

HALOGÉNEZETT SZÉNHYDROGÉNEK

Elnevezés

Nyíltláncú, telített

általános név: halogénalkán
alkil-halogenid

CH_3Cl
klórmétán
metil-klorid

$\text{CH}_3\text{CH}_2\text{Cl}$
klóretán
etil-klorid

$\text{CH}_3\text{CH}_2\text{CH}_2\text{Cl}$
1-klórpropán
propil-klorid

$\text{CH}_3\text{CH}(\text{Cl})\text{CH}_3$
2-klórpropán
izopropil-klorid

$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$
1-klórbután
butil-klorid

$\text{CH}_3\text{CH}_2\text{CH}(\text{Cl})\text{CH}_3$
2-klórbután
szek-butil-klorid

$\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{Cl}$
izobutil-klorid

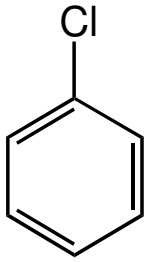
$\text{CH}_3\text{C}(\text{CH}_3)_2\text{Cl}$
terc-butil-klorid

Telítetlen

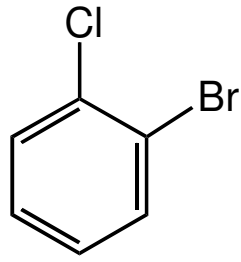
$\text{CH}_2=\text{CH}-\text{Cl}$
vinil-klorid

$\text{CH}_2=\text{CH}-\text{CH}_2-\text{Cl}$
allil-klorid

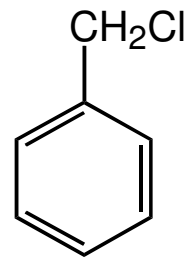
Aromás



klórbenzol

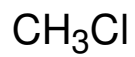


1-bróm-2-klórbenzol

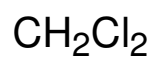


benzil-klorid

Többértékű



klórmétán
metil-klorid



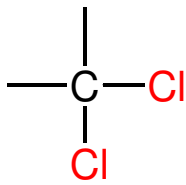
diklórmétán
metilén-klorid



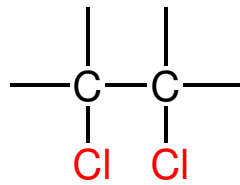
triklórmétán
kloroform



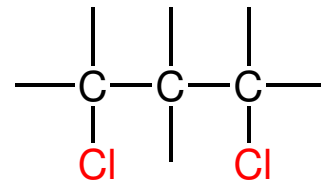
tetraklórmétán
szén-tetraklorid



geminális



vicinális



diszjunkt

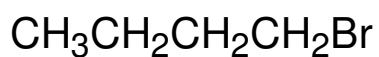
Kötésrendszer

	Kötéshossz (pm)	Kötési energia (kJ/mól)
C—F	141	488
C—Cl	177	326
C—Br	194	278
C—I	212	210

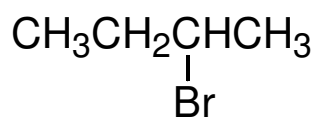
FIZIKAI TULAJDONSÁGOK

Forráspont (°C)

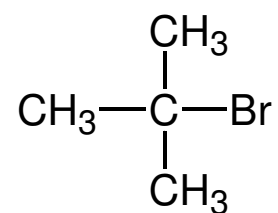
	F	Cl	Br	I
Me	-78	-24	-3	42
Et	-32	12	38	72



102 °C



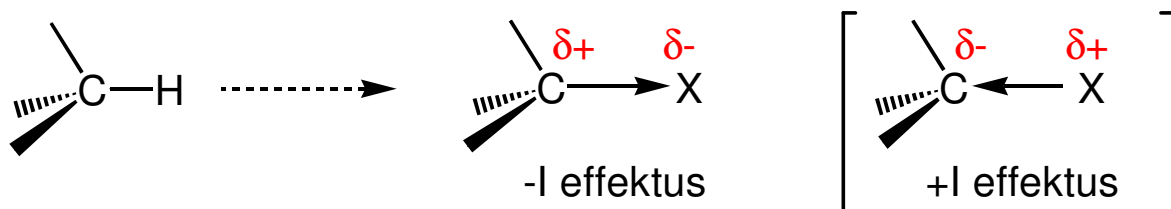
91 °C



73 °C

Dipólusmomentum

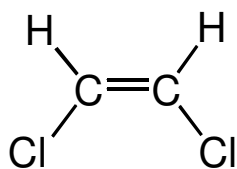
	C	H	F	Cl	Br	I
elektronegativitás	2.5	2.1	4.0	3.0	2.8	2.5



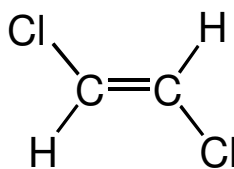
Példák

	CH ₃ F	CH ₃ Cl	CH ₃ Br	CH ₃ I
μ (D)	1.83	1.86	1.82	1.48

CH ₃ Br	CH ₃ CH ₂ Br	CH ₃ CH ₂ CH ₂ Br
1.82	1.88	1.93

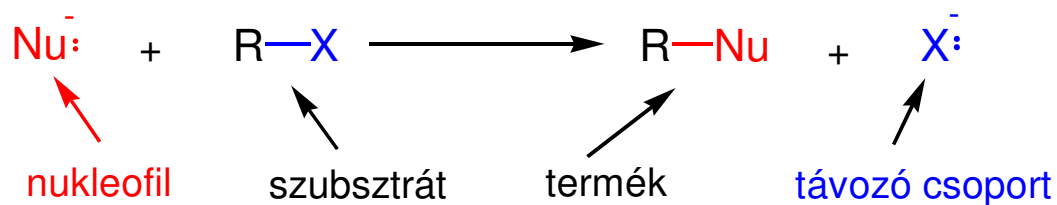


1.85

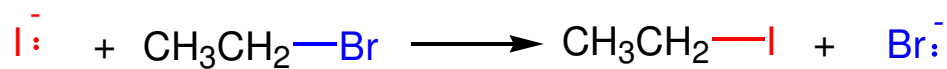
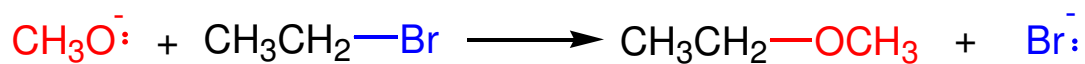
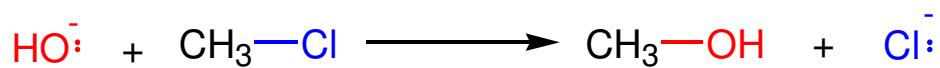


0

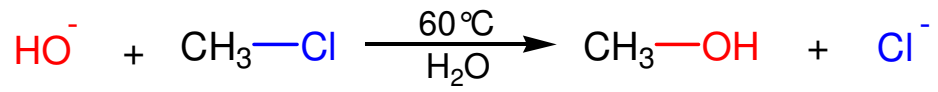
NUKLEOFIL SZUBSZTITÚCIÓS REAKCIÓK



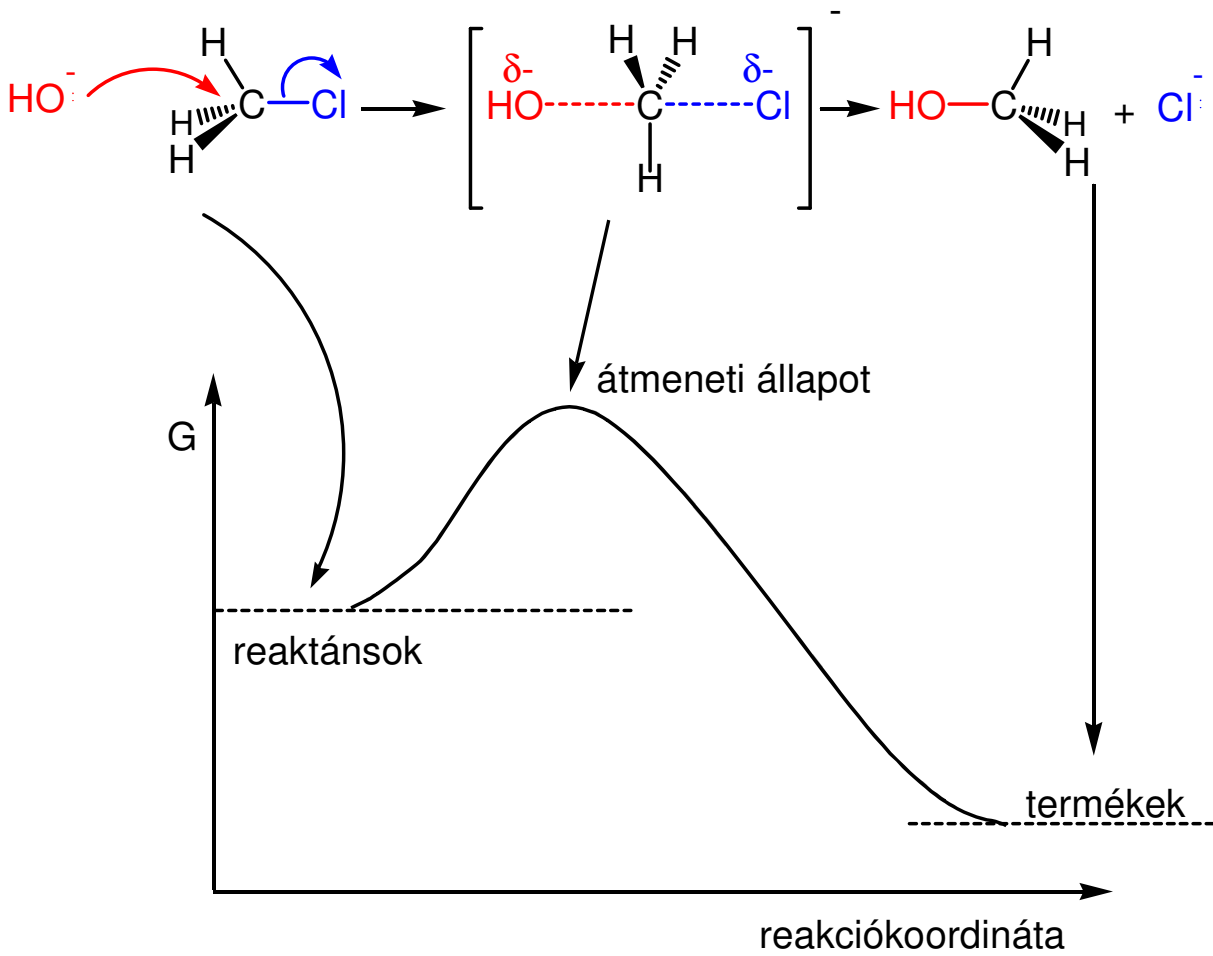
Példák



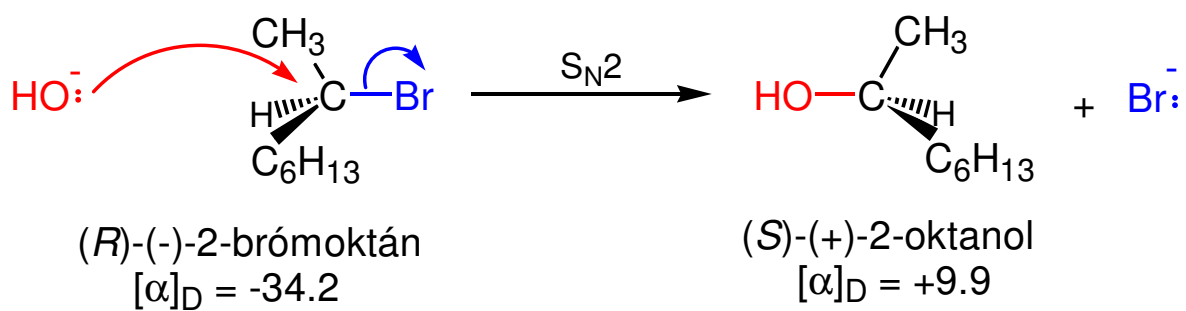
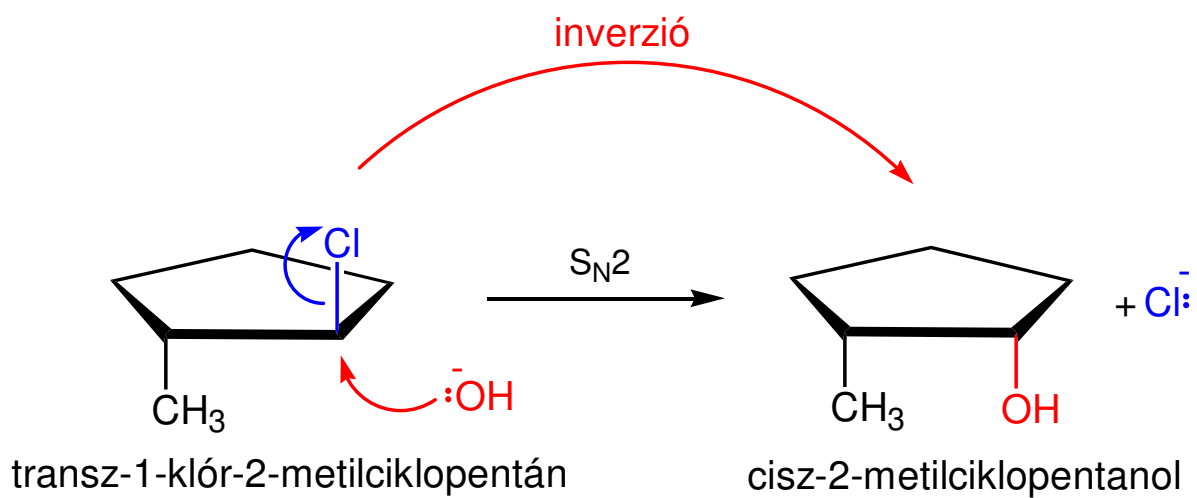
Az S_N reakciók mechanizmusa



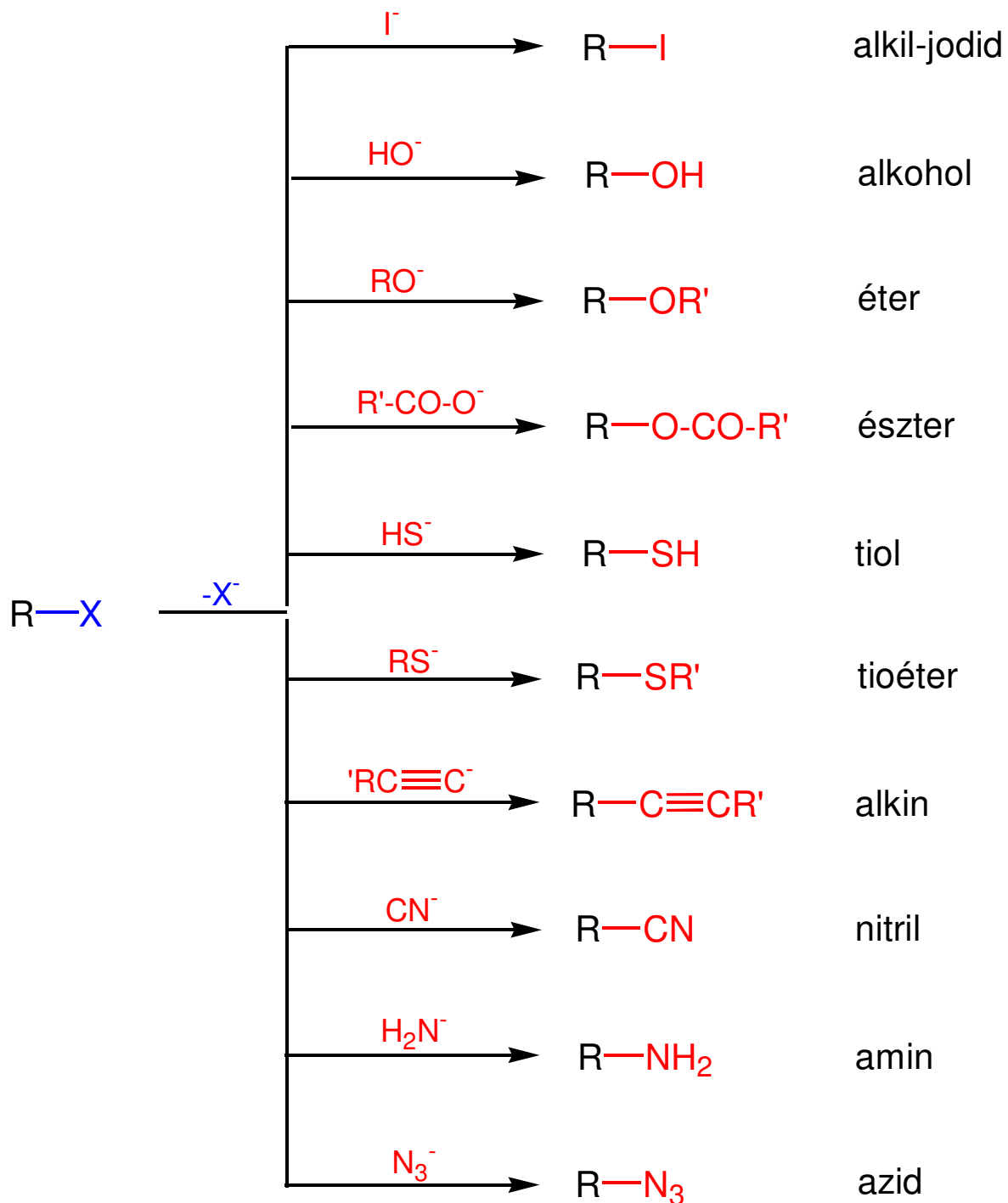
$$v = k[\text{CH}_3\text{Cl}][\text{OH}^-] \quad \text{-----} \rightarrow \boxed{\text{S}_{\text{N}}2}$$

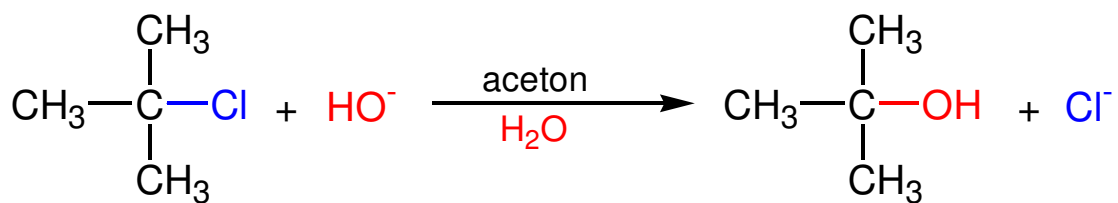


Az S_N2 sztereomechanizmusa

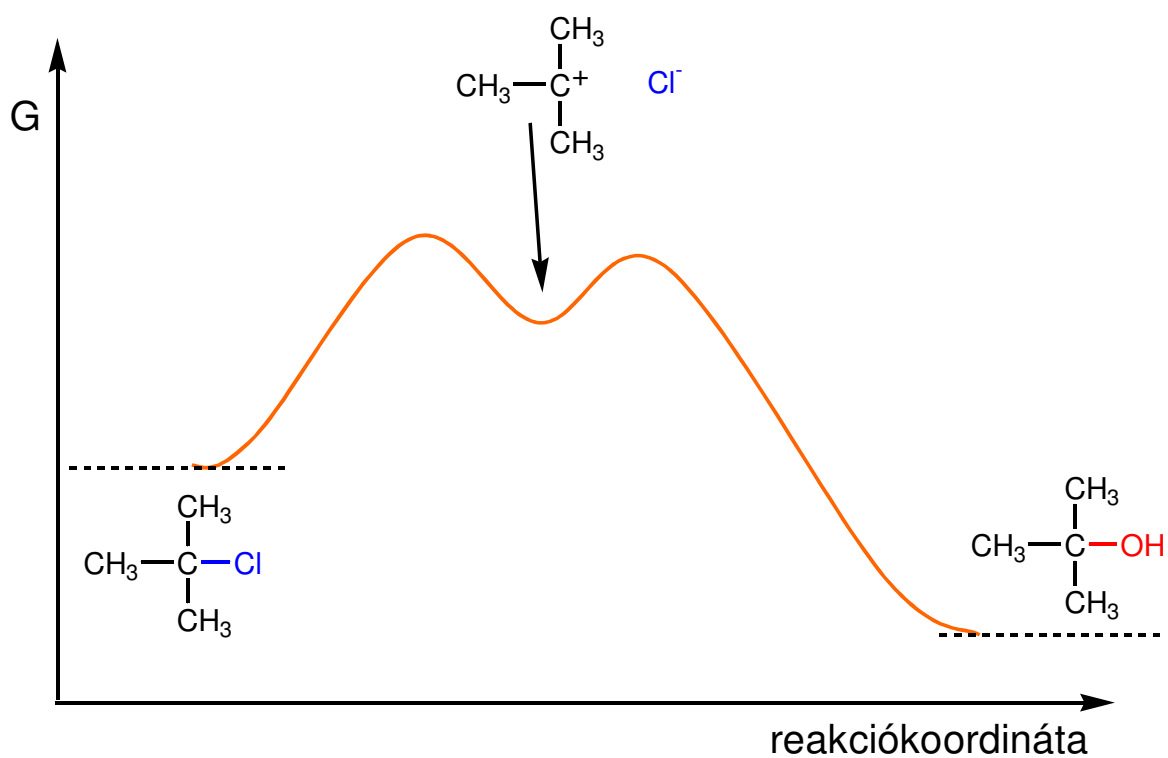
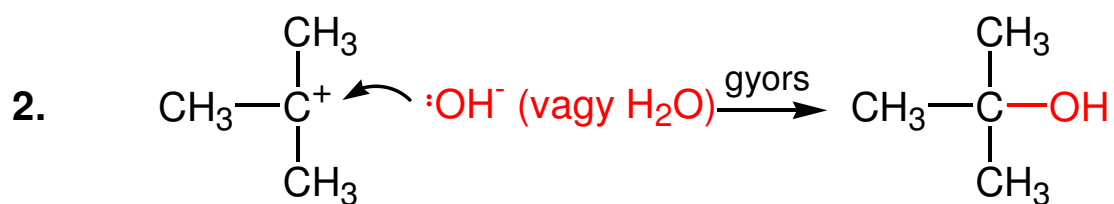
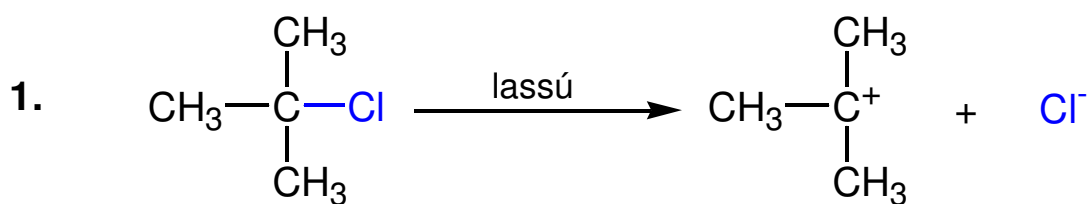


S_N2 reakcióval előállítható vegyületek típusai

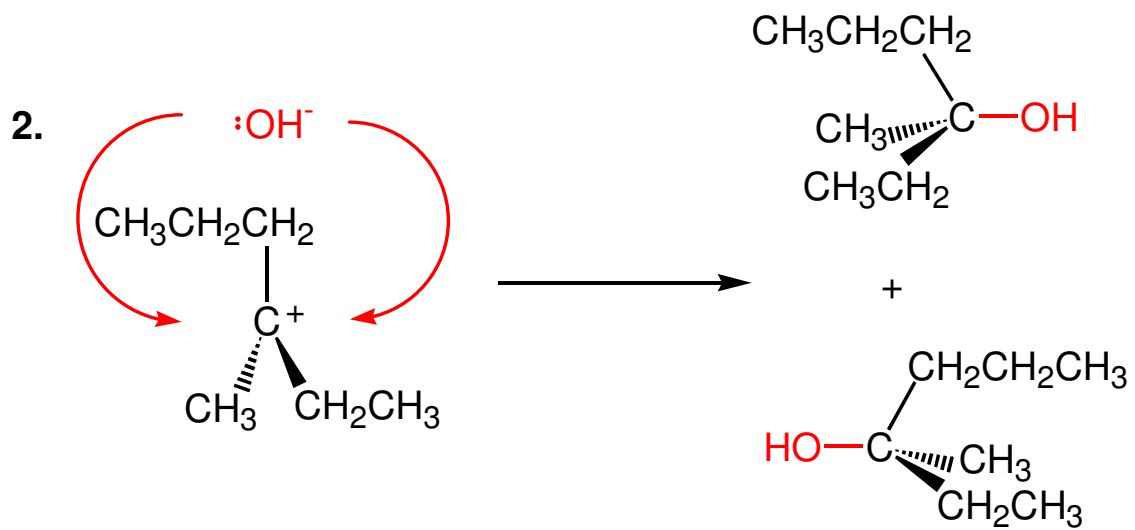
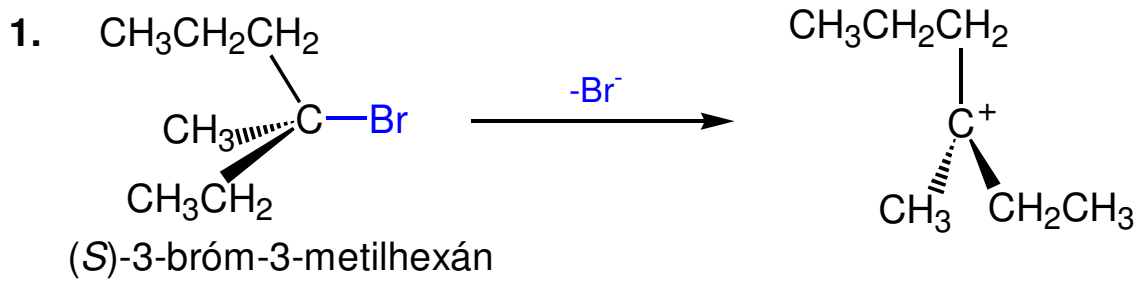




$$v = k[(\text{CH}_3)_3\text{CCl}] \longrightarrow \boxed{\text{S}_{\text{N}}1}$$

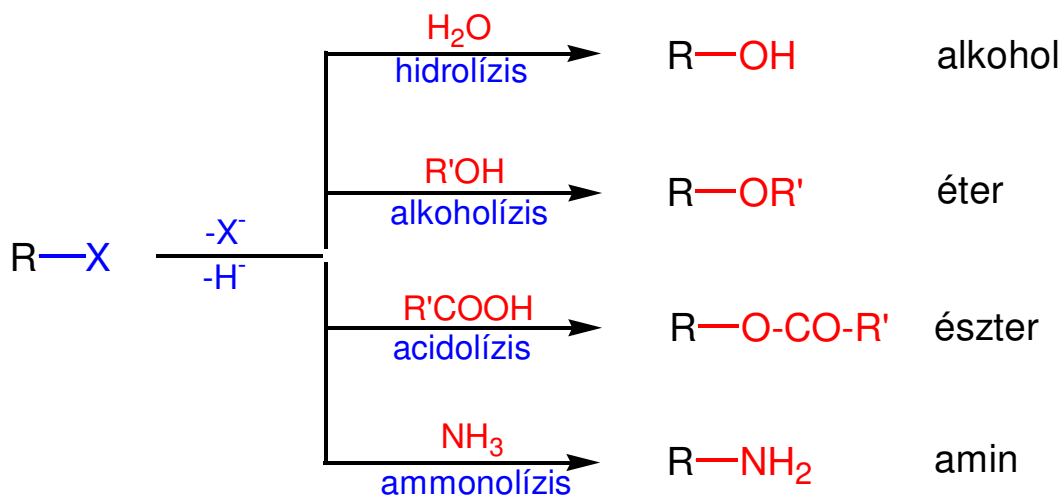


Az S_N1 sztereomechanizmusa

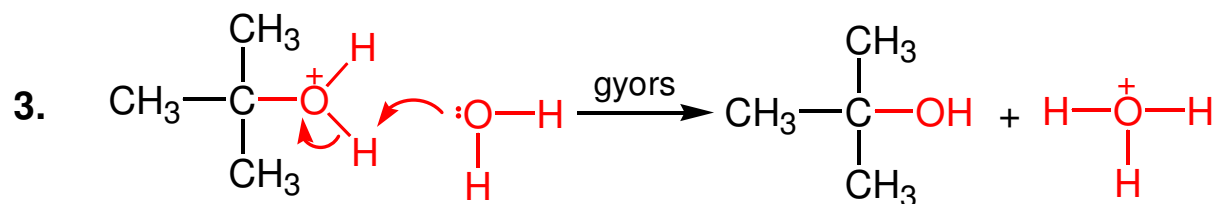
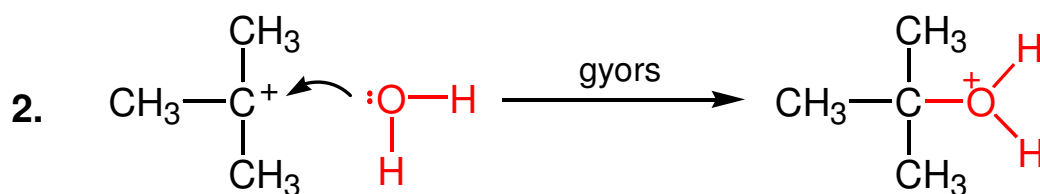
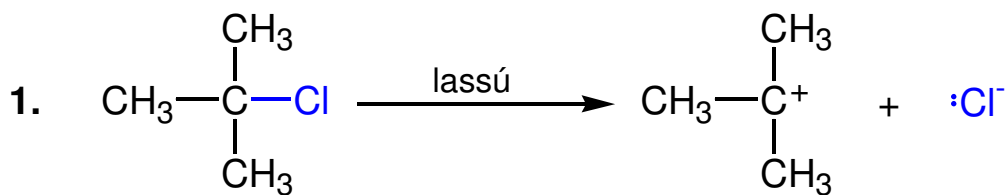


(S)-3-bróm-3-metilhexán $\xrightarrow{\text{racemizáció}}$ racém 3-metilhexán-3-ol

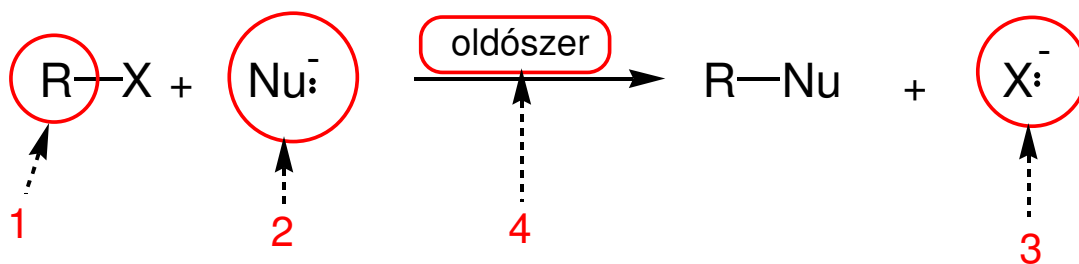
S_N1 típusú szolvólízises reakciók



Mechanizmus

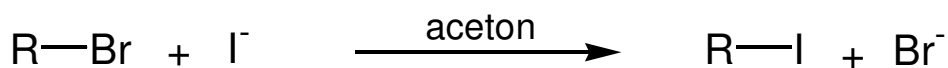


Az S_N reakciók sebességét befolyásoló tényezők

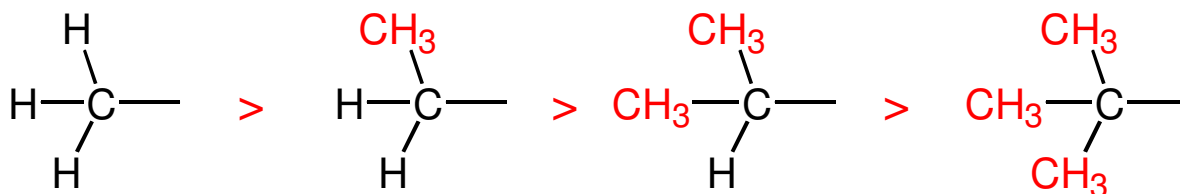


1 R-csoport

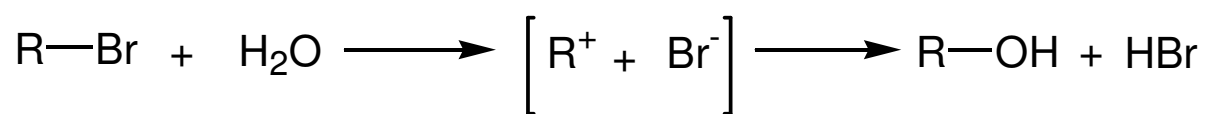
S_N2



R	k _{rel}
CH ₃ -	145
CH ₃ CH ₂ -	1
(CH ₃) ₂ CH-	0.008
(CH ₃) ₃ C-	0.0005

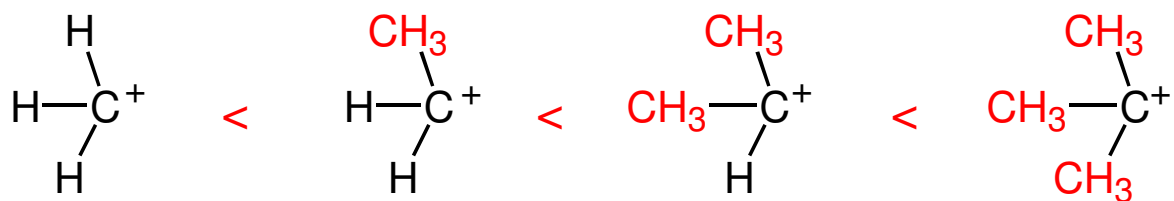


S_N1



R	k_{rel}
CH ₃ -	(1)
CH ₃ CH ₂ -	(1)
(CH ₃) ₂ CH-	12
(CH ₃) ₃ C-	10 ⁶

relatív stabilitás



2 Nukleofil reagens

S_N1 nem befolyásol

S_N2

a) bázicitás (azonos támadó atom esetén)



savi erősség

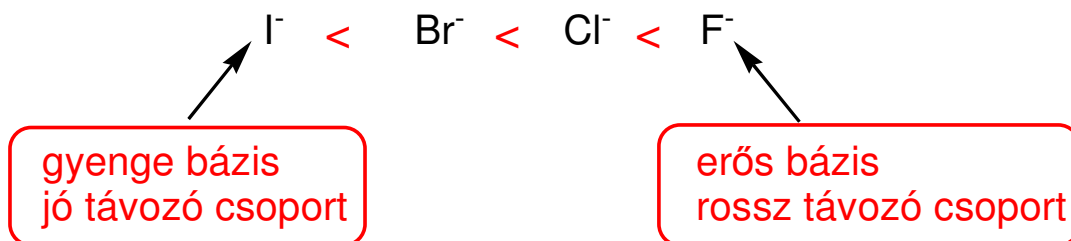


b) polározhatóság



3 Távozó csoport

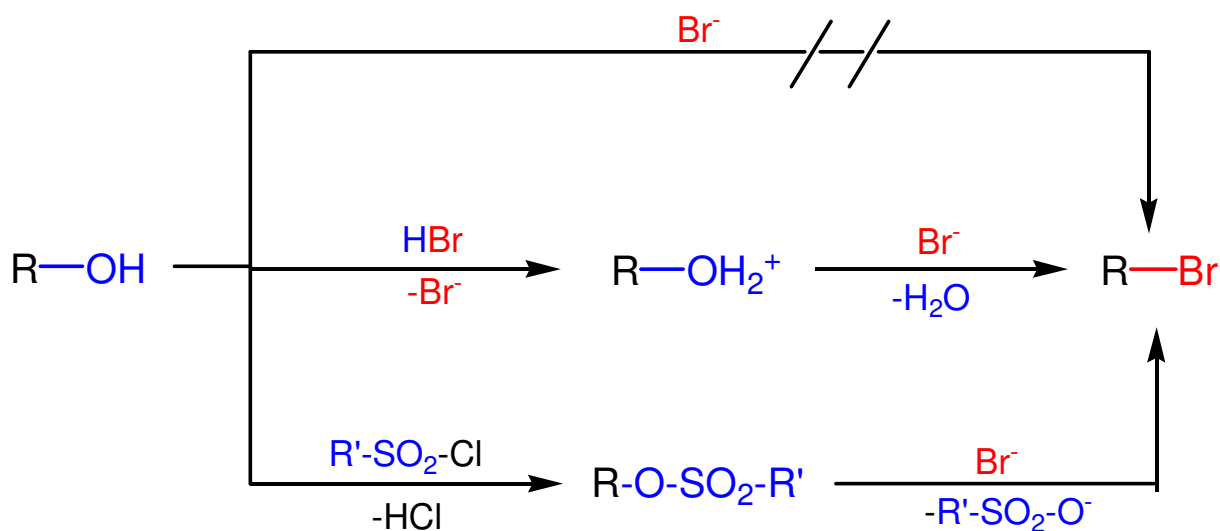
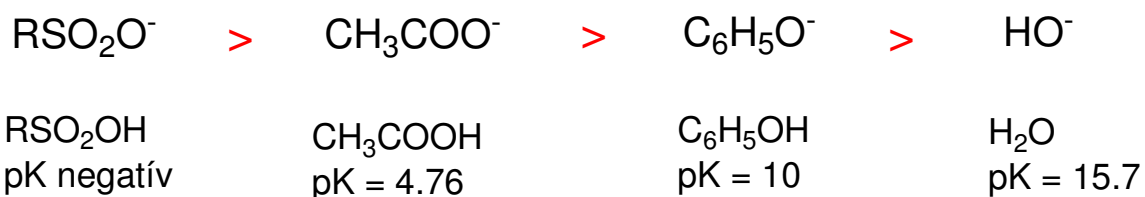
bázicitás



savi erősség

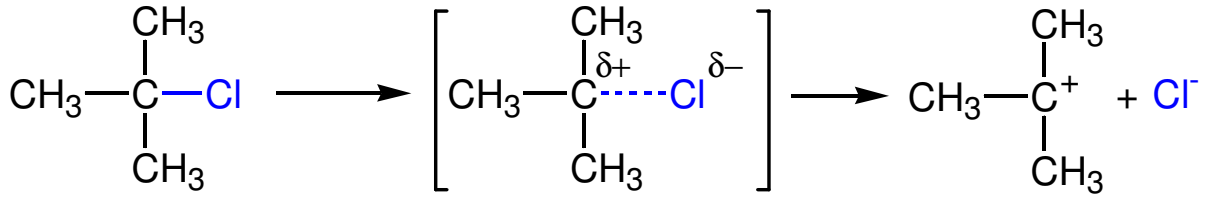


nem halogenid távozó csoportok



4 Oldószer

S_N1



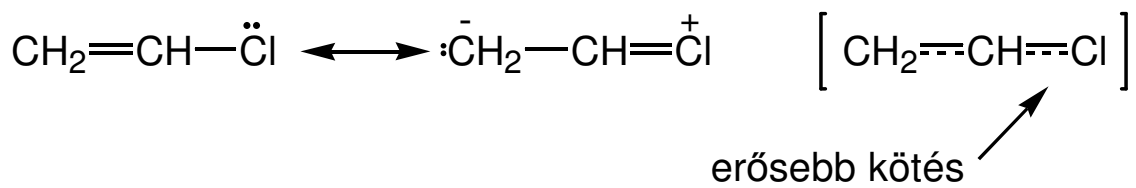
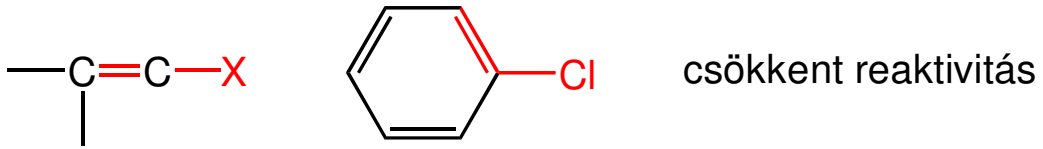
poláros oldószer segít

oldó- szer polaritás	protikus	aprotikus	dielektromos állandó
	H ₂ O		80
	HCOOH		59
		$\begin{array}{c} \text{O} \\ \\ \text{CH}_3-\text{S}-\text{CH}_3 \end{array}$	49
		H-CO-N(CH ₃) ₂	37
		CH ₃ CN	36
	CH ₃ OH		33
	CH ₃ CH ₂ OH		24
		CH ₃ -CO-CH ₃	21
	CH ₃ COOH		6

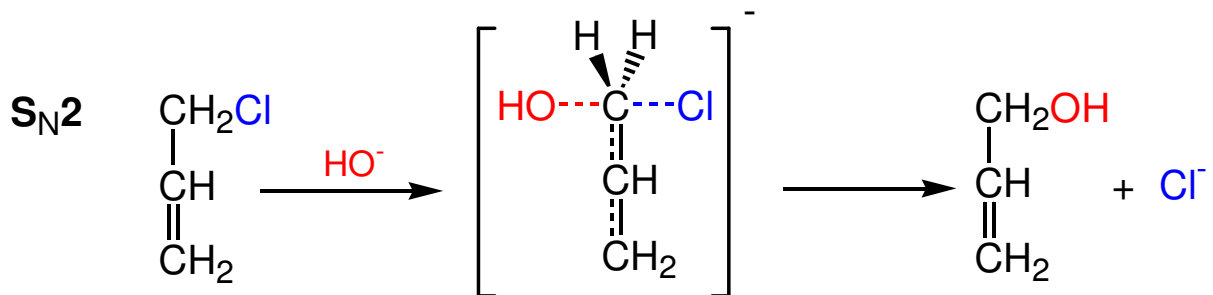
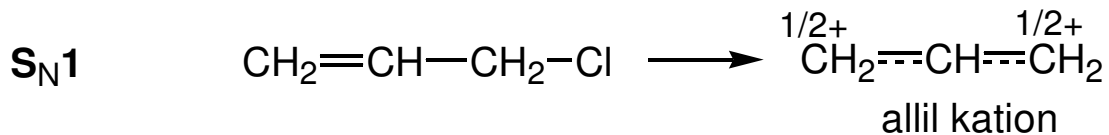
	S_N1	S_N2
Szubsztrát	tercier	primer
Nukleofil	semleges molekula gyakran oldószer (szolvólízis)	anion
Távozó csoport	gyenge bázis	gyenge bázis
Oldószer	poláros protikus	leggyakrabban poláros aprotikus

S_N REAKCIÓK TELÍTETLEN HALOGÉNEZETT SZÉNHYDROGÉNEKKEL

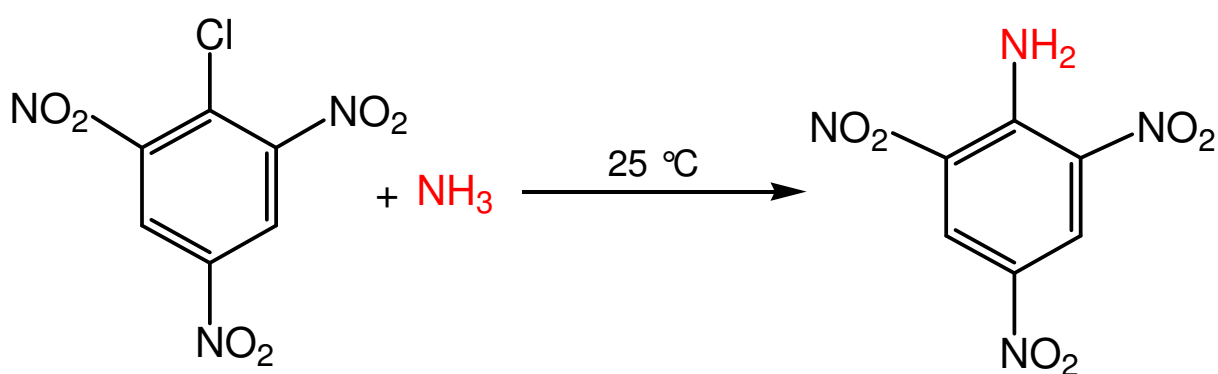
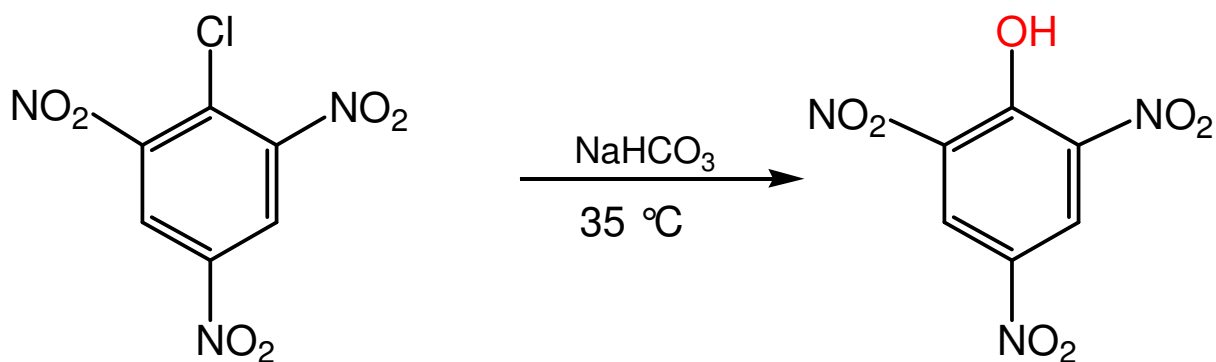
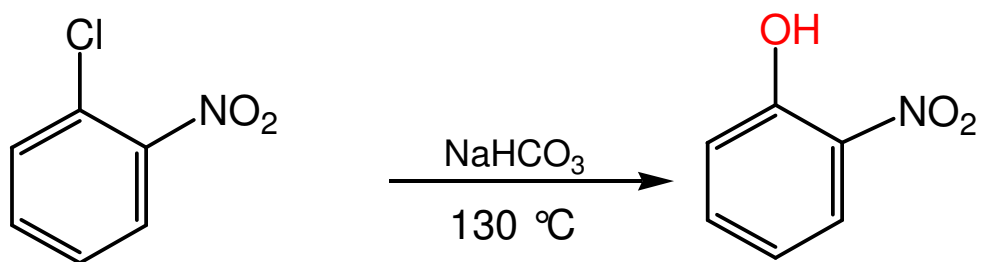
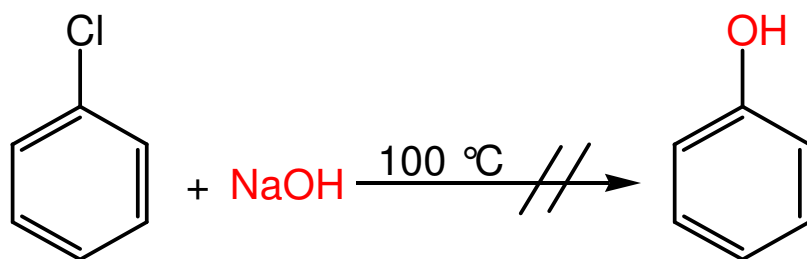
Vinil- és aril-halogenidek



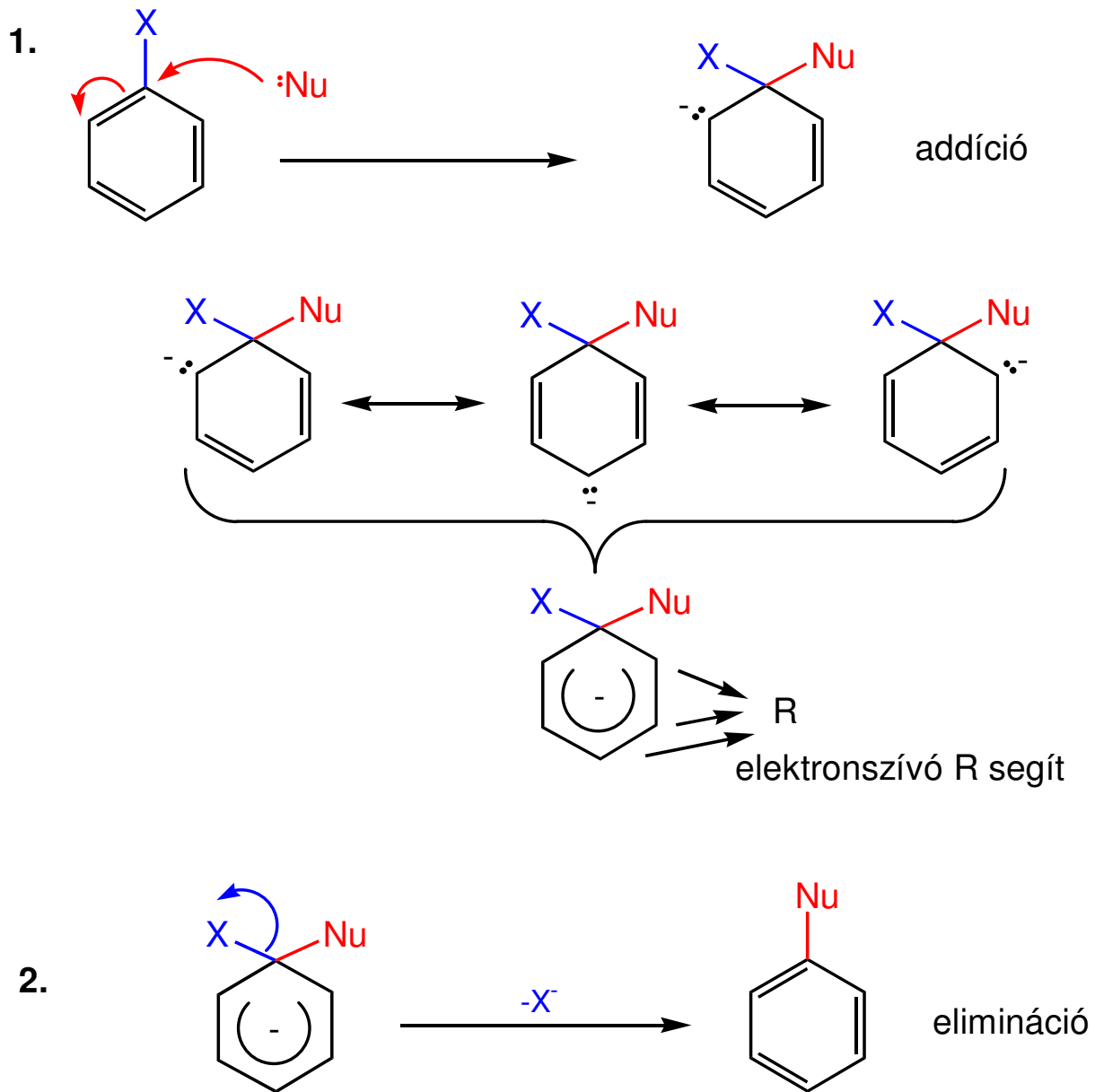
Allil- és benzil-halogenidek



AROMÁS NUKLEOFIL SZUBSZTITÚCIÓ



Mechanizmus



dönt

sorrend

Alifás S_N2

egylépéses

C-X erősség

F < Cl < Br < I

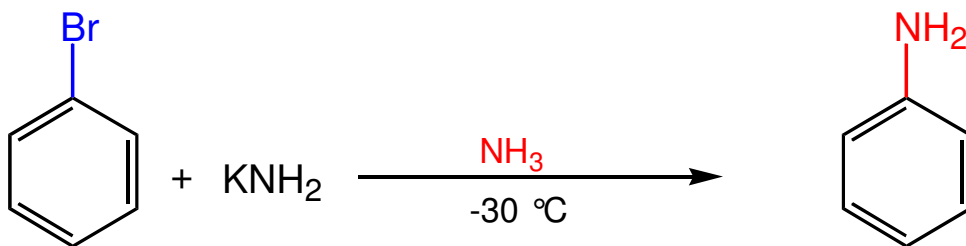
Aromás S_N2

kétlépéses

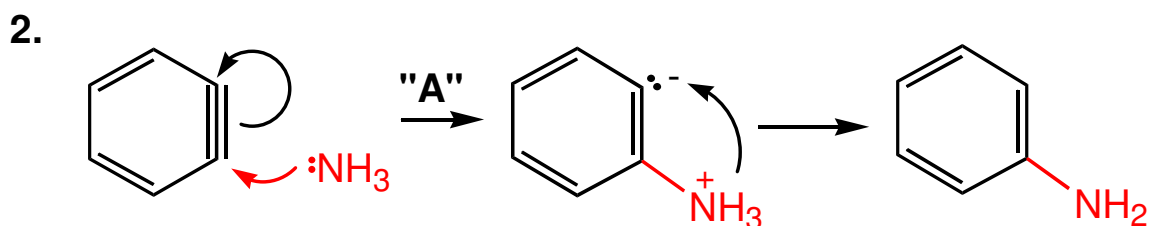
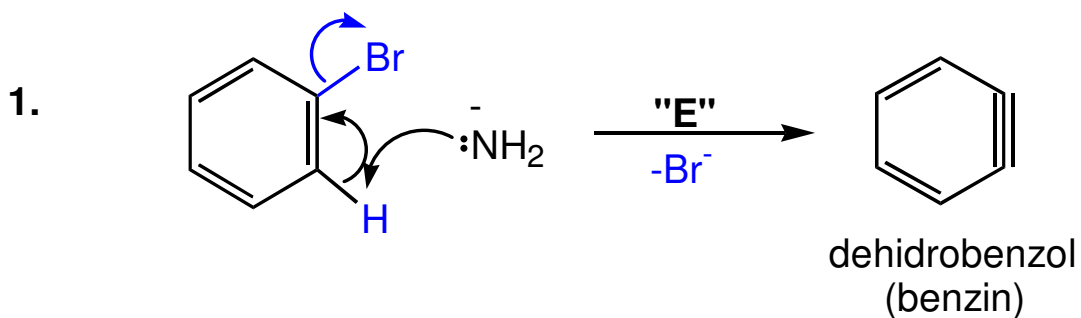
addíció C-re

F > Cl > Br > I

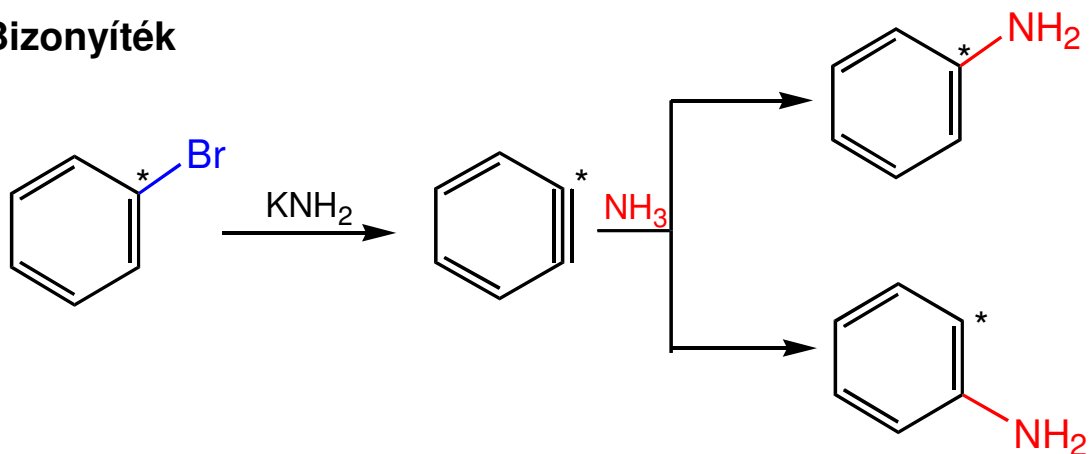
E-A mechanizmusú aromás nukleofil szubsztitúció



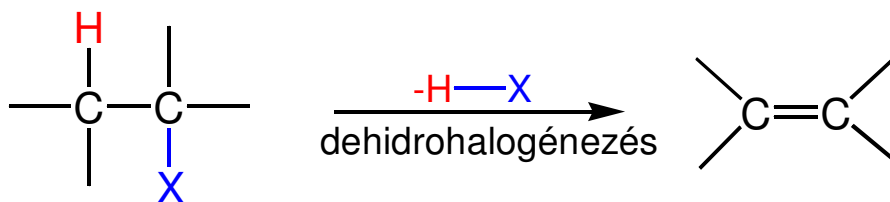
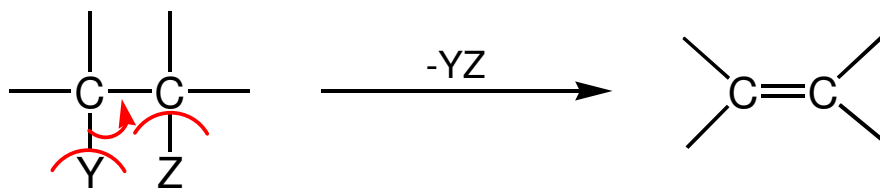
Mechanizmus



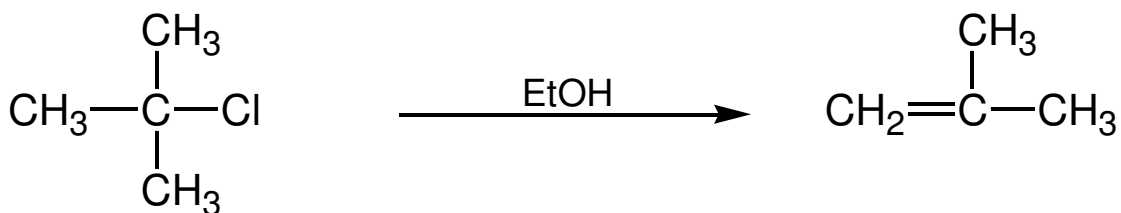
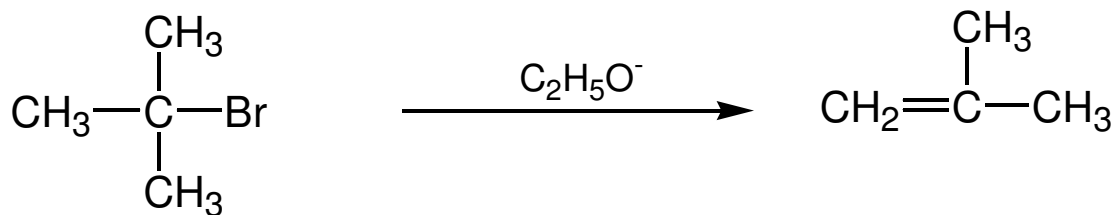
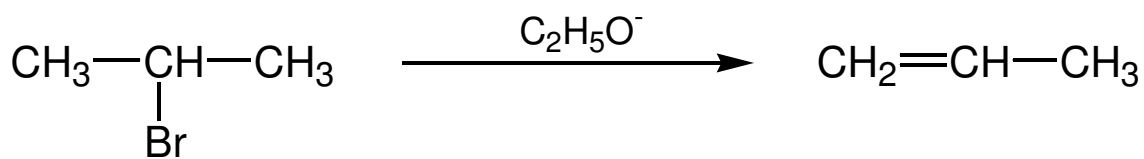
Bizonyíték



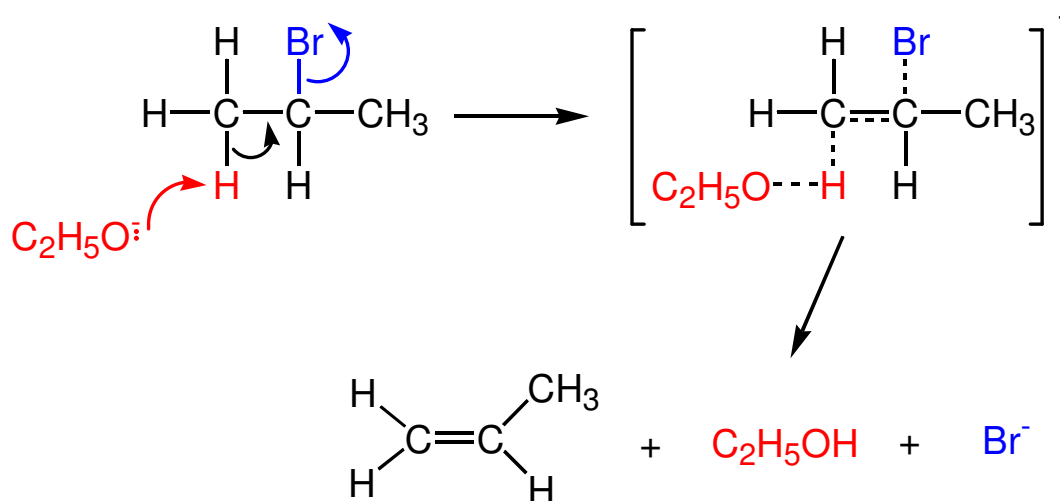
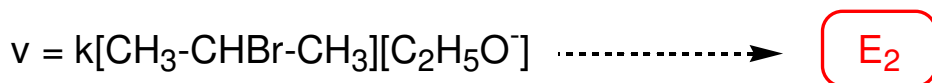
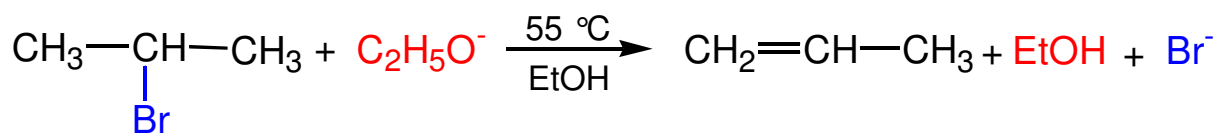
ELIMINÁCIÓS REAKCIÓK



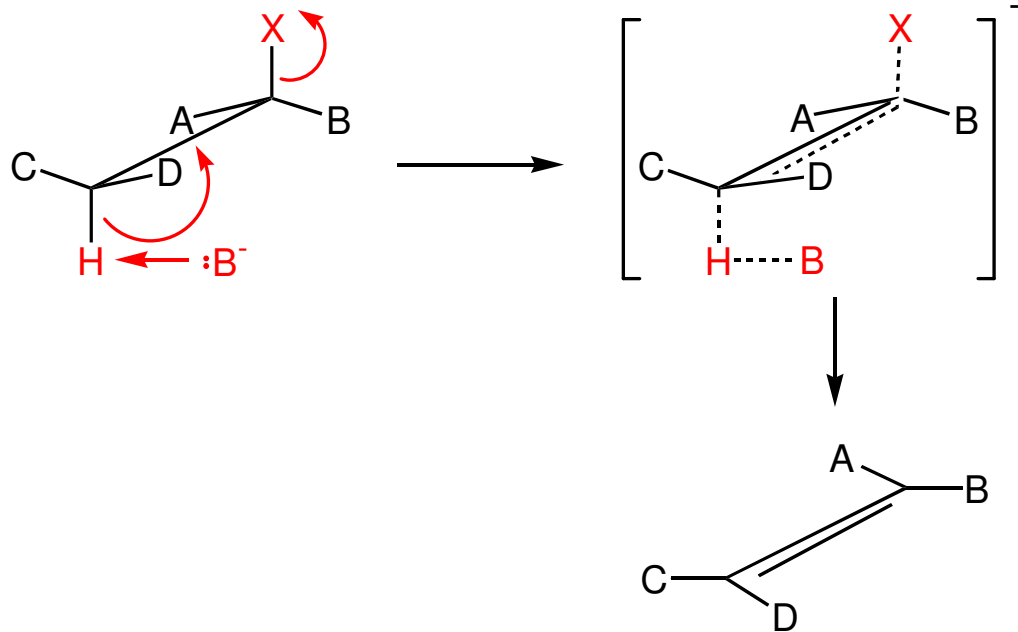
Példák



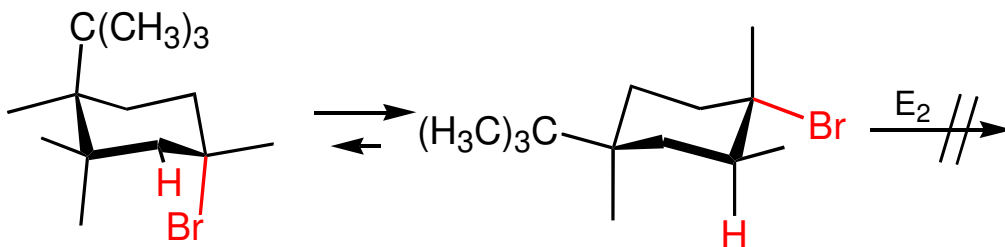
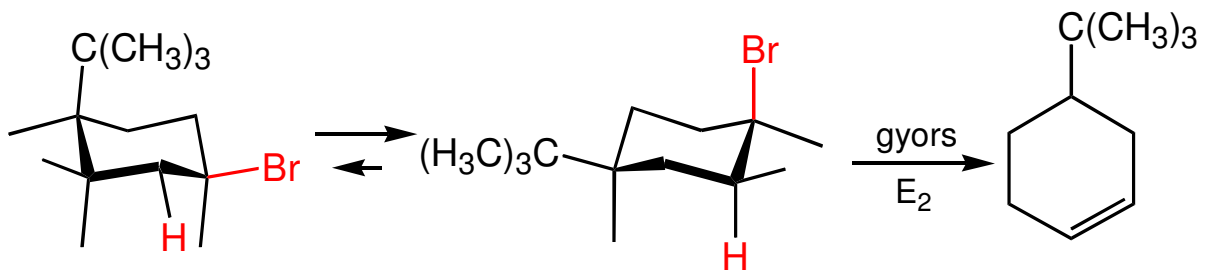
Az eliminációs reakciók mechanizmusa



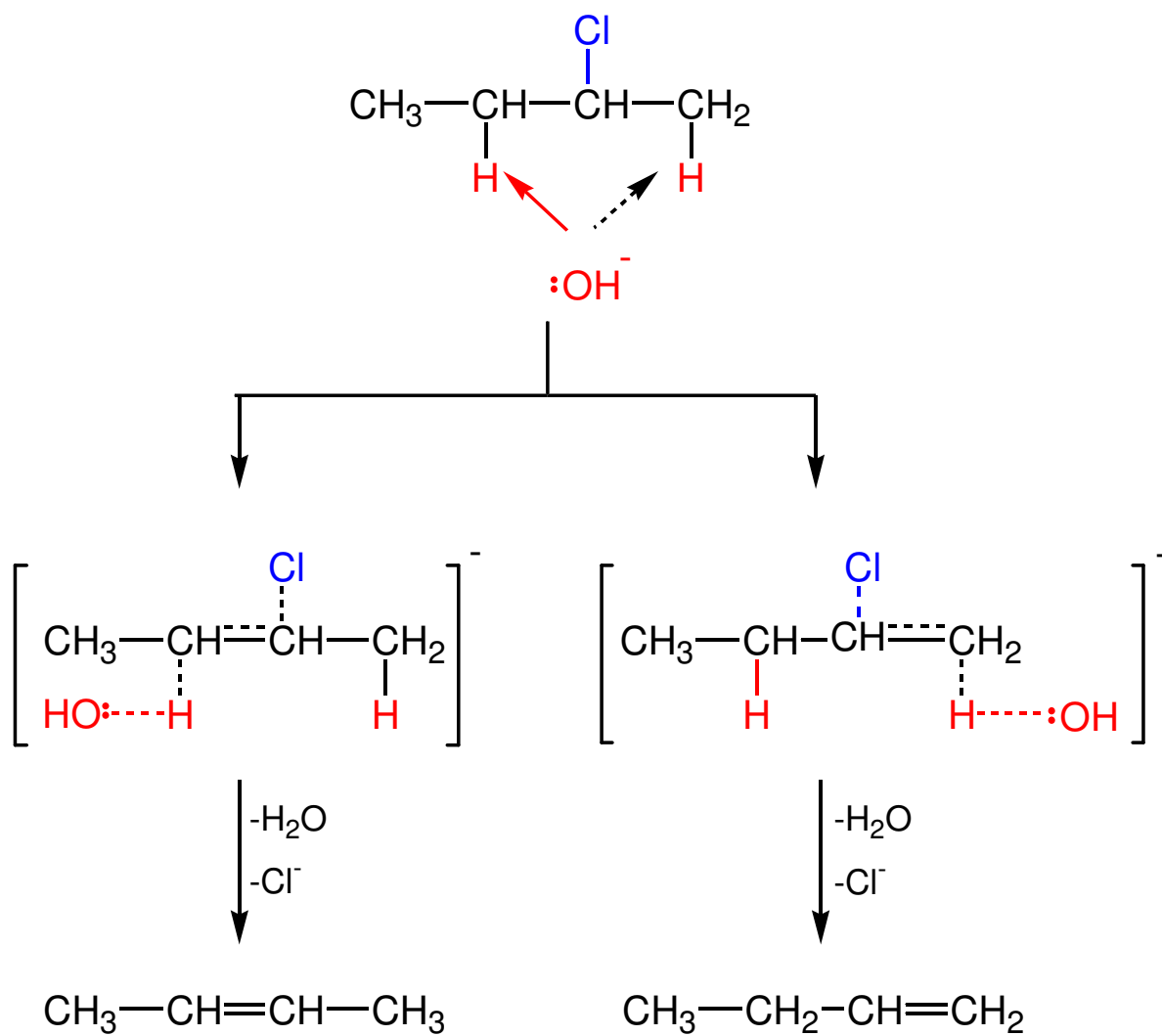
Az E₂ sztereomechanizmusa



Példa



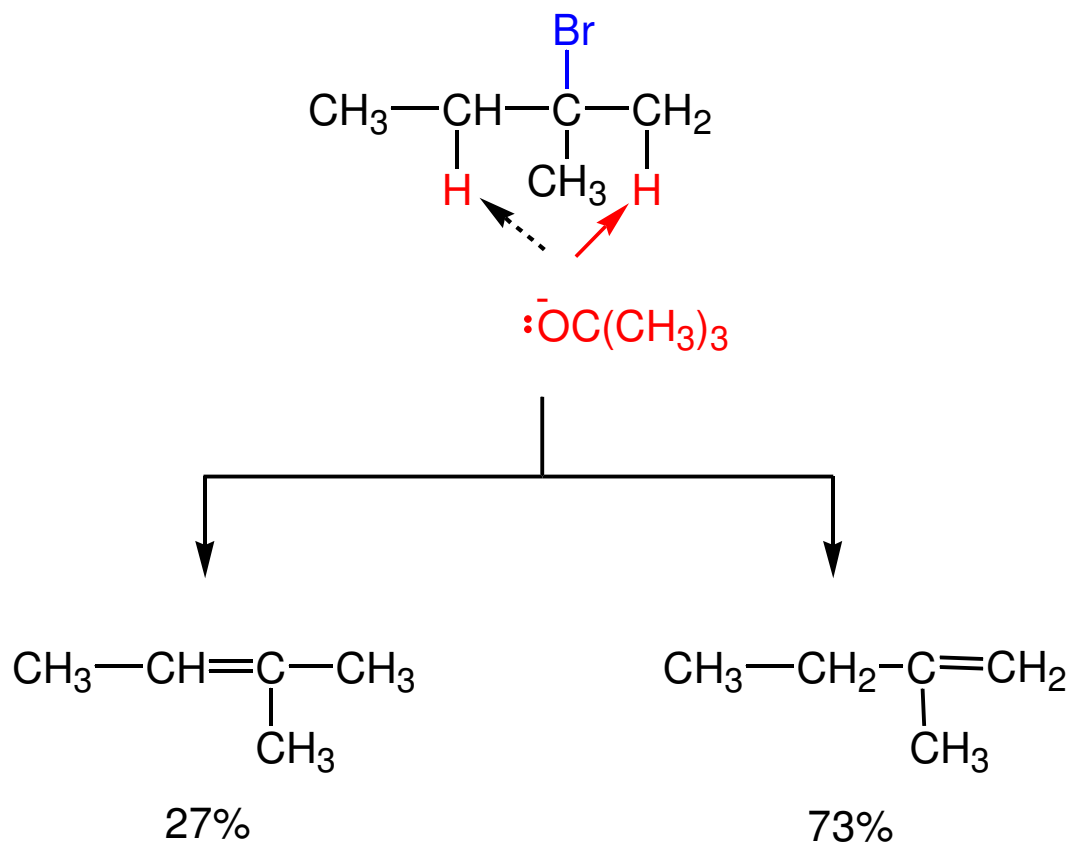
Termékösszetétel

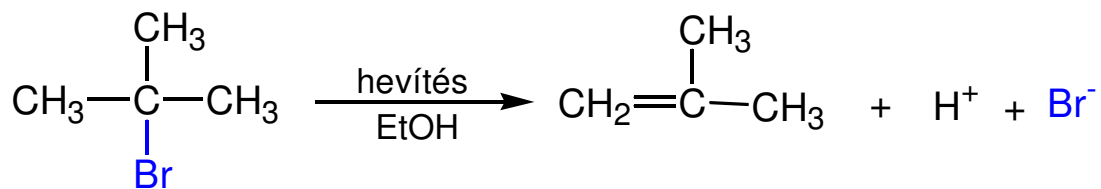


főtermék

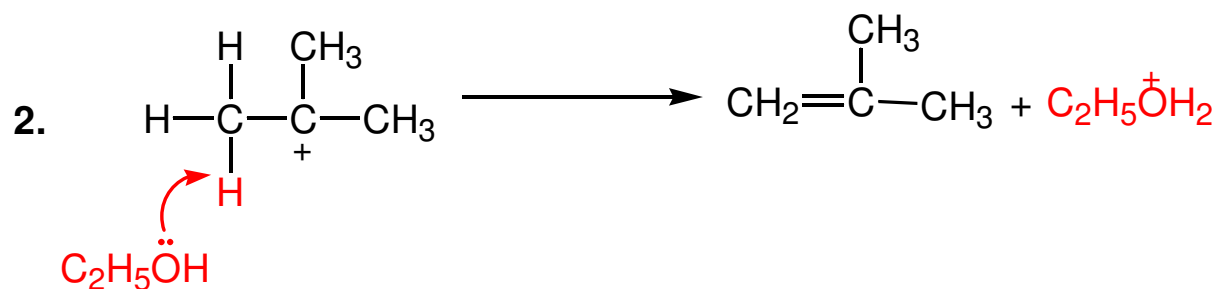
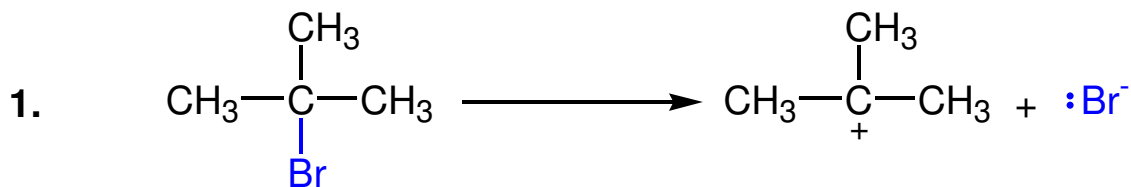
Zajcev szabály

E₂ reakció nagy térigényű bázissal

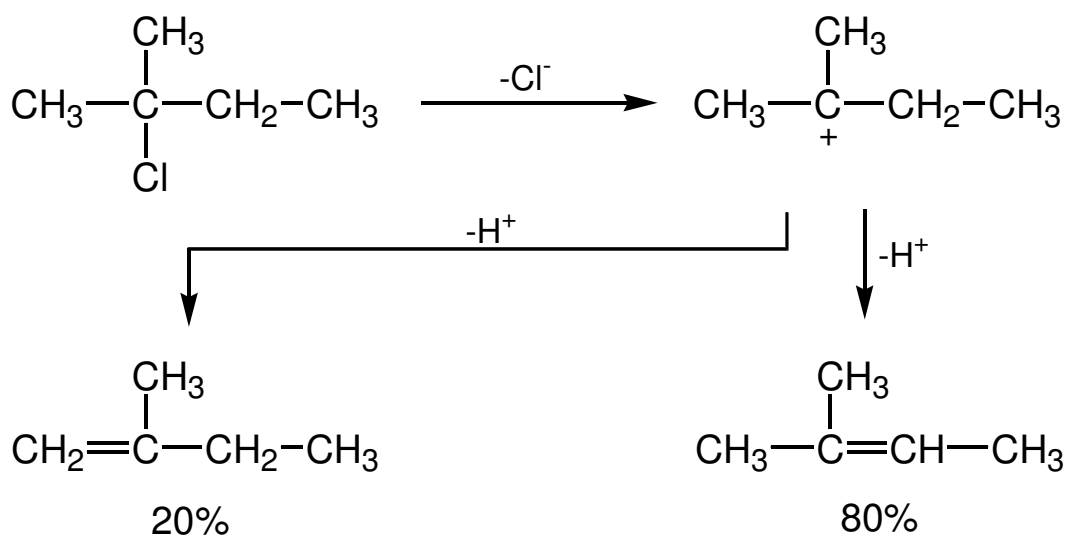




Mechanizmus



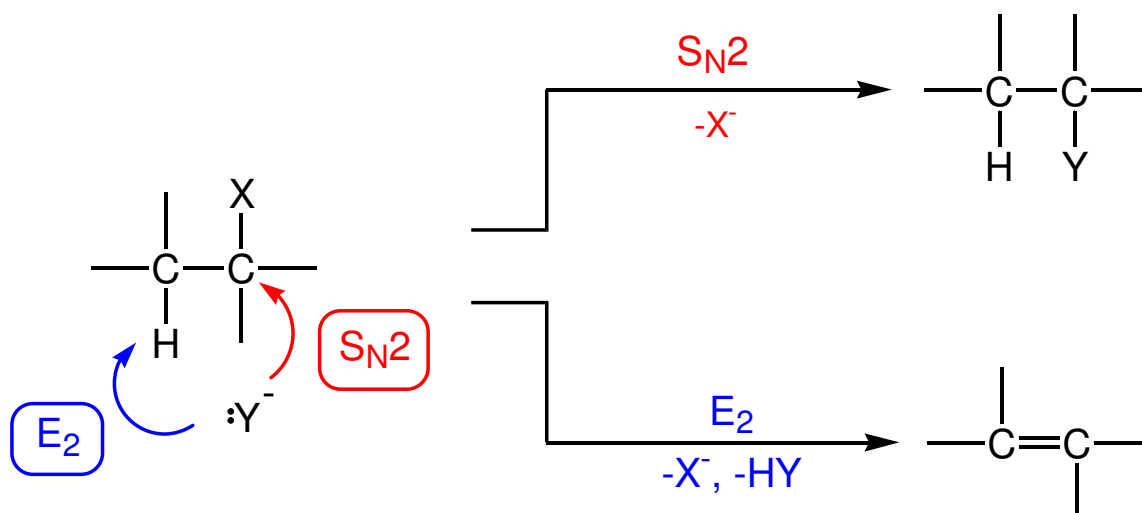
Termékösszetétel



Zajcev szabály

Párhuzamos reakciók

$Y:$ \longrightarrow nukleofil vagy bázis



1. R-csoport szerkezete

primer \longrightarrow S_N2

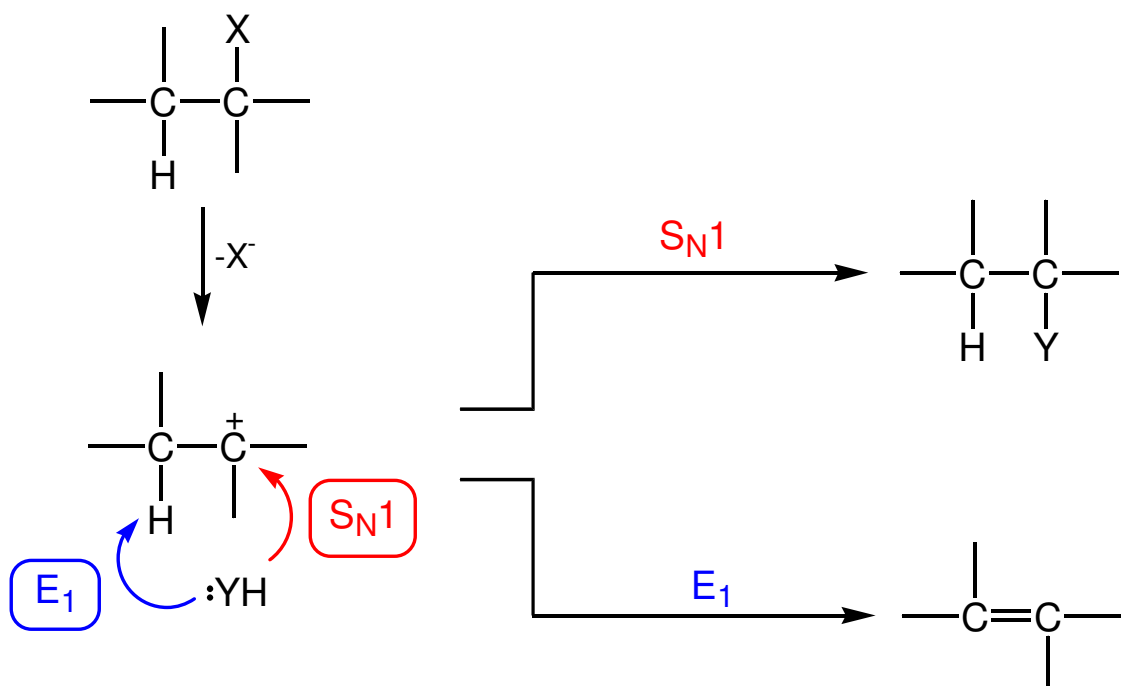
tercier \longrightarrow $E2$

2. Bázis, nukleofil

jó nukleofil, gyenge bázis (pl. I^- , CH_3COO^-) \longrightarrow S_N2

rossz nukleofil, erős bázis (pl. NH_2^- , H^-) \longrightarrow $E2$

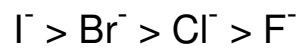
nagy térigényű bázis \longrightarrow $E2$



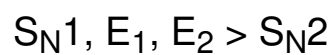
Egymás mellett lejátszódó reakciók \longrightarrow legtöbbször keveréktermék

Összefoglalás

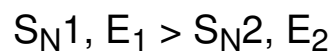
Halogénatom



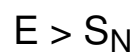
R-csoport növekvő rendűsége



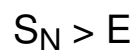
Oldószer polaritásának növelése



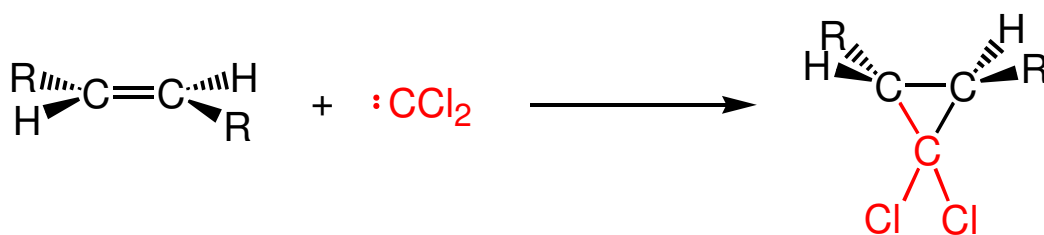
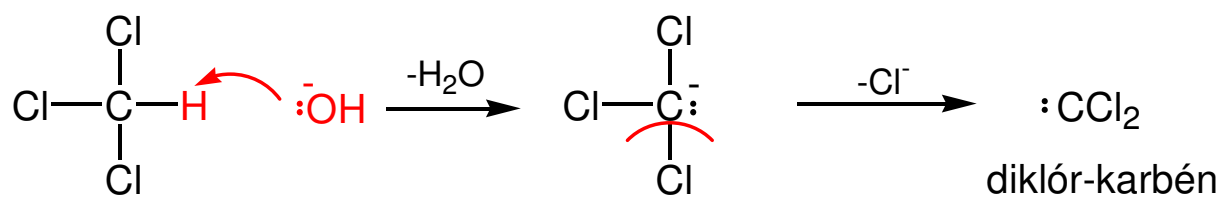
Erős bázis, gyenge nukleofil



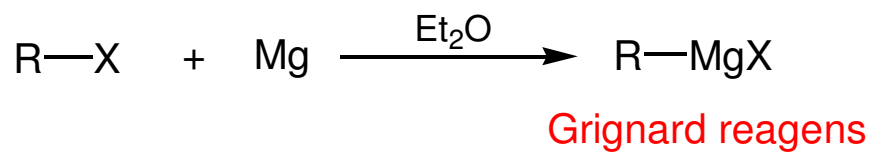
Gyenge bázis, jó nukleofil



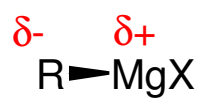
Az α -elimináció



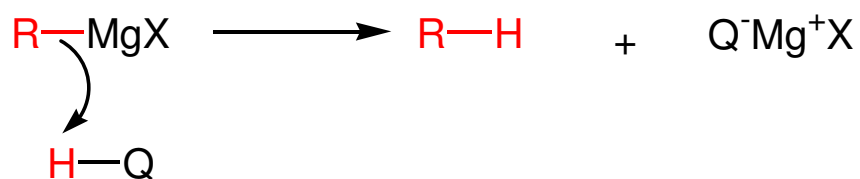
Halogénezett szénhidrogének reakciója magnéziummal



Szerkezet

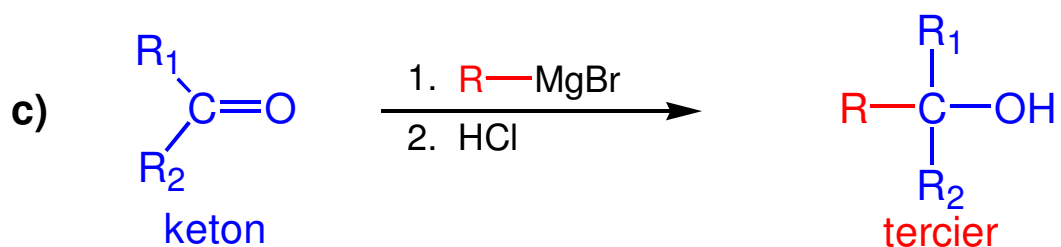
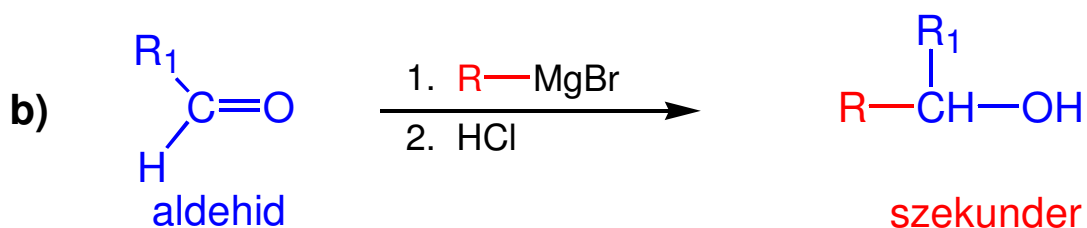
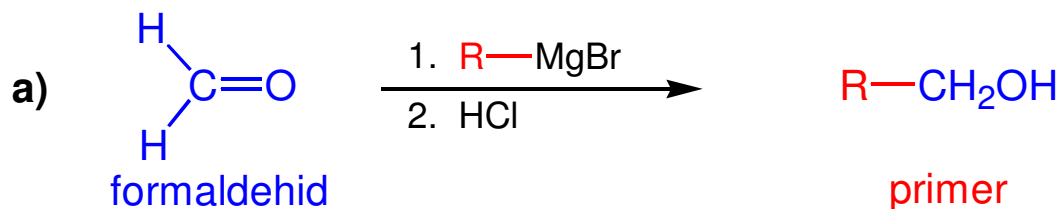
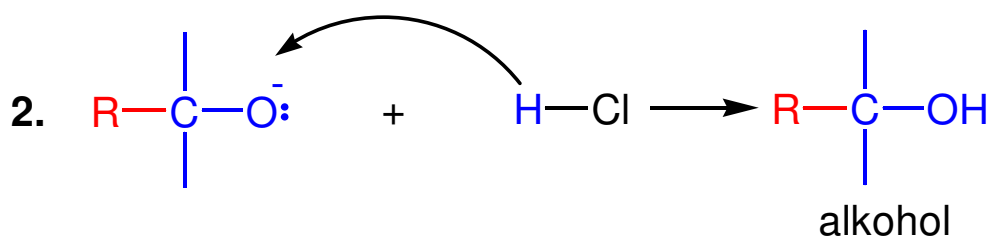
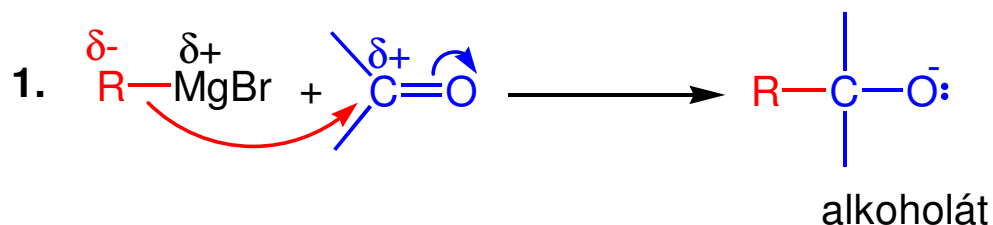


Bázikus jelleg

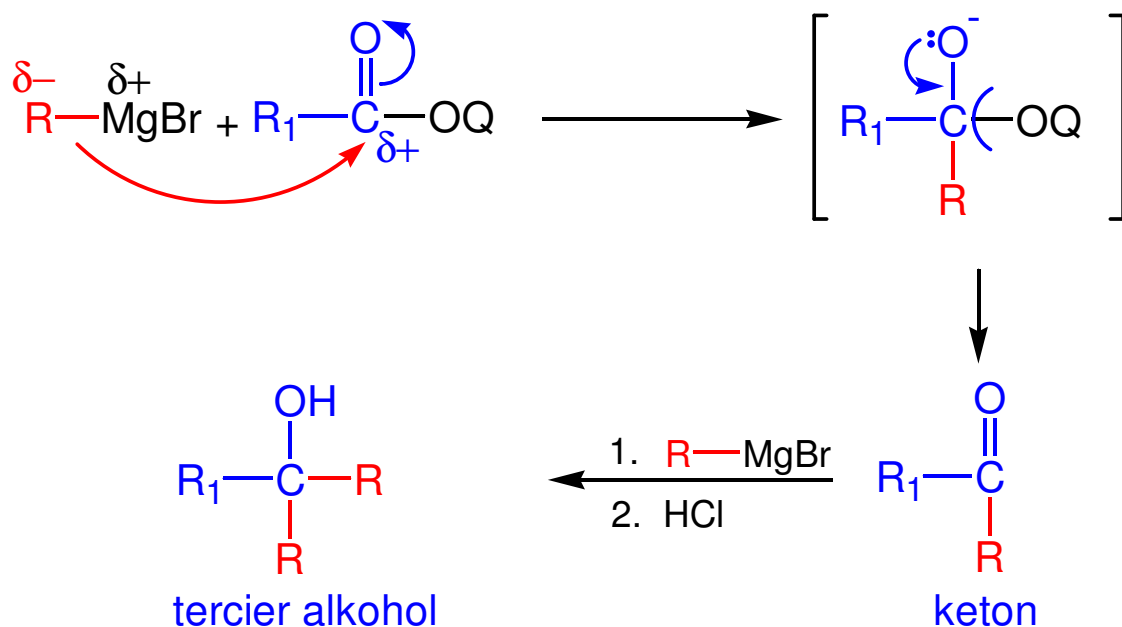


A Grignard reagens felhasználása szintézisekben

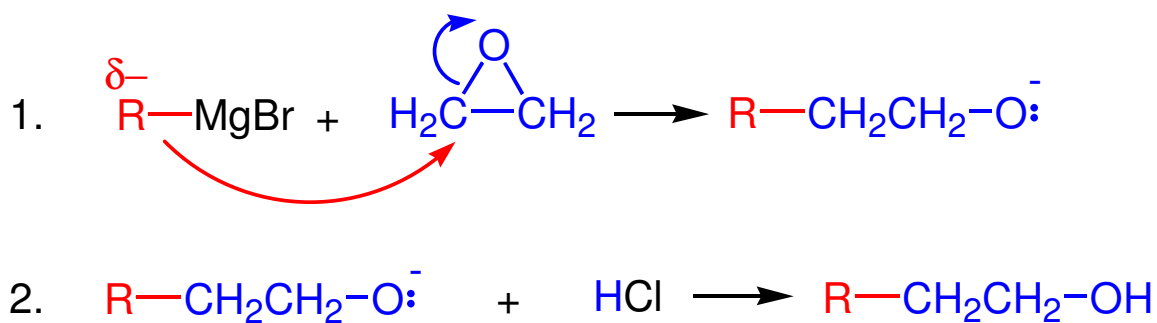
1. Reakció oxovegyületekkel; nukleofil addíció (Ad_N)



2. Reakció észterekkel



3. Reakció oxiránnal (epoxiddal)



4. Reakció széndioxiddal

