Chapter 11
Organic Reactions
Substitution-Elimination
Summary

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S_N2 or S_N1?

	S_N2	S_N1
Substrate	Primary or methyl	Tertiary
Nucleophile	Strong nucleophile	Weak nucleophile (may also be solvent)
Solvent	Polar aprotic solvent	Polar protic solvent, silver salts
Kinetics	[substrate][Nu]	[substrate]
Stereochemistry	Inversion	Racemic mixture
Rearrangement	No	Yes

Conditions of Elimination

Condition	E1	E2
Mechanism	1^{st} order	2^{nd} order
Rate	Dependent on only one chemical – the substrate	dependent on two chemicals – the substrate and Nu^-
Substrate	should form a stable carbocation	should be 1^o for better results
Nucleophile	Not dependent of Nu	should be strong base to cause elimination
Solvent	polar	Non polar
Competes	With SN1	With SN2
Stereochemistry	Not stereospecific (gives Zaitsev's product)	Stereospecific (needs the H and leaving group to be in anti periplanar)

Substitution or Elimination?

	Substitution	Elimination
Nucleophile strength	Strong Nu but weak base – S_N2	Strong Nu – E2
Nucleophile size	Small	Bulky
Substrate	Primary – S_N2	Tertiary - S_N1, E1 or E2
Temperature		Higher temp - > more E

E2 vs S_N2

3° halide and bulky base promote E2

E1 vs S_N1

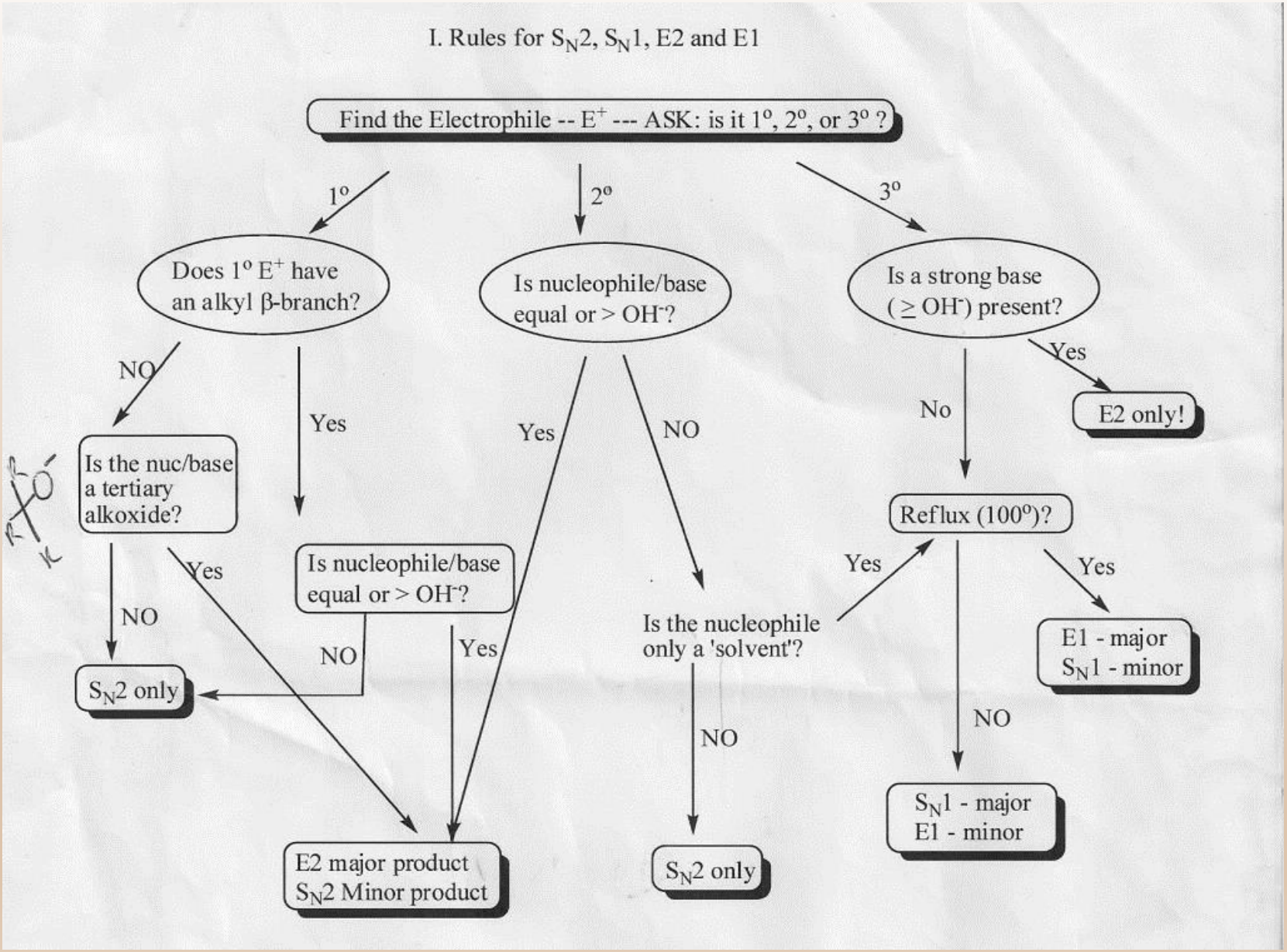
High heat promotes E1

Types of Alkyl Halides

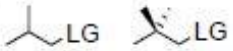
1° – will almost always give S_N2

2° – primarily S_N2 except when using a bulky base

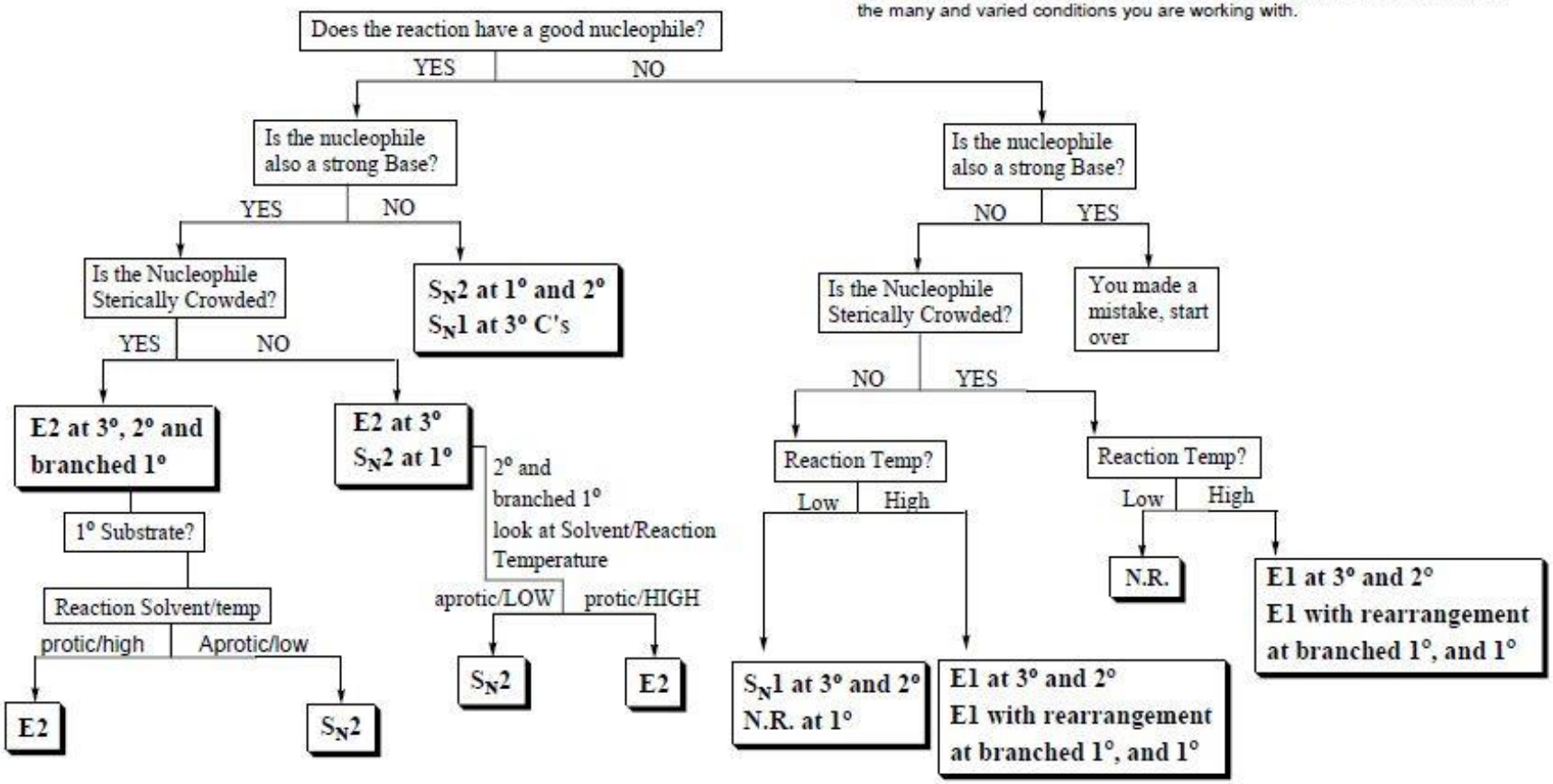
3° – S_N1, E1 or E2. Strong base and high temperature promotes E


I. Rules for S_N2, S_N1, E2 and E1
Find the Electrophile -- E^+ --- ASK: is it 1°, 2°, or 3° ?
1°
2°
3°
Does 1° E^+ have an alkyl β-branch?
Is nucleophile/base equal or > OH^-?
Is a strong base (≥ OH^-) present?
NO
Yes
Yes
NO
Yes
No
E2 only!
Is the nuc/base a tertiary alkoxide?
Reflux (100°)?
Yes
Is nucleophile/base equal or > OH^-?
Yes
Yes
Is the nucleophile only a 'solvent'?
NO
Yes
E1 - major
S_N1 - minor
NO
S_N2 only
NO
Yes
NO
S_N1 - major
E1 - minor
E2 major product
S_N2 Minor product
S_N2 only

A Simple Flow Chart Diagram

1) Identify the Substrate (it's the one with the leaving group!!)
2) identify the Nucleophile/Base (Its the one with the lone pair of electrons and/or the negative charge)
3) Define good Nucleophile as any nucleophile with a full negative charge
4) Define sterically hindered as secondary or tertiary
5) Define strong base as anion on Oxygen, Nitrogen, or Carbon
6) Branched 1^{o} = 

Caveat: Thius will help predict the major product of a particular reactions. This does NOT mean it will be the only product formed, but only will help you consolidate the many and varied conditions you are working with.



Key Words/Concepts

- Substitution Reaction
- Elimination Reaction
- Nucleophile
- Electrophile
- Leaving group
- 1^{st} order reaction (unimolecular)
- 2^{nd} order reaction (bimolecular)
- Transition state
- Rate determining step
- Carbocation
- Polar protic solvent
- Polar aprotic solvent
- Non polar solvent
- Solvolysis