Course 343 Lecturer Gellman

Day Monday Date 9/21/15

Notes Taken By Kirandeep Deol Total # of Pages 3

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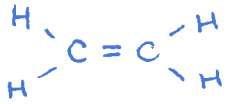
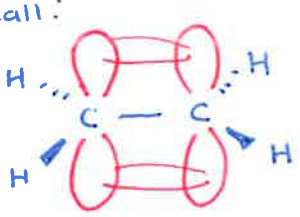
Recall: Alkenes

- hydrocarbons that contain at least one C=C (double bond)

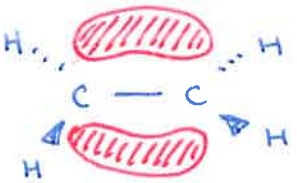
simplest:  "ethene or ethylene"

- Double bond has σ component and π component (source of reactivity)

Recall:



or



Thus, all six atoms in one plane.

π-e⁻ density is above and below that plane

(focus on π e⁻'s because of their reactivity)

Consider bond strengths:

Typical C-C σ ~ 90 kcal/mol

C=C π ~ 60 kcal/mol

π bond strength leads to the structural phenomenon of "stereoisomerism" - forms that differ only in the spatial arrangement of atoms

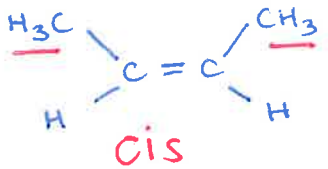
Example

$CH_3-CH=CH-CH_3$

isomers of 2-butene (4 carbon, alkene, position of π bond)

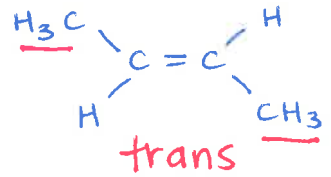
⇒ read SH.2 on nomenclature (name → drawing ONLY)

- 2 stereoisomers of 2-butene



cis

VS.

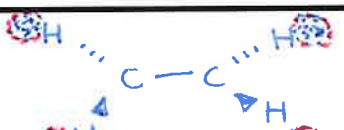


trans

cis-trans interconversion "costs" ~60 kcal/mol

↳ must break π bond.

anti-bonding orbital



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Perspective - rotation about C-C single bond is rapid at or over RT

This interconversion "costs" ~3.3 kcal/mol.

Note: Contrast w/constitutional isomerism

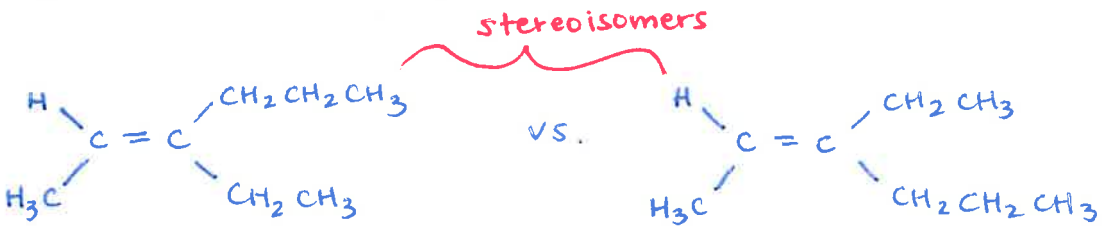
- different bonding relationship among atoms

$CH_3CH_2CH=CH_2$ 1-butene

General Classification Scheme for ALKENE STEREOISOMERS

E. vs. Z

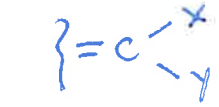
consider:



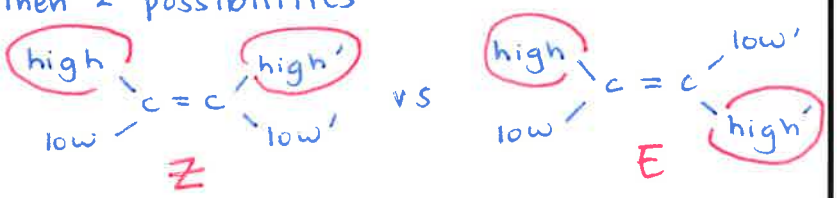
E vs Z

↓ entoegen ↓ zusammen

RULES of PRIORITY among molecular fragments



Then 2 possibilities -



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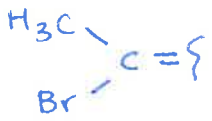
Priority Assignment rules:

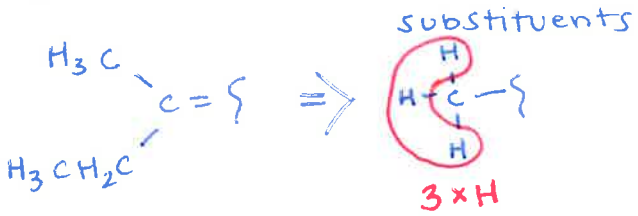
① Consider atoms directly bonded to the sp^2 carbon

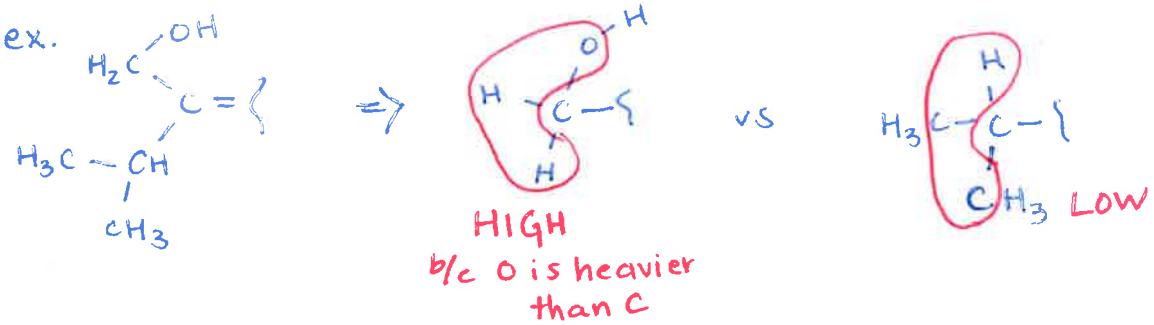
- higher atomic # => higher priority

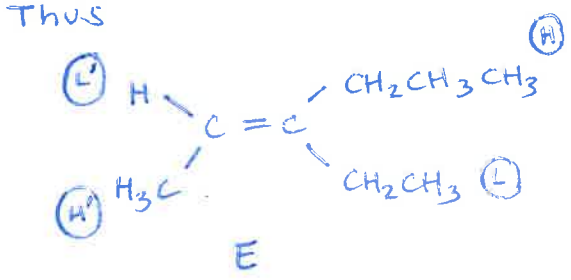
ex. 

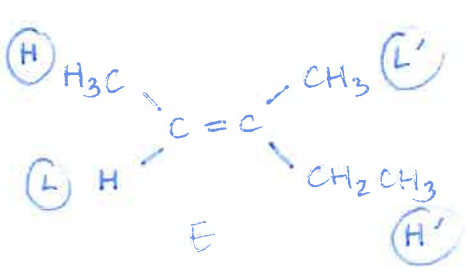
Br higher priority than C

② If no distinction based on rule #1, then consider the next set of atoms.

ex. 

ex. 

Thus 



Extracting structural possibilities from molecular formula info.

"unsaturation number" (U)