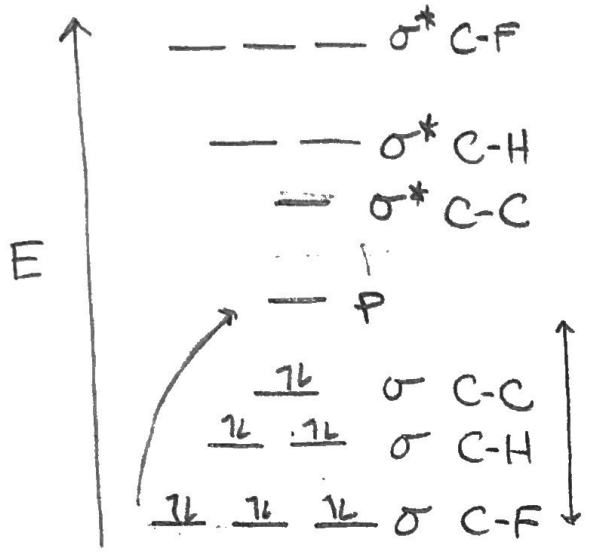
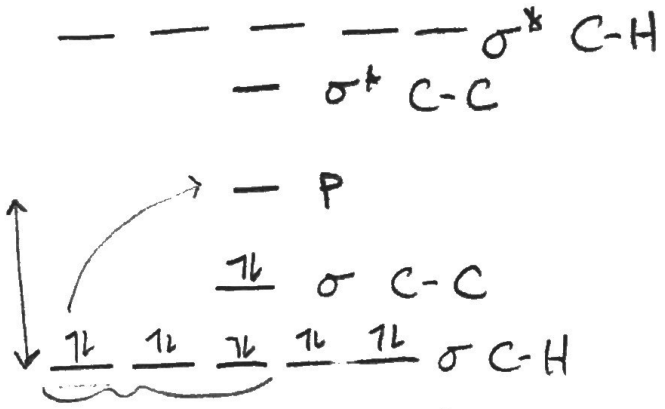
Intro to MO Theory - HW Solns

D.1 $F_3C-\overset{\oplus}{C}H_2$ $H_3C-\overset{\oplus}{C}H_2$



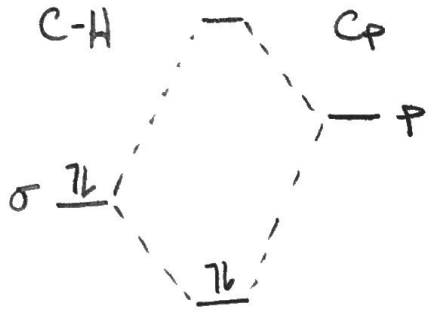


Can participate in hyperconjugation

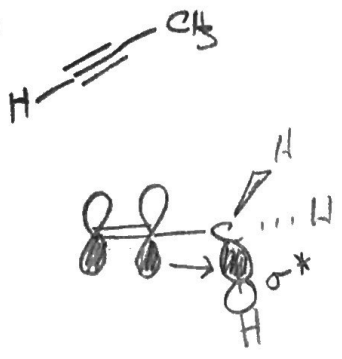
Smaller energy gap = better interaction

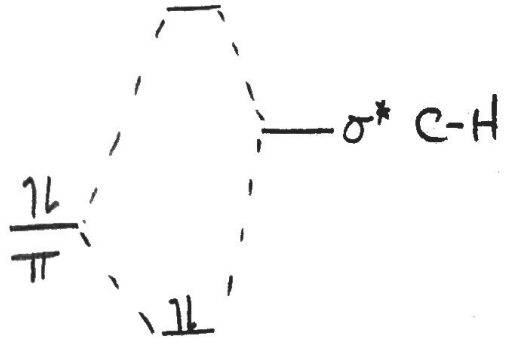
The hyperconjugation is better in $H_3C-\overset{\oplus}{C}H_2$ than in $F_3C-\overset{\oplus}{C}H_2$

MO Interaction:

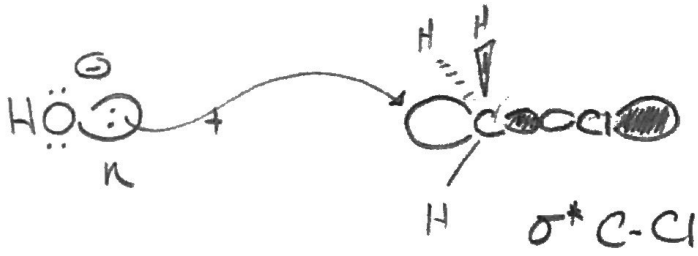


D.3



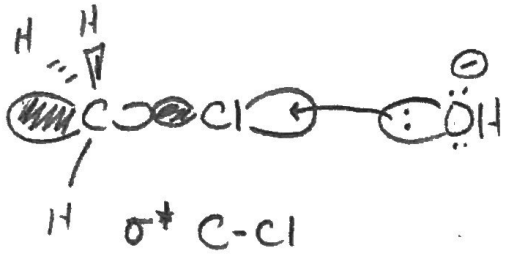


D.5



Correct approach to σ^* at the C

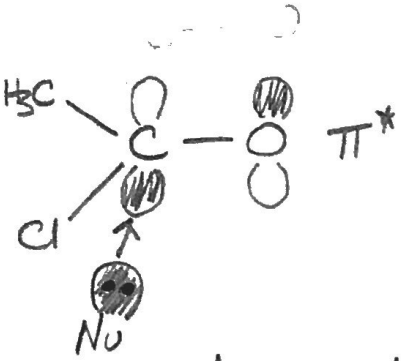
It is allowed (constructive orbital overlap) for $HO^{\ominus}$ to approach σ^* from the Cl side



This does not happen, however, due to electrostatics.

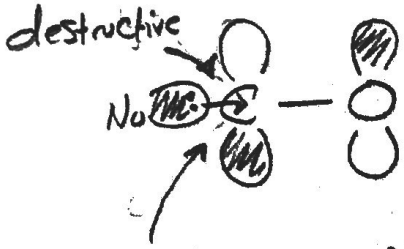
This is a site of high e⁻ density reacting with another site of high e⁻ density, which is not favorable.

D.7 Nu will react with the LUMO, which is the π^* orbital



preferred approach

If nu approaches directly along the C=O bond



Constructive

no net gain = does not occur

D.8

11 σ* orbitals

— π*

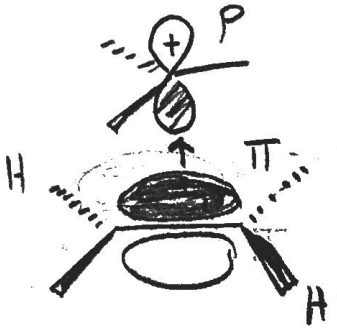
12 σ* orbitals

— p LUMO

HOMO — π

11 σ orbitals

12 σ orbitals



Constructive interaction