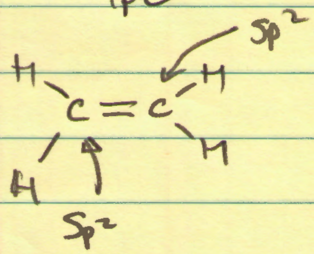
Br 57

Alkenes

- contain double bonds and have generic formula

  C_nH_{2n-2} where $n = 1, 2, 3 \ldots$

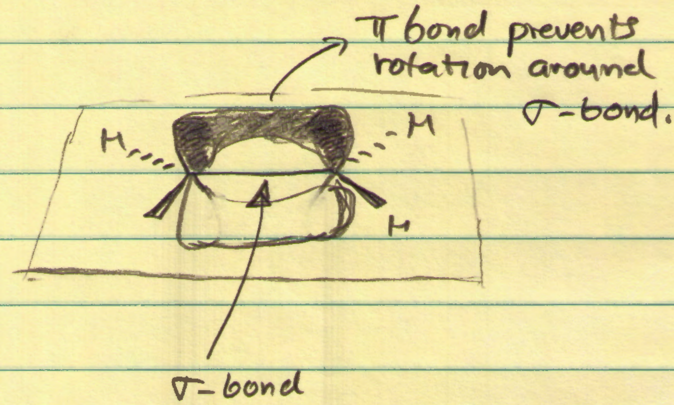
Shape



sp^2 = trigonal planar

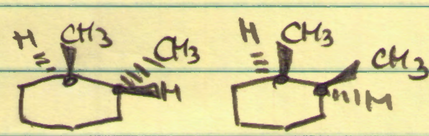
∴ molecule at left is flat on page.

In perspective drawing



Cis/Tran Isomerism

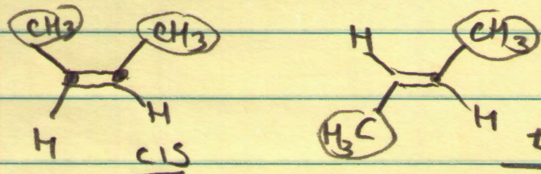
Recall



trans cis

Note: The carbons that have substituents that cause these to be referred to as 'cis' or 'trans' also have an H attached

Likewise



cis trans

Br 5-2

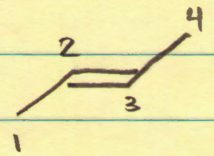
Naming alkenes

① Find longes chain that contains the double bond

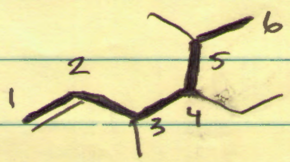
② # chain so C=C gets lowest #

③ Indicate location of C=C by using lowest #

④ Name and locate (w/number) substituents as done w/ alkanes



trans-2-butene

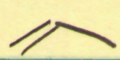
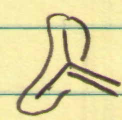


1-hexene → 'ene' suffix

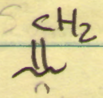
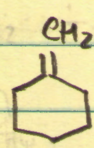
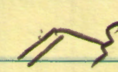
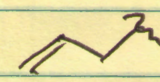
3-methyl
5-methyl } 3,5-dimethyl

3,5-dimethyl-1-hexene

Common Names (CN)

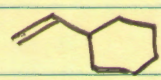
	$H_2C=CH_2$		
CN	Ethylene	Propylene	Isobutylene
IUPAC	Ethene	Propene	2-methylpropene 2-methyl-1-propene

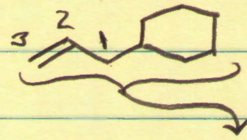
Substituents

				
CN	methylene	methylidenecyclohexane	Vinyl	allyl
IUPAC	methylidene		ethenyl	2-propenyl

-yl indicates substituent

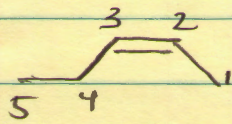
Br 5-3



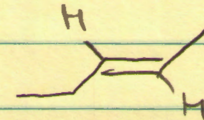


IUPAC: ethenylcyclohexane 2-propenyl cyclohexane
CN: vinyl " allyl "

Cis/Trans Revisited

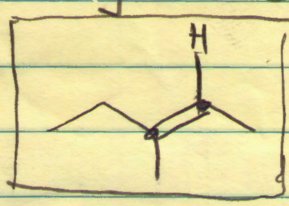


cis-2-pentene



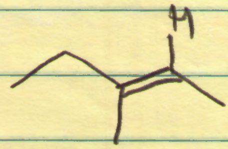
trans- 2-pentene

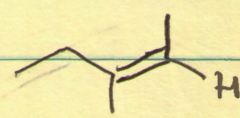
Can you use "cis/trans" for the following?



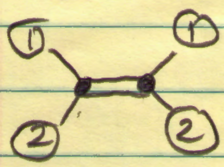
NO! each C of the double bond does not have at most 1 H.

How do you distinguish



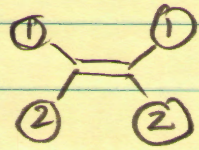
from


Use E/Z System
↳ same priority rules as those used for S/R configuration assignments: Cahn-Ingold-Prelog



Assign priorities 1 and 2 to the substituents each atom of C=C holds

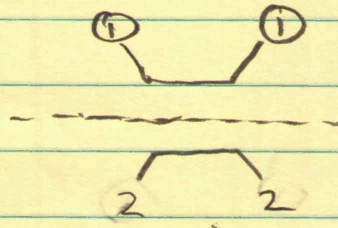
Br 5-4



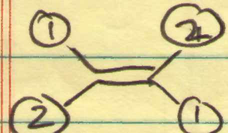
1 gets 1st place

2 gets 2nd place

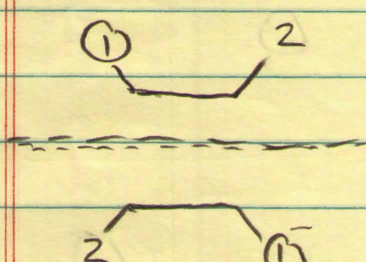
Are the 1s on same side of double bond



yes! ∴ (Z)ussamen

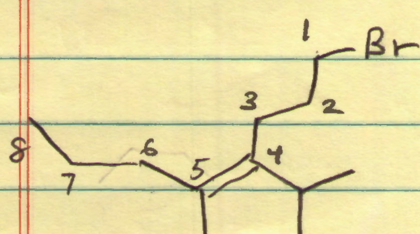


The 1s are on opposite sides of double bond



∴ (E)ntgegen

entgegen (in German) = "in opposite"



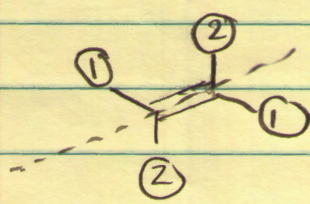
4-octene

4-isopropyl IUPAC: (1-methylethyl)

5-methyl

1-bromo

(E)-1-bromo-4-isopropyl-5-methyl-4-octene



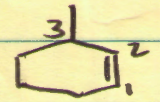
E

Br 5-5

Cycloalkenes (Naming)

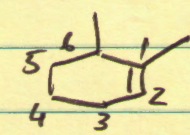
① Ring C=C are # 1 and 2 always

② Substituents are named so they get the lowest # when C=C are 1 and 2



3-methyl$\underbrace{\text{cyclohexene}}$

Note, there is no need to say 1-cyclohexene because that is implied if C=C gets assigned as 1 and 2

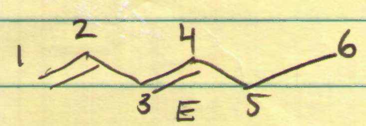


substituent on C=C dictates # of C1, the other C of C=C is # 2

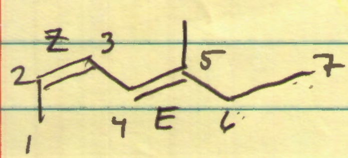
1,6-dimethylcyclohexene

NOT 2,3-dimethyl______

Polyenes



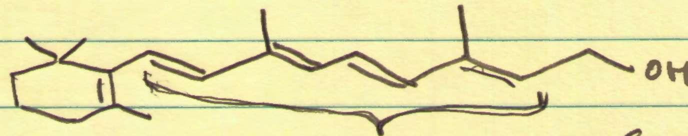
1,3-hexadiene



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

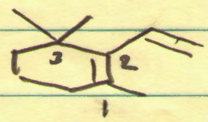
Br 5-6

Vitamin A



all-trans or (all E)

Name using IUPAC names for substituents



cyclohexene

2- ethenyl

1,3,3 - trimethyl

Reminder: Alkenes have a molecular Formula of $C_n 2n$ where as a <u>saturated alkane</u> has 2 additional hydrogen atoms represented by $C_n 2n \underline{+2}$
"plus 2"

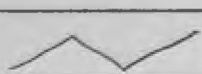
So, you can see that for one double bond in a alkene H_2 is lost from the saturated alkane formula

If two double bonds are present in a <u>di</u>ene, (i.e. two double bonds are present then this molecule loses $H_2 + H_2$ (or $2 H_2$)

For each unit of H_2 lost, this is referred to as the Index of Hydrogen Deficiency (IHD)

"Index of H_2 units Lost"

Compare



butane

C_4H_{10}

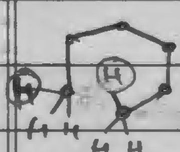
1,3-butadiene

C_4H_6

butadiene lost 2 H_2 units compared to the saturated butane $\therefore$ butadiene has an IHD = 2

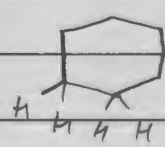
Note: when a carbocycle ring is formed there is an IHD = 1. There is 1 IHD per ring.

Examples:



hexane

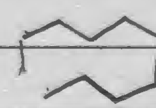
C_6H_{14}



cyclohexane

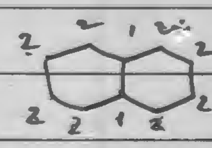
C_6H_{12}

This lost 1 H_2 compared to hexane



decane

$C_{10}H_{22}$



[4.4.0]-bicyclodecane

$C_{10}H_{18}$

hydrogen # listed on each carbon to confirm

This compound lost 2 H_2 when 2 rings were form

∴ For every double bond and ring ~~an~~ IHD can be registered.

∴ if you are given the molecular formula of a compound, you can calculate the IHD which will be a total of the double bond and/or rings

In class, we calculated the IHD for

$C_6H_6N_2O$: ① Our goal was to transform this to a formula containing C and H only.

Let's look at a simple molecule like ethanol

$\Rightarrow$ MF : $\underline{C_2H_6O}$

we know ethanol has $\underline{\text{NO}}$ double bonds or rings ∴ it has an IHD = 0. Let's check

C_2H_6O

Note: Oxygen does not affect the Hydrogen count compared to $\underline{\text{a saturated } C_2 \text{ alkane}}$: C_2H_6

So C_2H_6O is equivalent to a "C/H" Formula of C_2H_6

saturated C_2 alkane: $\quad C_2H_6$

minus C_2H_6O equivalent: $\quad \underline{-\,C_2H_6}$

$$H_0 \times \frac{IHD}{H_2} = \emptyset \text{ IHD}$$

Let's look at ethylamine

There are NO double bonds or rings

∴  $IHD = \emptyset$. Let's check

C_2H_7N compared to saturated C_2 alkane C_2H_6

→ this is saturated too! i.e. no double bonds ∴ N brings an additional H to the formula, so an H must be subtracted when evaluating the C/H equivalent

∴ C_2H_7N

→ C_2H_6 this is the same as C_2H_6 ∴ the $IHD = \emptyset$

Back to

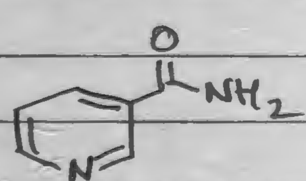
$C_6H_6N_2O$ a saturate C_6 alkane is C_6H_{14}

$C_6H_6N_2$ (we know Oxygen does not affect the Hydrogen (#) in a formula)

C_6H_4 (we know that every N brings an additional Hydrogen over the saturated C/H formula so 2 H are deducted when we remove both Nitrogens

$$
\begin{array}{lr}
\text{saturated } C_6 \text{ alkane:} & C_6H_{14} \\
\text{minus } C_6H_6N_2O \text{ equivalent:} & -\ C_6H_4 \\
\hline
 & H_{10} \times \dfrac{\text{IHD}}{H_2} = 5 \text{ IHD}
\end{array}
$$

This formula came from



Note: 1 ring
4 double bonds

5 IHD