

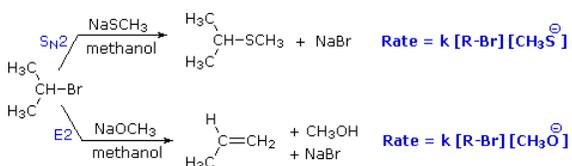
## 8.4: The E2 Mechanism

E2, bimolecular elimination, was proposed in the 1920s by British chemist Christopher Kelk Ingold. Unlike E1 reactions, E2 reactions remove two substituents with the addition of a strong base, resulting in an alkene.

### Introduction

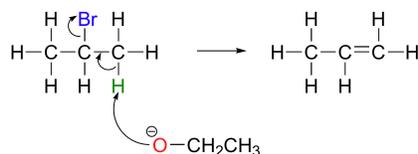
E2 reactions are typically seen with secondary and tertiary alkyl halides, but a hindered base is necessary with a primary halide. The mechanism by which it occurs is a single step **concerted** reaction with one transition state. The rate at which this mechanism occurs is second order kinetics, and depends on both the base and alkyl halide. A good leaving group is required because it is involved in the rate determining step. The leaving groups must be coplanar in order to form a pi bond; carbons go from  $sp^3$  to  $sp^2$  hybridization states.

To get a clearer picture of the interplay of these factors involved in a reaction between a nucleophile/base and an alkyl halide, consider the reaction of a 2°-alkyl halide, isopropyl bromide, with two different nucleophiles. In one pathway, a methanethiolate nucleophile substitutes for bromine in an  $S_N2$  reaction. In the other (bottom) pathway, methoxide ion acts as a base (rather than as a nucleophile) in an elimination reaction. As we will soon see, the mechanism of this reaction is single-step, and is referred to as the E2 mechanism.



### General Reaction

Below is a mechanistic diagram of an elimination reaction by the E2 pathway:

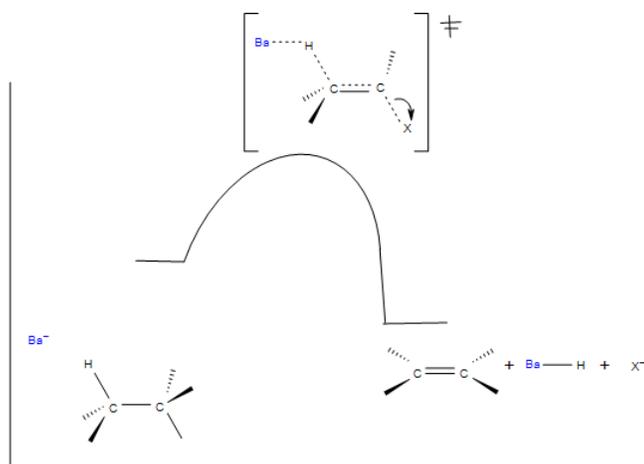


In this reaction Ba represents the base and Br represents a leaving group, typically a halogen. There is one transition state that shows the concerted reaction for the base attracting the hydrogen and the halogen taking the electrons from the bond. The product be both eclipse and staggered depending on the transition states. Eclipsed products have a synperiplanar transition states, while staggered products have antiperiplanar transition states. Staggered conformation is usually the major product because of its lower energy confirmation.

An E2 reaction has certain requirements to proceed:

- A strong base is necessary especially necessary for primary alkyl halides. Secondary and tertiary primary halides will proceed with E2 in the presence of a base ( $\text{OH}^-$ ,  $\text{RO}^-$ ,  $\text{R}_2\text{N}^-$ )
- Both leaving groups should be on the same plane, this allows the double bond to form in the reaction. In the reaction above you can see both leaving groups are in the plane of the carbons.
- Follows Zaitsev's rule, the most substituted alkene is usually the major product.
- Hoffman Rule, if a sterically hindered base will result in the least substituted product.

### E2 Reaction Coordinate



### The Leaving Group Effect in E2 Reactions

**As Size Increases, The Ability of the Leaving Group to Leave Increases:** Here we revisit the effect size has on basicity. If we move down the periodic table, size increases. With an increase in size, basicity decreases, and the ability of the leaving group to leave increases. The relationship among the following halogens, unlike the previous example, is true to what we will see in upcoming reaction mechanisms.



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