Course 343 Lecturer Gellman

Day Wed. Date 9/23/15

Notes Taken By Kirandeep Deol Total # of Pages 3

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"Structural insights from Molecular Formulas"

- unsaturation # (u) / degree of unsaturation
  - for molecular formula w/more than a handful of atoms esp. carbon's, many ways to form bonds

However, the possibilities are limited by the relative amounts of C and other elements.

Alkane w/out rings - max # of C and H

$C_nH_{(2n+2)}$

i.e. C_5H_{12} 

Note, branch points do not affect formula.

form a ring or a double bond => lose 2H

ie C_5H_{10}  etc

∴ one ring or one double bond = one degree of unsaturation

For hydrocarbons:

$$U = \frac{2C + 2 - H}{2}$$

C = # of carbons

H = # of hydrogen

ie. For C_5H_{12}, U = ∅

C_5H_{10}, U = 1

C_5H_8, U = 2 

More general:

$$U = \frac{2C + 2 + N - H}{2}$$

[* oxygen is irrelevant]

Now

C = # of carbon

N = # of nitrogen

H = # of hydrogens or HALOGENS

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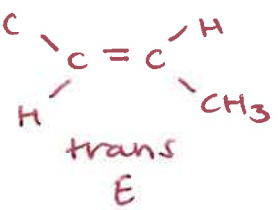
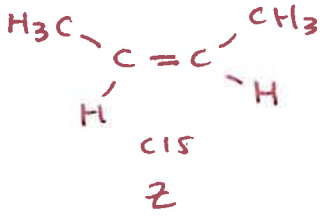
- See TEXT for details & examples

Fundamental Question: relationship between molecular structure and stability

ie 

vs 

Which is more stable? why?

→ most effectively answered by comparing isomers

* otherwise apples vs. oranges

Several ways to approach: all involve heats of rxn.

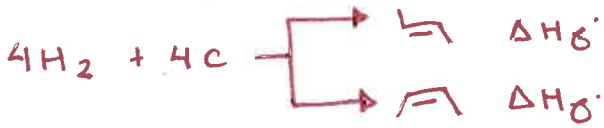
heat released in a rxn ("exothermic")
heat absorbed in a rxn ("endothermic")

To compare isomeric 2-butene, consider rxns that form them from a single set of starting materials or that convert them to identical products

3 approaches

① Heats of formation (ΔH_f°)

General: form a molecule from its elements (1atm, 25°C)



← "more stable" than cis isomer

∴ standard free enthalpy difference (ΔH), E vs. Z is 1.0 kcal/mol

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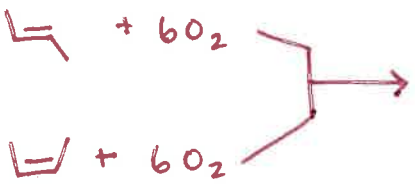
② Heats of combustion (ΔH_c°)



ΔH_c°

-646.8 kcal/mol

-647.8 kcal/mol

* same conclusion: ⌐ more stable than ⌐

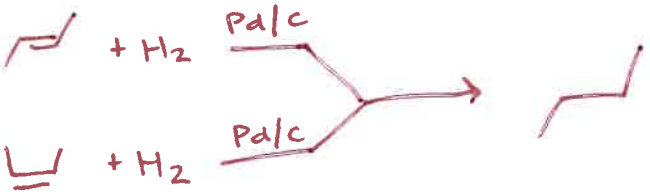
③ Heat of hydrogenation (ΔH_h°)

General: rxn of alkenes - addition of H_2 across C=C, requires metal catalyst.

ie. $CH_3CH_2-CH=CH_2 + H_2 \xrightarrow{Pd/C} CH_3CH_2-\underset{H}{\overset{|}{C}}H-\underset{H}{\overset{|}{C}}H_2$

Pd/C ⇒ Pd metal on finely divided carbon (maximize exposed surface of expensive metal).

Thus



(ΔH_h°)

-27.6 kcal/mol

-28.6 kcal/mol