$S_N 1? E1? S_N 2? E2? How Will I Know??$



What are the reactions?

Compare each of the criteria on this chart. See which reaction has the most factors going for it.

	S _N 1	E1	S _N 2	E2
Reaction mechanism	2-step w/ a carbocation	2-step w/ a carbocation	Concerted	Concerted
Strength of nucleophile	Can be mediocre, must be non-basic	Can be mediocre, must be basic	Strong, non-basic, non- bulky	Strong AND basic
Leaving group ability	Must be great	Must be great	Can be mediocre	Can be mediocre
Solvent	Polar Protic	Polar Protic	Polar aprotic	Polar aprotic
Primary Substrate	No reaction	No reaction	Highly favored	Favored only w/ a strong base
Secondary substrate	Only w/ a non-basic nucleophile or if the carbocation is resonance stabilized	Only if the carbocation is resonance stabilized	Need strong non-basic nucleophile, otherwise will compete with E2	Favored with strong base
Tertiary substrate	Favored with non-basic nucleophile	Competes with SN1	No reaction	Can occur but ONLY with a strong base
Stereochemistry	gives (almost) totally racemic product, see #2 below	Bulky groups will prefer opposite sides	Walden inversion	"H" must be able to go antiperiplanar

What are the leaving groups?

Great: I-, Br- Cl- OTs-, OCF₃-, OMs⁻, and H₂O (not OH⁻)

Mediocre: F, CH₃COO, NH₃, (not NH₂-)

Bad: OH-, OCH₃, NH₂

What are the solvents?

Polar Protic: Acetic acid, H2O, ROH, NH₃.

Polar Aprotic: DMF, nitromethane, acetone, acetonitrile, DMSO, ethyl

acetate.

Non-polar: alkanes, cycloalkanes, toluene, benzene, ether.

What are the nucleophiles?

VERY GOOD Nu: I-, HS-, RS-Good Nu: Br-, HO-, RO-, CN-, N₃-

Fair Nu: NH₃, Cl⁻, F⁻, RCO₂⁻

Weak Nu: H₂O, ROH VERY Weak Nu: RCO₂H What are the bases?

Very Strong: NH₂, H, HC≡C Strong: RO-, HO-,

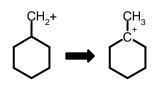
Mediocre: RNH₂, Na₂CO₃

Weak: NH₃, CN⁻, RCOO⁻, Cl⁻, Br⁻,

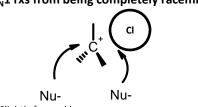
I⁻, NaHCO₃

And don't forget....

1) Carbocations WILL rearrange if they can

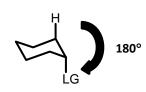


2) Solvent-Separate Ion Pairs (SSIP) Keep S_N1 rxs from being completely racemic



Slightly favored here

3) E2 need antiperiplanar H's, or no rxn.



Will rearrange to a more stable cation.

The leaving groups partially blocks one face, keeping it from being totally racemic.

Must be able to rotate the H into a 180° angle or no rxn. Can happen with rings sometimes.