

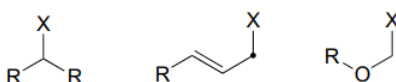
## 8.7: SN1 or SN2? Predicting the Mechanism

First of all, it is important to understand that the  $S_N1$  and  $S_N2$  mechanism models are just that: models. While many nucleophilic substitution reactions can be described as proceeding through 'pure'  $S_N1$  or  $S_N2$  pathways, other reactions - in particular some important biochemical reactions we'll see later - lie somewhere in the continuum between the  $S_N1$  and the  $S_N2$  model (more on this later). With that being said, here are some guidelines to help you predict whether a reaction is likely to have more of an  $S_N1$  or  $S_N2$  character.

First, look at the electrophile: as stated above, an  $S_N1$  reaction requires that a relatively stable carbocation intermediate be able to form. An  $S_N2$  reaction requires a relatively unhindered electrophilic center. Therefore, methyl and primary carbon electrophiles will react by the  $S_N2$  pathway, and tertiary carbon electrophiles will react by the  $S_N1$  pathway.

Secondary carbon electrophiles, or primary carbon electrophiles adjacent to a potential carbocation-stabilizing group (double bond or heteroatom) can react by either or both pathways. The reasoning here is that these electrophiles are unhindered (favoring  $S_N2$ ), but can also form stabilized carbocation intermediates (favoring  $S_N1$ )

Can react by  $S_N1$  or  $S_N2$



Next, look at the nucleophile. More powerful nucleophiles, particularly anionic nucleophiles such as hydroxides, alkoxides or thiolates, favor an  $S_N2$  pathway: picture the powerful nucleophile 'pushing' the leaving group off the electrophile. Weaker, uncharged nucleophiles like water, alcohols, and amines, favor the  $S_N1$  pathway: they are not nucleophilic enough to displace the leaving group, but will readily attack a carbocation intermediate.

Finally look at the solvent in the reaction. As a general rule, water and other protic solvents (for example methanol or ethanol) favor  $S_N1$  pathways, due to the ability of the solvents to stabilize carbocation intermediates, combined with their tendency to weaken the nucleophile by enclosing it in a 'solvent cage'. In laboratory reactions, the presence of a polar aprotic solvent such as acetone or dimethylformamide points to the probability of an  $S_N2$  reaction.

### Factors favoring the two pathways

#### Factors favoring the $S_N1$ pathway:

- hindered electrophile
- potential for a tertiary, secondary, or resonance-stabilized carbocation intermediate
- uncharged nucleophile
- protic solvent such as water

#### Factors favoring the $S_N2$ pathway:

- Unhindered (methyl or primary) electrophile
- powerful, anionic nucleophile
- polar aprotic solvent

[Video tutorial: nucleophilic substitution reactions](#)

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