

Course 343

Instructor Hockenberger

Day Mon

Date 12/9/2013

Notes Taken By Adam

Total # of Pages

Submit notes to the Undergraduate Chemistry Office for posting.
PLEASE COMPLETE NOTES IN INK AND DO NOT STAPLE.

Final Exam: Friday, Dec 20th 10:05 - 12:05

- Room: Social Science 6210 (all students)

Office hours: this week: Mon, Wed, Fri 12-1 pm

next week: Mon, 16th Dec 11 am - 1 pm

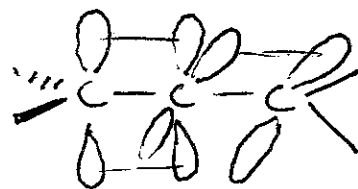
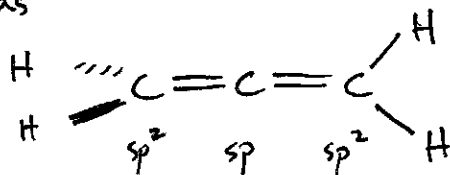
Ch 15 - Dienes, Resonance, and aromaticity (skip 15.2)

Problems: 3-5, 11-24, 27-30, 33-45, 50-73

Dienes: hydrocarbons containing 2 C=C double bonds

Three types:

1) Cumulenes or allenes: one C is involved in both double bonds



orthogonal π bonds

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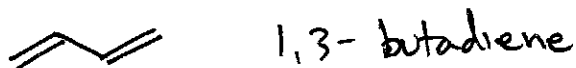
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2) Conjugated dienes: the two C=C share a bond between them

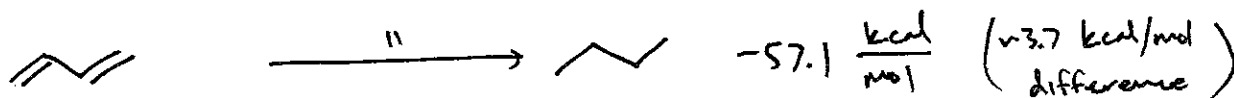
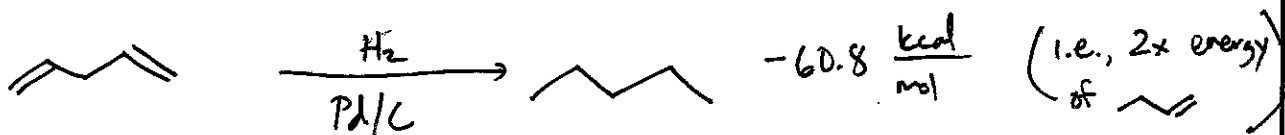
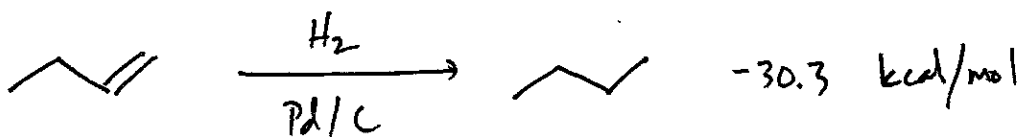


this type of diene results in new reactivity
 (i.e. Diels-Alder rxn)

3) "Ordinary" diene: ≥ 1 sp^3 C between the two double bonds



Look at heat of hydrogenation (ΔH_h) to observe differences for conjugated dienes



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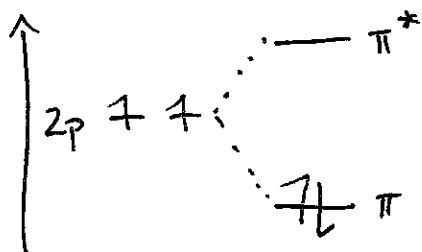
• What is the origin of this 3.7 kcal difference in stability?

~~Area~~ - Delocalized π -bonding

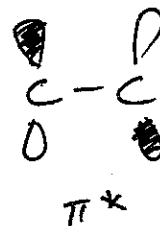
• Localized π bonding: π electrons shared between just two atoms

• Delocalized: π electrons shared between more than 2 atoms

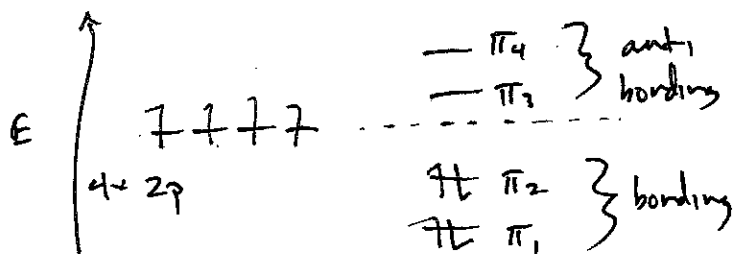
Recall: Ch 4, p 126



graphical drawing



• Molecular orbitals for



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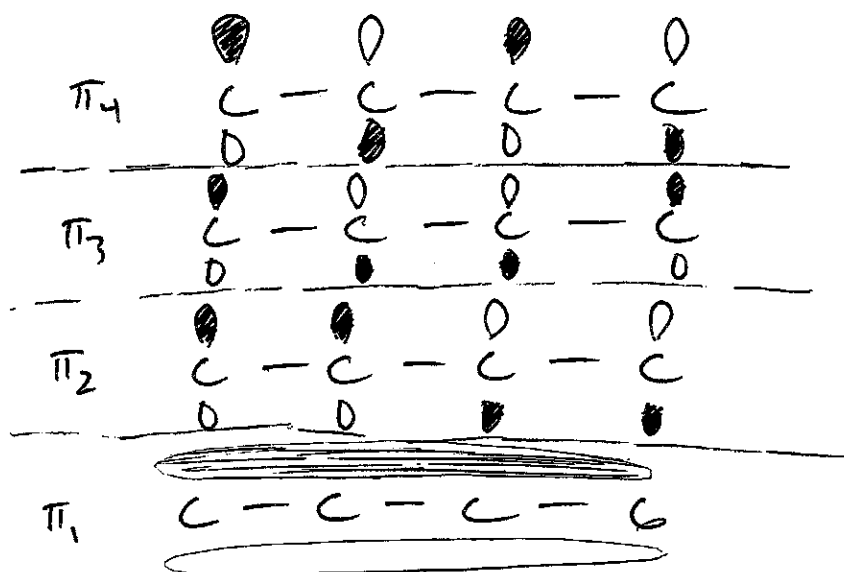
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Consequences/observations:

1) For π_1 the electrons are fully delocalized over all 4 carbons of a conjugated diene

2) - i.e., there is some π character between C_2 and C_3



2) The # nodes increases ~~the more~~ from $\pi_1 \rightarrow \pi_4$

- more nodes = higher energy

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• Structural consequences

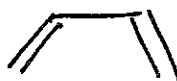
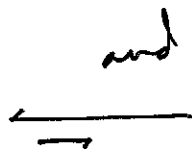
1) Conjugated dienes prefer conformations in which all 4 C's are in one plane (to allow orbital overlap)

- 2 different possible conformations fulfill this requirement for 1,3-butadiene

s = single bond (between C2 + C3)



s-trans



s-cis

• s-trans form is more stable due to steric repulsion for s-cis

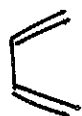
• however, both forms still exist in equilibrium with each other

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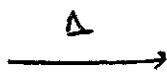
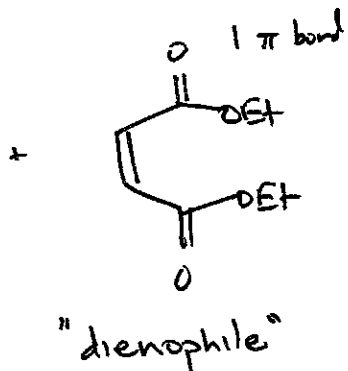
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Reactions of conjugated dienes: Diels-Alder rxn

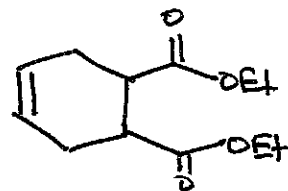
2 π bonds



diene



1 π , 2 σ



6-membered ring

Mechanism: concerted cycloaddition

