

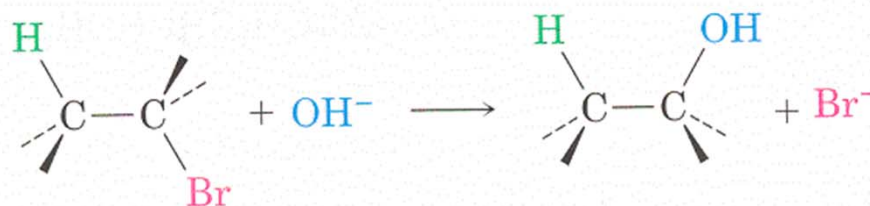
할로젠화 알킬의 제거반응

목차

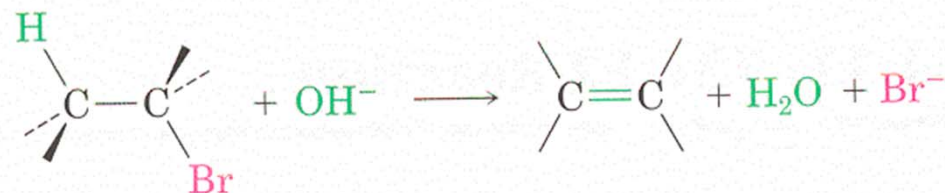
- 제거반응
- E2반응
- 제거반응과 Cyclohexane의 형태
- 중수소 동위원소 효과
- E1반응
- 요약

제거반응

Substitution



Elimination



이웃한 수소를 공격하여 HX를 제거하고 alkene
을 만드는 반응

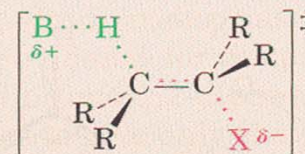
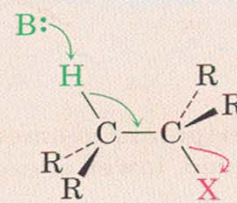
제거반응

Mechanism of the E2
reaction of an alkyl halide.
The reaction takes place
in a single step through a
transition state in which
the double bond begins
to form at the same time
as the H and X groups are
leaving.

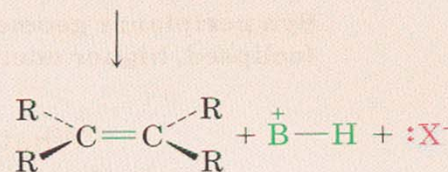
refer to
Mechanisms
& Movies

Base (B:) attacks a neighboring
hydrogen and begins to remove the
H at the same time as the alkene
double bond starts to form and the
X group starts to leave.

Neutral alkene is produced when
the C-H bond is fully broken and
the X group has departed with the
C-X bond electron pair.



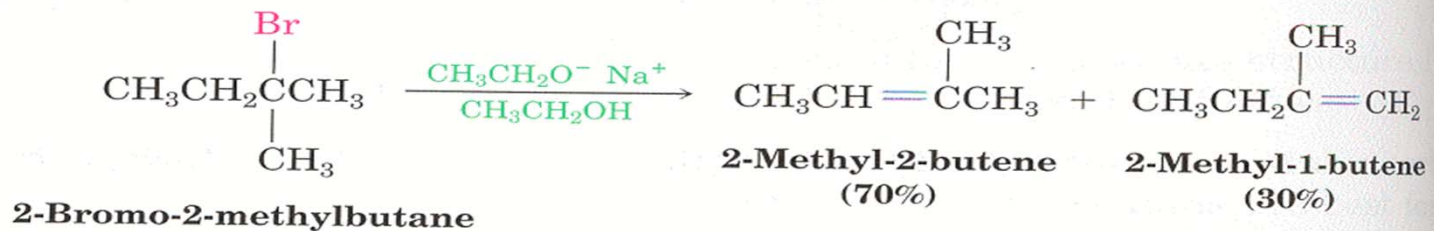
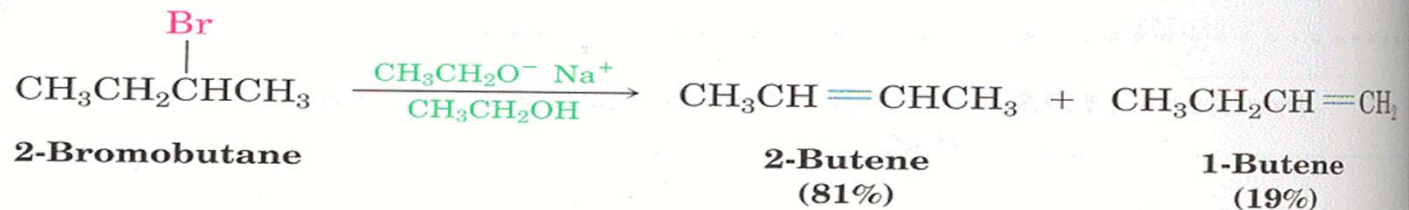
Transition state



Zaitsev의 규칙

- 할로젠화 알킬로부터의 HX 제거반응에서 치환이 많이 된 알켄이 주생성물이 된다.

Zaitsev's rule In the elimination of HX from an alkyl halide, the more highly substituted alkene product predominates.



E2 반응 (elimination, bimolecular)

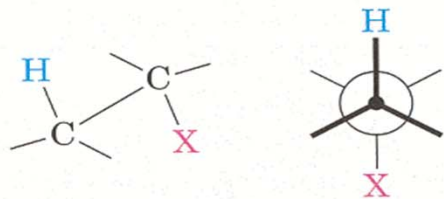
- 하이드록시 이온, 알콕시 이온과 같은 강한 염기와 반응시 일어남
- 준평면(periplanar) 기하구조로 반응함
- 이차반응 속도식을 보인다.

$$\text{반응속도} = k * [\text{RX}] * [\text{Base}]$$

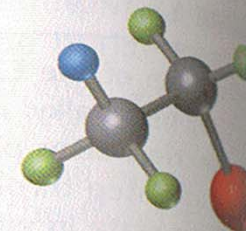
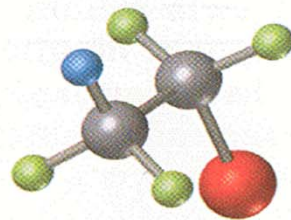
준평면 기하구조

- H와 X가 분자의 같은 쪽에 있는 신 준평면 (syn periplanar)
- H와 X가 분자의 반대쪽에 있는 안티 준평면 (anti periplanar)

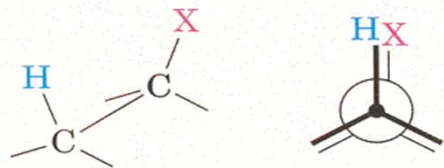
준평면 기하구조



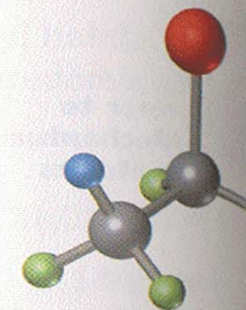
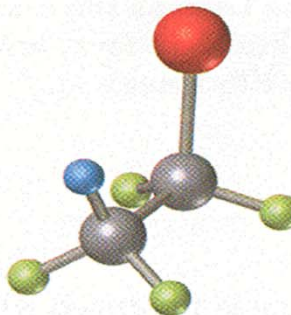
Anti periplanar geometry
(staggered, lower energy)



Stereo View



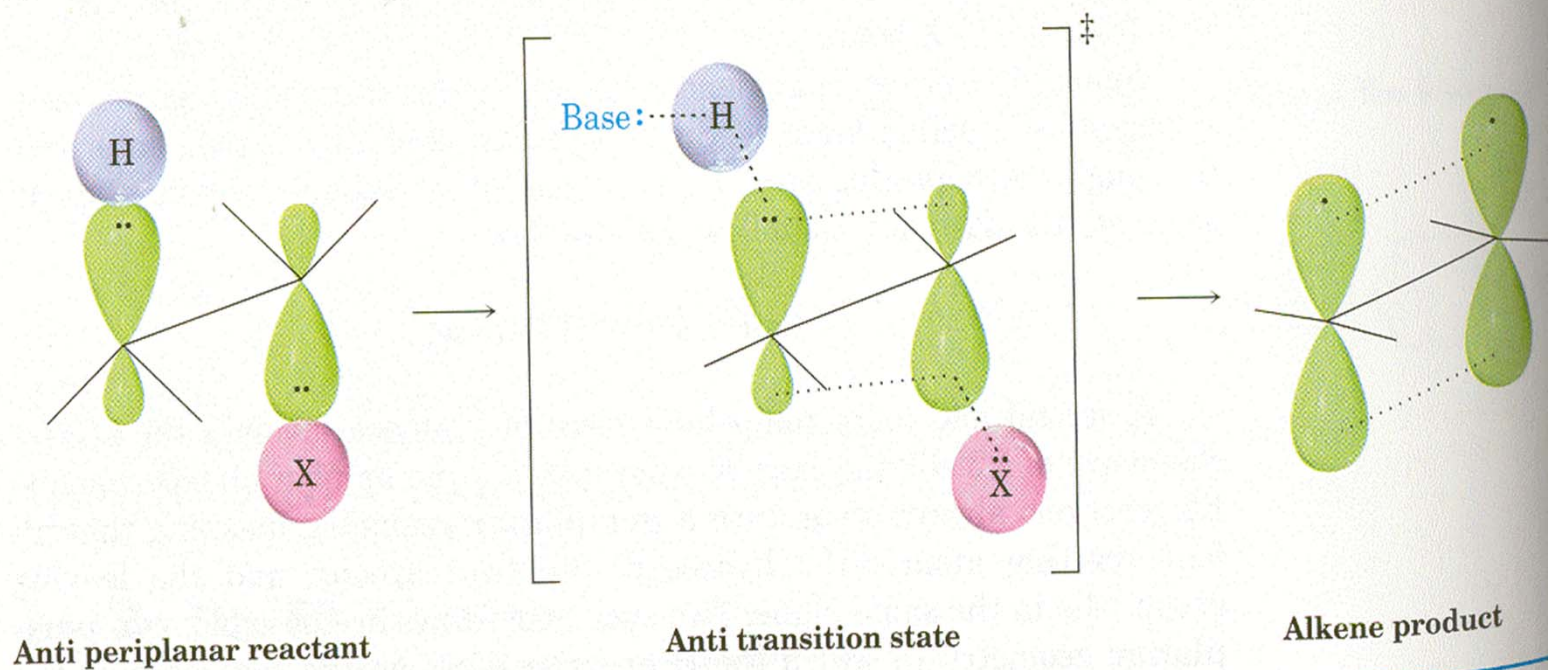
Syn periplanar geometry
(eclipsed, higher energy)



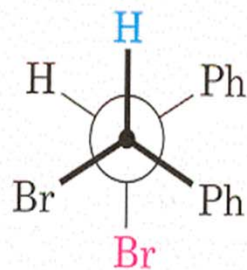
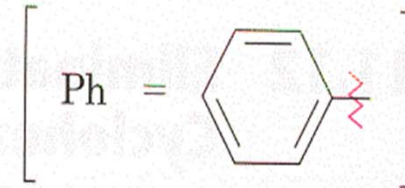
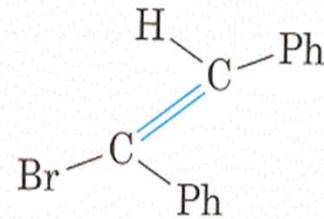
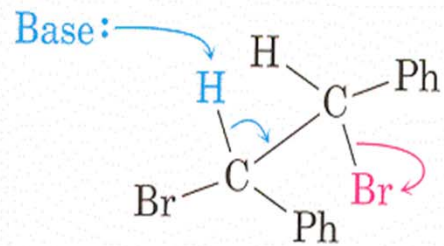
Stereo View

준평면 기하구조

The transition state for the E2 reaction of an alkyl halide with base. Overlap of the developing p orbitals in the transition state requires periplanar geometry of the reactant.



준평면 기하구조



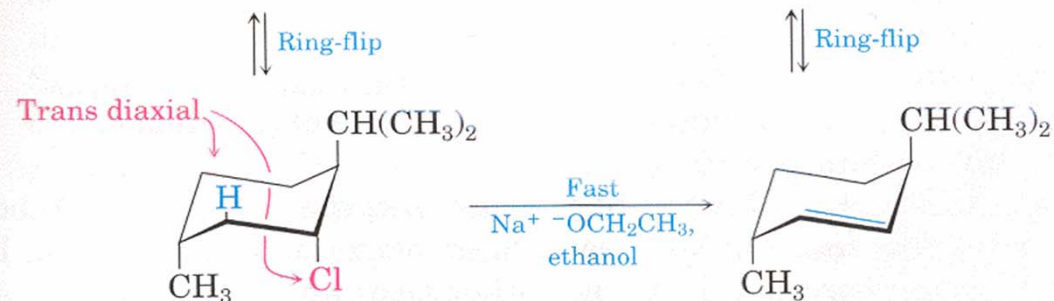
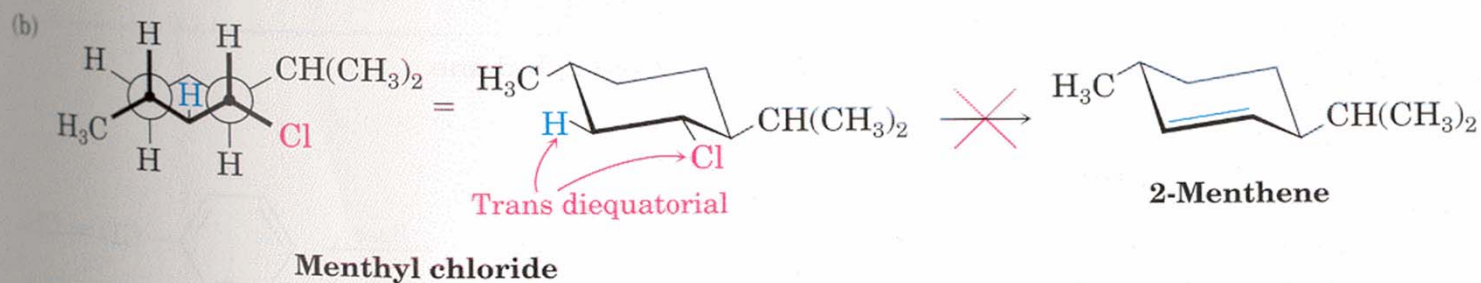
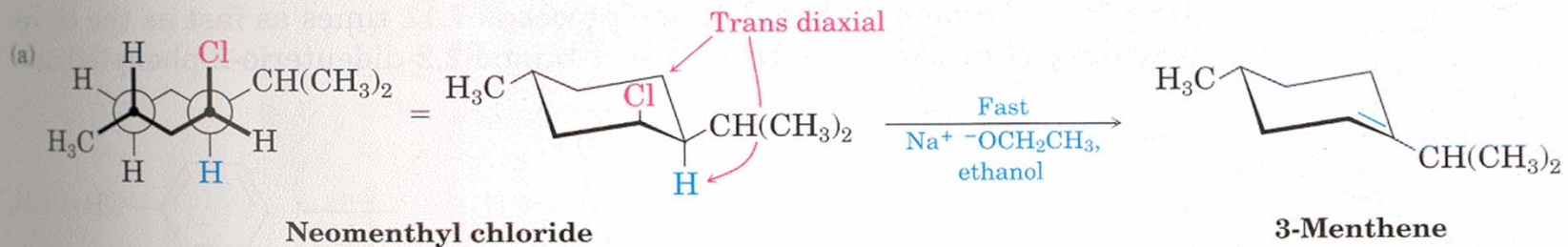
meso-1,2-Dibromo-
1,2-diphenylethane
(anti periplanar geometry)



(*E*)-1-Bromo-
1,2-diphenylethylene

제거반응과 Cyclohexane의 형태

Dehydrochlorination of menthyl and neomenthyl chlorides. (a) Neomenthyl chloride loses HCl from its more stable conformation, but (b) menthyl chloride must first ring-flip before HCl loss can occur.



중수소 동위원소 효과

Faster reaction



1-Bromo-2-phenylethane

Slower reaction



1-Bromo-2,2-dideuterio-2-phenylethane

Deuterium isotope effect:

같은 조건하에서 C-H결합은 C-D결합보
약하다

E1 반응 (elimination, unimolecular)

- 흔히 치환 반응 및 제거 반응 생성물의 혼합물로 얻어진다.
- 기하구조적 요건이 필요하지 않다.
- 중수소 동위원소 효과가 없다.
- 일차반응 속도식을 보인다.

$$\text{반응속도} = k * [\text{RX}]$$

E1 반응

Mechanism of the E1 reaction. Two steps are involved, the first of which is rate-limiting, and a carbocation intermediate is present.



refer to
Mechanisms
& Movies

Spontaneous dissociation of the tertiary alkyl chloride yields an intermediate carbocation in a slow, rate-limiting step.

Loss of a neighboring H^+ in a fast step yields the neutral alkene product. The electron pair from the C-H bond goes to form the alkene π bond.

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