Course CHEM 343 Lecturer Gellman

Day Wed 1:20PM Date 12/7/11

Notes Taken By Patrick Total # of Pages 2

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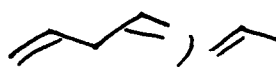
Recall: 3 classes of dienes

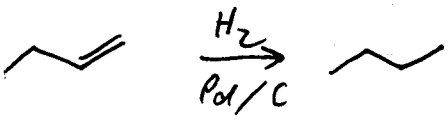
1) allenes (=•=)

2) conjugated dienes (=—=)

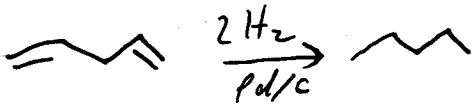
3) others ( , etc) → ≥ 1 sp^3 (b/w C=C unites (~regular alkene) bonding

Focus on conjugated dienes – ex. of delocalized

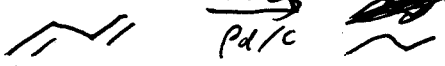
consider heats of hydrogenation (ΔH_h°, kcal/mol)



ΔH_h = −30.3



−60.8 (about 2 × C=C)

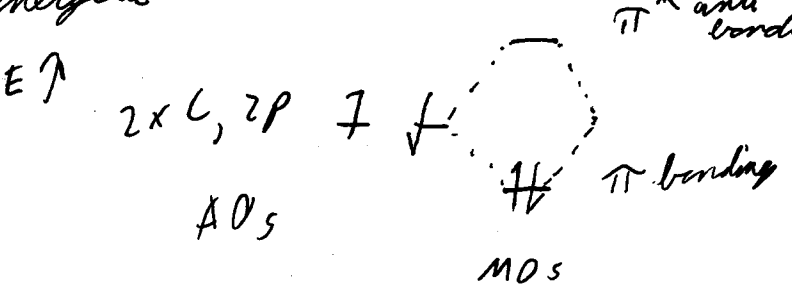


−57.1 (3.7 kcal/mol less than 2 C=C)

stability in conjugated diene relative to isolated C=C

- To understand origin of this extra stability (from e⁻ delocalization) consider π MO analysis
- Begin by recording π MO analysis of simple alkene ($CH_2=CH_2$)

1) Energetic considerations



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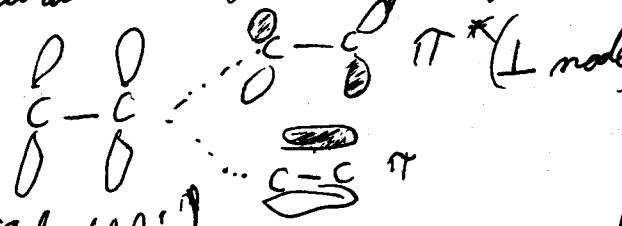
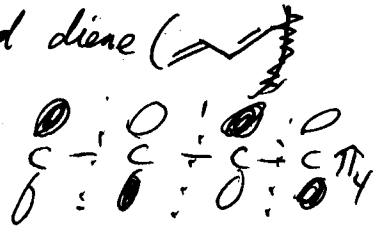
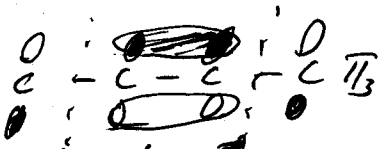
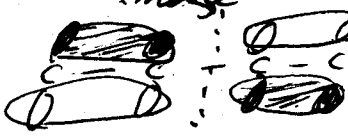
2) Spatial distribution of e^-'s

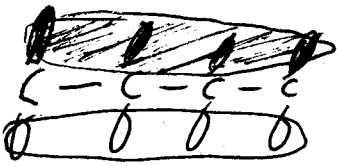


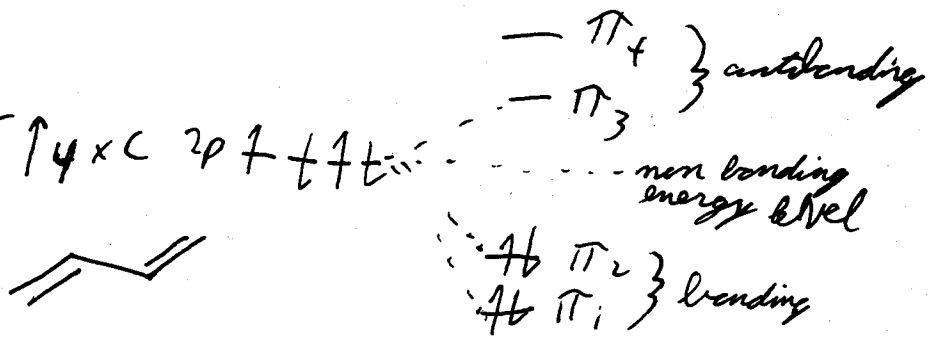
Extend this MO analysis to conjugated diene (for ex.)









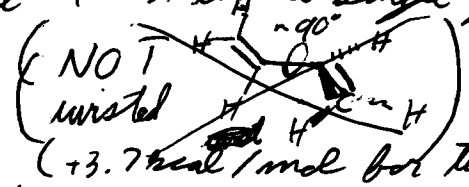


- Note: # of ⊥ nodes increases as we move up. More ⊥ nodes => higher energy (e's don't like confinement)
- Significance of π_1: $H_2C=CH-CH-CH_2$
- Note: The drawing corresponds most closely to π_2
  - π_1 rationalizes energy stabilization

Structural consequences of π_1 (delocalized over 4C)

- Conformational preferences of conjugated diene
  - prefer to have all 4 C's in a single plane ("planar")

or



UV spectroscopy § 15.2 → ignore