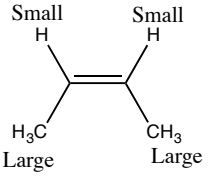
Intermediates - Often non-stable molecules that occur during reactions for short periods of time (ex. cation, anion, radical)

Review of alkene nomenclature and examples

2 double bonds →	diene	2 triple bonds →	diyne
3 double bonds →	triene	3 triple bonds →	triyne
4 double bonds →	tetraene	4 triple bonds →	tetrayne

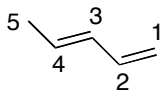


Trans (opposite)
E (Entgegen, opposite)

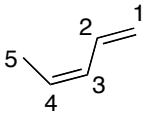


Cis (same side)
Z (Zusammen, same side/together)

The two molecules below are stereoisomers, and both are conjugated.

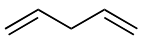


E-1,3-pentadiene



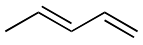
Z-1,3-pentadiene

The two molecules below are constitutional (structural) isomers.
1,4-pentadiene is not conjugated. It has double bonds separated by **2** single bonds.



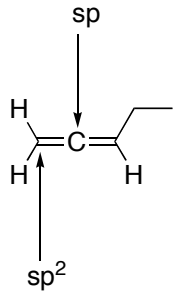
1,4-pentadiene

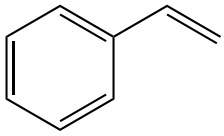
NOT conjugated



E-1,3-pentadiene

1,2-pentadiene, shown below is not conjugated. It has **cumulated** double bonds. This molecule is an **allene** and is a structural isomer with respect to the above 1,3-pentadienes.

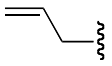
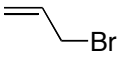




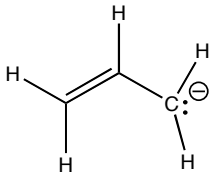
Styrene

Degrees of unsaturation: 5

Nomenclature of Allyl and Vinyl Groups (the squiggly line represents attachment to any group)

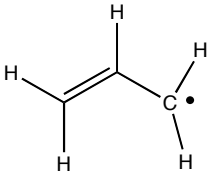
Allyl Group	Example	Vinyl Group	Example
	 allyl bromide		 vinyl chloride

Allyl (Allylic) intermediates include:



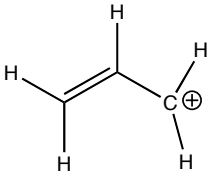
Allyl anion

Has 8 e^- at C
C is negative



Allyl radical

Has 7 e^- at C
C is neutral but reactive



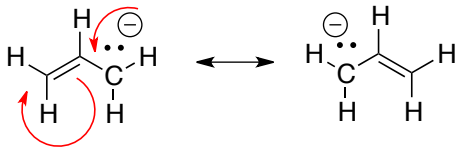
Allyl cation

Has 6 e^- at C
C is positive

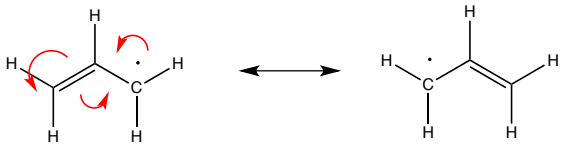
All are conjugated intermediates. The excess or deficient electrons at the carbon atom are conjugated to the double bond.

All are stabilized through resonance structures.

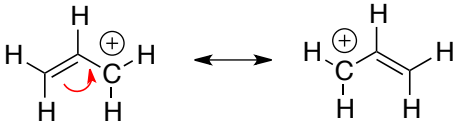
Allyl Anion:

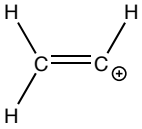


Allyl Radical:



Allyl Cation:





Vinyl cation is not conjugated

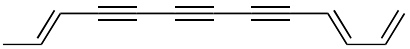
Conjugated Molecules & Systems – Nomenclature

Cyclobutadiene

Formally conjugated

Cyclohexatriene/ Benzene

Aromatic system



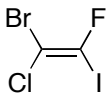
(3*E*,11*E*)-trideca-1,3,11-trien-5,7,9-triyne

The above compound is part of a plant defense mechanism (anti-nematode) from canola to kill predatory worms.

All double bonds and triple bonds in the above compound are conjugated.

It is a derivative of a tridecane (13 carbons). Know the names of the first 20 alkanes. Begin numbering at the end of the longest chain with maximum number of multiple bonds so as to give the first multiply bonded carbon the lowest number. There is no stereochemistry in the triple bonds because they are linear (180°). Stereochemistry is only potentially possible in the molecule's double bonds.

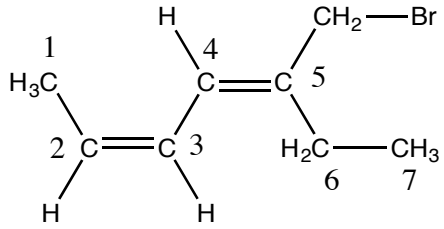
Another example for nomenclature below: Is this an E or Z alkene (olefin)?



First of all, look at the highest priority (based on the atomic number of the atom directly attached) on either side of the double bond.

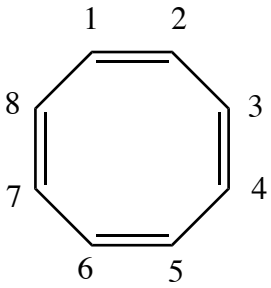
I is higher priority relative to F
Br is higher priority relative to Cl
Therefore it is an E double bond, as the high priority groups are on opposite sides of the double bond.
The name is (E)-1-bromo-1-chloro-2-fluoro-2-iodoethylene.

More examples

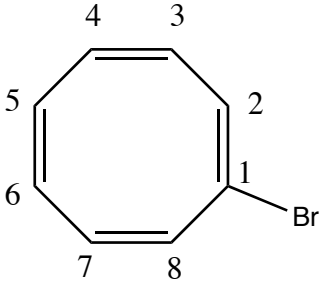


(2Z,4E)-5-(bromomethyl)-2,4-heptadiene

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 largest group on C5



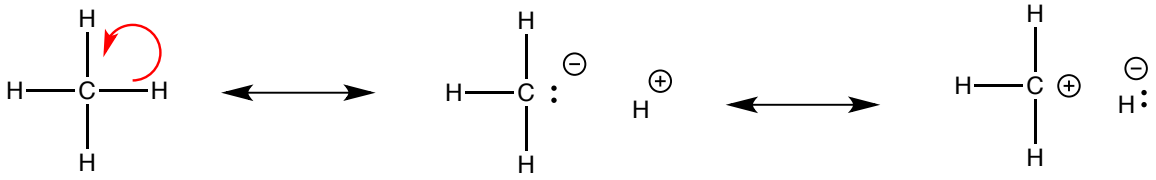
1,3,5,7-cyclooctatetraene



1-bromo-1,3,5,7-cyclooctatetraene

Resonance Forms

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



Separation of charge is BAD

Shown below are the resonance forms of sodium nitrate ($NaNO_3$). Conjugation stabilized molecules. The anion on oxygen is a conjugated anion. The nitrogen cation is not conjugated. Resonance forms are connected by a double-headed arrow.