

Theoretical Aspects Of Physical Organic Chemistry: The SN2 Mechanism

	SN2	SN1	E2	E1
rate law	rate = k[substrate][nucleophile]	rate = k[substrate]	rate = [substrate][base]	rate = k[substrate]
stereochemistry	inversion occurs at site of the substitution	full or partial racemization	anti periplanar loss of H and leaving group	stereochemistry is lost
substrate effect on the rate	Works well (fast) for CH3 and primary substrates; very slow for tertiary substrates so E2 faster; secondary substrate successful with good nucleophile that is not strongly basic.	Fastest for tertiary and secondary allylic or tertiary allylic substrate; extremely slow (fails) for primary substrates; slow with secondary substrate.	Faster than SN2 with tertiary substrate; slower than SN2 with primary substrate; faster than SN2 when strong base used with secondary substrate.	Fastest for tertiary and secondary allylic or tertiary allylic substrate; extremely slow for primary substrates; slow with secondary substrates. (See temperature.)
leaving group effect on rate	sulfonate > I- > Br- > Cl- > H2O (H2O is lost from alcohols) :OH-, :H-, :NH2-, :F-, etc FAIL	I- > Br- > Cl- > H2O (H2O loss from tertiary alcohols is common.) :OH-, :H-, :NH2-, :F-, etc FAIL	Br- > Cl-; sulfonate favors SN2 (H2O loss from alcohols cannot occur under the alkaline conditions) :OH-, :H-, :NH2-, :F-, etc FAIL	Most common is tertiary halide or water from secondary or tertiary in dehydration with hot acid.
nucleophile/base effect on rate	I- > Br- > Cl- > SH- > OH- > CH3- > NH2- > OH- > OCH3 > F- (This group favors E2 with secondary substrates.) HS-, CH3S-, :CN, RSP-, etc. give SN2 with secondary substrate	Rate independent of nucleophile concentration, but more of product come from better nucleophile. Any nucleophile more basic than HCO3- give E2 rather than SN1.	Faster with stronger base. Use anion of first row element to favor E2 over SN2 with secondary substrate. Any anion more basic than HCO3- gives E2 with tertiary substrate.	Rate independent of base strength When strong base present the reaction will occur by E2.
solvent effect on rate	Rate accelerated by use of polar aprotic solvent such as DMSO or DMF.	Requires polar protic solvent to form the carbocation intermediate	Favored by polar protic solvent, especially with secondary substrates, so that competing SN2 is slowed.	Requires polar protic solvent to form the carbocation intermediate.
temperature effect on rate	Rate is increased at higher temperature but less than rate of E2. Use lowest temperature that gives satisfactory reaction rate.	Rate is increased at higher temperature, but not as much as rate of competing E1. Use lowest temperature that will give ionization.	Rate is increased at higher temperature much more than is the rate of a competing SN2 reaction.	Rate is increased at higher temperature much more than is the rate of a competing SN1 reaction.

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