Course CH 343 sec 003 Lecturer Sam Hellman

Day Wednesday 1:20 Date 9/21/11

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"In the news" (Website)

- Molecules w/very long C-C bonds (>1.70 Å)

Compare: CH_3-CH_3 1.54 Å

Recall: Relationships between molecular structure and Brønsted acidity...

1) Periodic Trends

a) Acidity increases along a row left to right

(Rationale: Parallels electronegativity increase

Ex: CH_4 vs NH_3 vs OH_2 vs F-H

Consider: conjugate bases

$^{\ominus}CH_3$ vs. $:\ddot{O}H$

- Oxygen is better at "dealing with" excess $e^{\ominus}$ because it is very electronegative

b) Acidity increases down a column

(see text for rationale)

Ex: H-OH pKa ~ 16

H-SH pKa ~ 7

c) Charge Effect

Ex: $H_3\overset{\oplus}{O}-H$ vs H_2N-H

- Same idea as $H_3O^{\oplus}$ vs H_2O

pKa ~9 ~35

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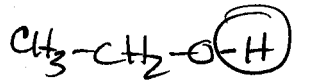
3. Polar Substituent Effects

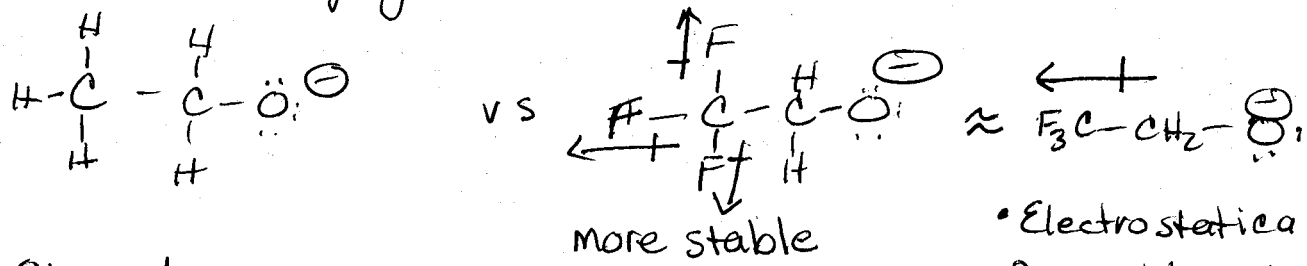
• Electronegative substituents can stabilize conjugate base

Ex:



pKa ~ 16 vs pKa ~ 12 ← Don't need to know pKa #; just know the trend!

Consider conjugate bases:



more stable

• Electrostatically favorable interaction

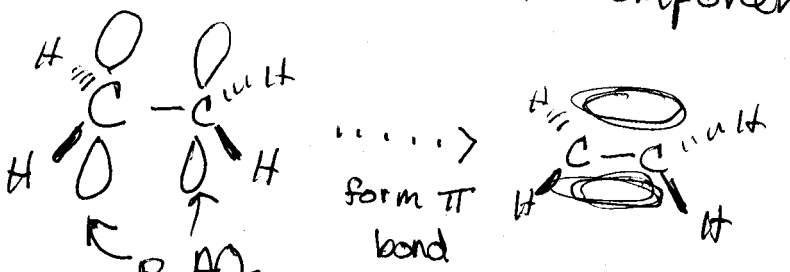
Chap 4 - Alkenes (contain C=C) ← structures only

Rec. Probs: 1, 2, 5-10, 12-26, 29-37, 39+40, 41-43, 46-58, 55-58, 60-66, 68

Alkene vs Alkane

• Simplest alkene: $H_2C=CH_2$ "ethene" (common name: ethylene)

Recall: MO - focus on π component



• π electrons are less tightly held than σ bonds
∴ π bonds are sites of reactivity

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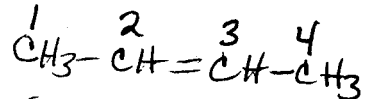
Consider bond energies (what it would 'cost' to break the bond)

Typical C-C σ bond ~90 Kcal/mol

Typical C-C π bond ~ 58 Kcal/mol

↳ strong enough to lead to stereoisomerism in alkenes

Consider:



Read nomenclature in § 4.2a

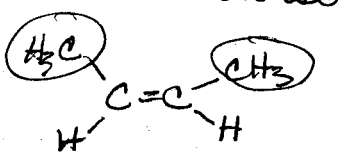
(2)-Butene → location of the double bond

↳ alkene

↓

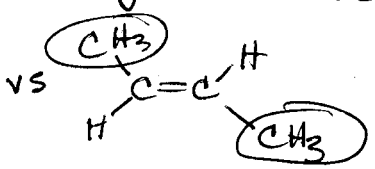
4 carbons

Two stereoisomers of 2-butene



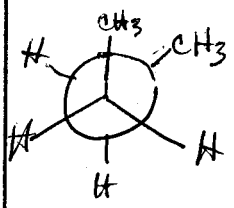
cis-2-butene

vs

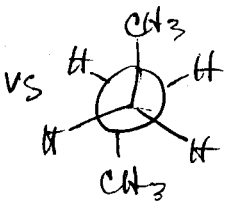


trans-2-butene

Recall:



vs



← Very rapid interconversion

- Small E barrier 63 Real/mol)

Compare to alkene at 58 Kcal/mol

- Stable to interconversion at room temp

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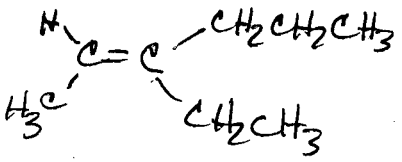
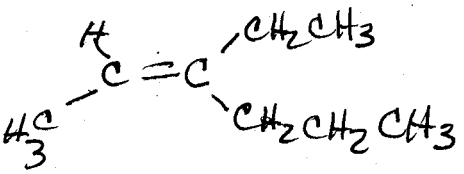
General Nomenclature for Alkene Stereoisomers

Z vs E



vs

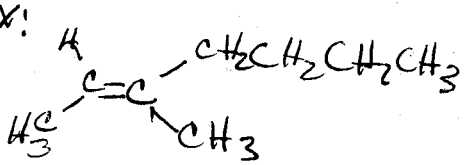


stereoisomers

Note:

Stereoisomer vs constitutional isomer
↳ different bonding relationship

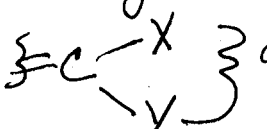
Ex:



is a constitutional isomer of these

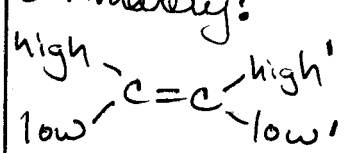
Assign E vs Z

- Start by focusing on individual alkene carbons

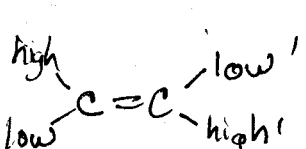


assign priority @ X + Y

Ultimately:



Z



E

Rules for assigning priority to molecular fragments