(10) **Today**

Competition between S_N1, E1, S_N2, and E2

Chap 12: Mass Spectrometry Introduction

Next Class (11)

pseudo-Monday

Chap 12: Mass Spectrometry and Infrared Spectroscopy

(12) **Second Class from Today**

Chap 12: Mass Spectrometry and Infrared Spectroscopy

Third Class from Today (13)

Test 1 on Chap 11

S_N2/E2

- strong base
  good nucleophile
- α-C 3° no S_N2
  only E2 possible
- α-C 2° ... it depends
  on the Nu/base
  access is only so so, so
  strong bases do E2
- α-C 1° S_N2
  preferred
  for elimination add heat

S_N1/E1

weak base
so so Nu

3°, 2° ... a mix

S_N1 + E1

/ \

cold hot

1° not possible

Conjugate Acid	pK_a	Nucleophile
HI	–10	I^-
HBr	–9	Br^-
HCl	–7	Cl^-
$CH_3OH_2^+$	–2.5	CH_3OH
H_3O^+	–1.7	HOH
HF	3.2	F^-
H_2S	7.0	HS^-
$HC{\equiv}N$	9.1	$^-C{\equiv}N$
NH_4^+	9.4	NH_3
CH_3CH_2SH	10.5	$CH_3CH_2S^-$
CH_3OH	15.5	CH_3O^-
HOH	15.7	HO^-
HCCH	25	HCC^-

weak bases S_N2 on 2° α-C

$S_N1/E1$

SO SO

SO SO

SO SO

weak bases S_N2 on 2° α-C

strong bases

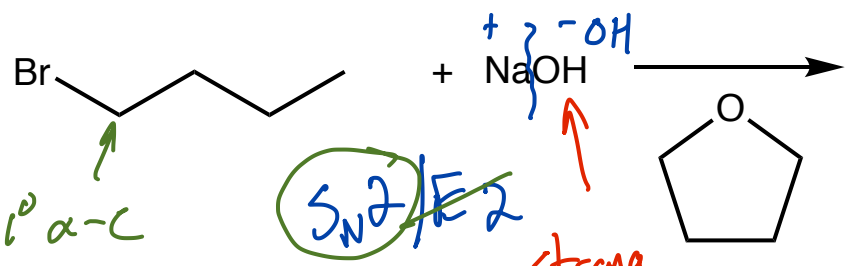
E2 on 2° α-C

good Nu

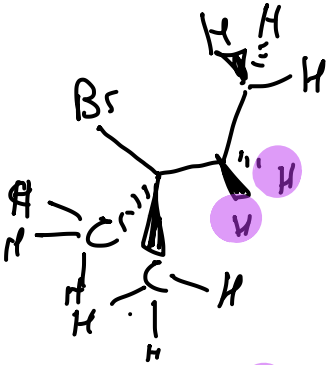
Competition

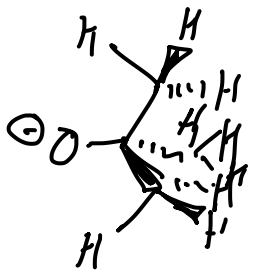
1. bimolecular or unimolecular
good Nu
strong base
so so
weak base

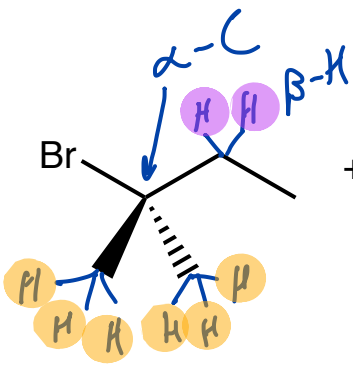
2. α-C?
1° → S_N2 unless Δ
3° → E2
2° strong base? yes E2
NaBr no S_N2

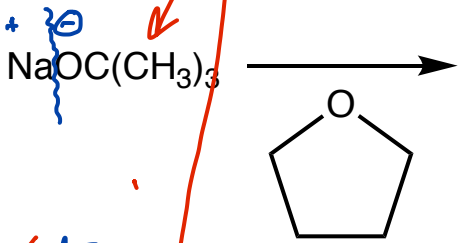


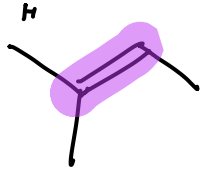
strong base



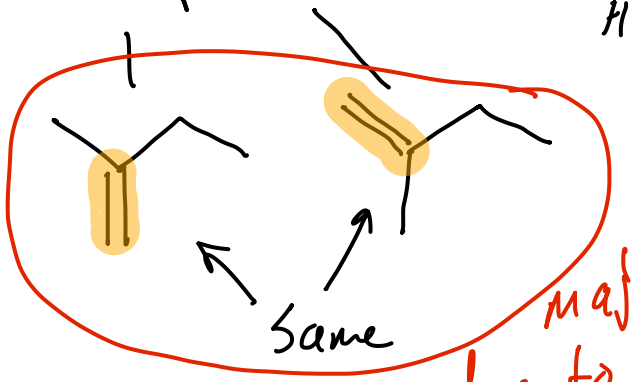






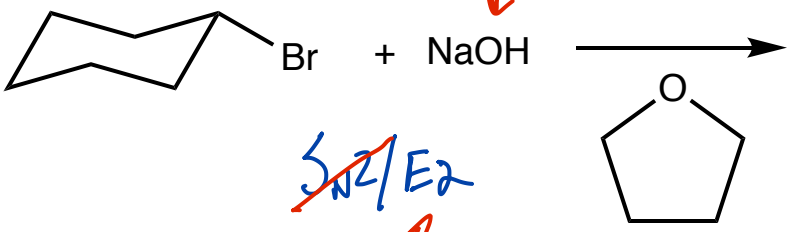


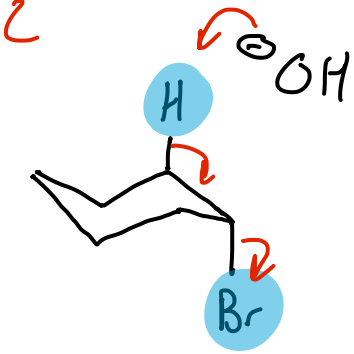
2-methyl-1-butene

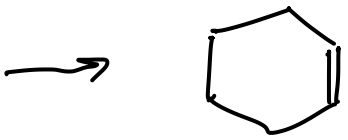


major due to big base exception

S_N2 not possible at 3° α-C







H_2O

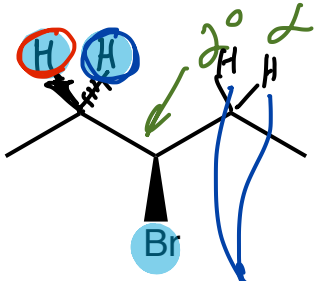
NaBr

S_N2/E2

strong base forces E2 on 2° α-C

1. "bi" or "uni" 2. α-C ?

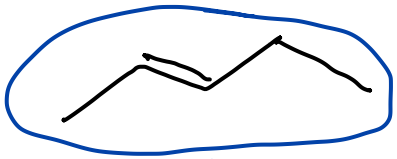
Competition



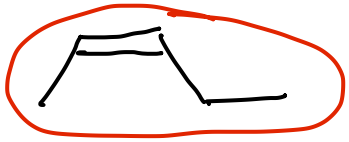
2° α-C + strong base so E2

+ NaOH → (EtOH)

S_N2/E2



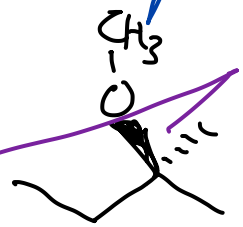
more stable major product



these do get removed but the same products form

3° α-C. S_N can form

+ CH_3OH →



same! C is not chiral

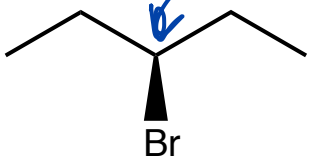
$H^{\oplus}$ $Cl^{\ominus}$

S_N1/E1

weak base so SO Nu

no added heat predominates

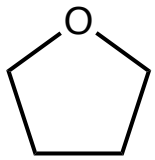
so substitution even though $HOCH_3$ could come in from the front, it would make the same product, so just draw one



2° α-C

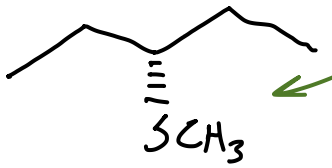
+ $^{\ominus}SCH_3$

+ $NaSCH_3$ →



S_N2/E2

good Nu weak base



only this stereoisomer forms