Electronic Supplementary Material (ESI) for Chemistry Education Research and Practice.

ELECTRONIC SUPPLEMENTARY INFORMATION

Generalized rubric for level of explanation sophistication for nucleophiles in organic chemistry reaction mechanisms

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This electronic supplementary information (ESI) contains constructed response item prompt variations and reaction mechanisms used in this study.

ORGINAL PROMPT

Part A: Describe in full *what* you think is happening on the molecular level for this reaction. Be sure to discuss the role of the reactant and intermediate.

Part B: Using a molecular level explanation, explain *why* this reaction occurs. Be sure to discuss why the reactants form the products shown.

MORE CUED PROMPT

Part A: Describe in full detail the sequence of events that occur at the molecular level for this reaction. Be sure to discuss the role of each reactant and intermediate.

Part B: Using a molecular level explanation, explain why each of the reactants and intermediates interact.

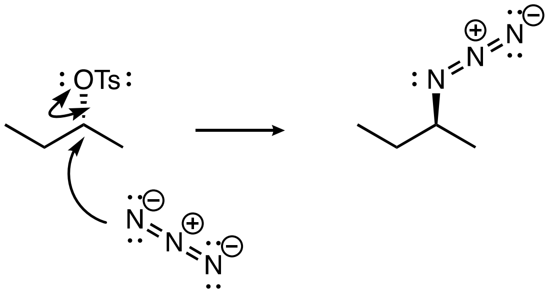
REACTION MECHANISMS

Note: functional groups and reactions are hyperlinked in this table.

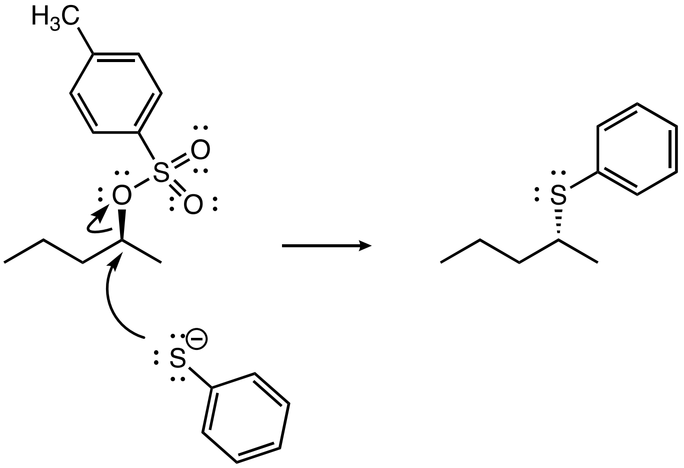
Functional group	Reaction	Variations
Alkyl halide	Bimolecular nucleophilic substitution (S_N2)	4
	Unimolecular nucleophilic substitution (S_N1)	8
Alkene	Halogenation/hydrohalogenation	5
	Halohydrin formation	3
	Hydration/dehydration	4
Alkyne	Alkylation	1
Alcohol	Conversion to good leaving group, then S_N2	4
	Epoxidation/ring-opening	6
Aromatic ring	Acylation	1
	Addition-elimination	1
	Alkylation	1
	Azo coupling	1
	Electrophilic aromatic substitution	6
	Nucleophilic aromatic substitution	2
Carbonyl	Acyl substitution	3
	Aldol addition/condensation	2
	Alpha-halogenation	1
	Condensation of an ester/diester	2
	Conjugate addition	2
	Enamine/imine synthesis	2
	Esterification	1
	Grignard	6
	Hemiacetal/acetal formation	4
	Hydration/dehydration	2
	Hydrolysis	1
	Reduction	9
	Saponification	1
Conjugated diene	Electrophilic addition	2

BIMOLECULAR SUBSTITUTION (S_N2)

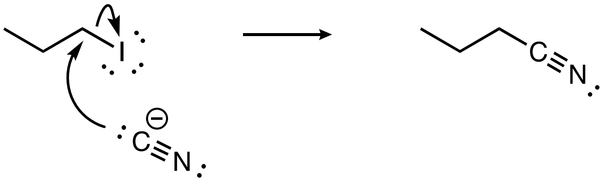
Consider the mechanism for the S_N2 reaction between (R)-sec-butyl 4-methylbenzenesulfonate and azide to form (S)-2-azidobutane.



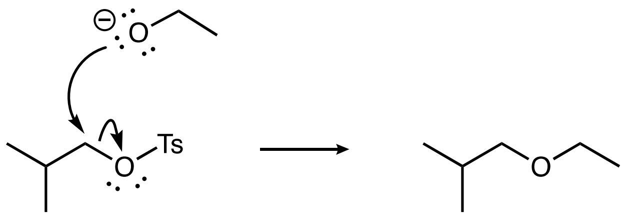
Consider the mechanism for the S_N2 reaction between (*S*)-pentan-2-yl-4-methylbenzenesulfonate and benzenethiolate to form (*R*)-pentan-2-yl(phenyl)sulfane.



Consider the mechanism for the S_N2 reaction between 1-iodopropane and cyanide to form butyronitrile.

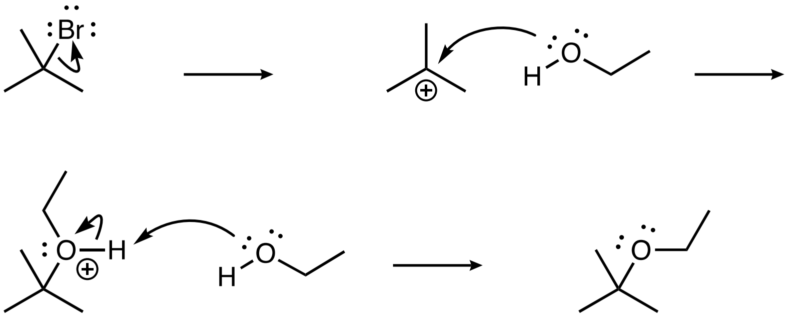


Consider the mechanism for the S_N2 reaction between isobutyl 4-methylbenzenesulfonate and ethoxide to form 1-ethoxy-2-methylpropane.

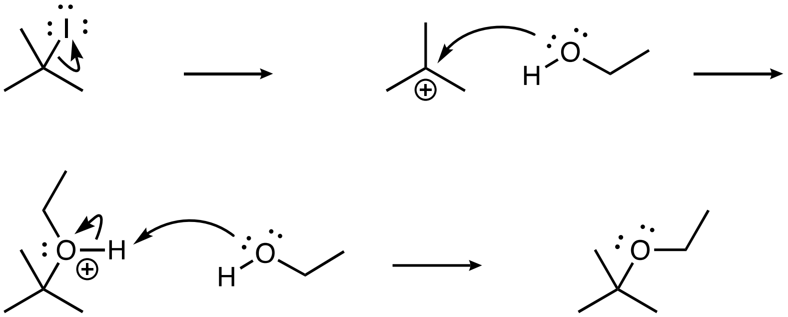


UNIMOLECULAR SUBSTITUTION (S_N1)

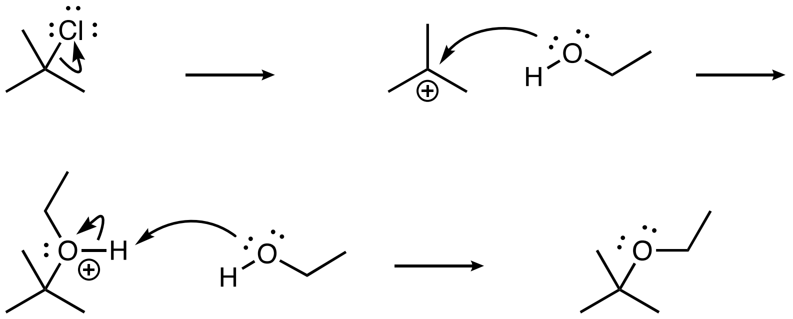
Consider the mechanism for the S_N1 reaction between *t*-butyl bromide and ethanol to form ethyl *t*-butyl ether.



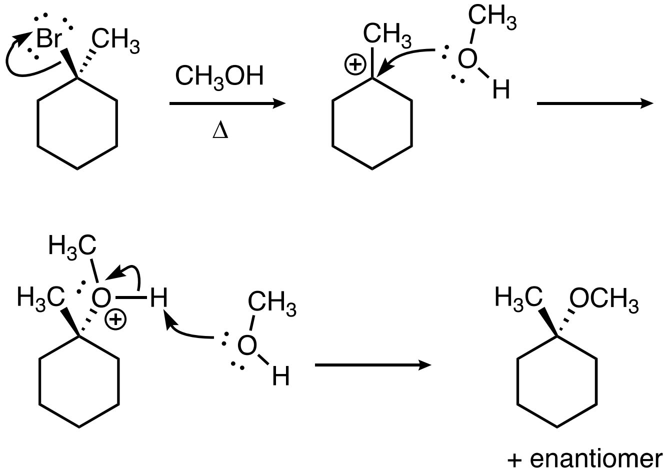
Consider the mechanism for the S_N1 reaction between *t*-butyl iodide and ethanol to form ethyl *t*-butyl ether.



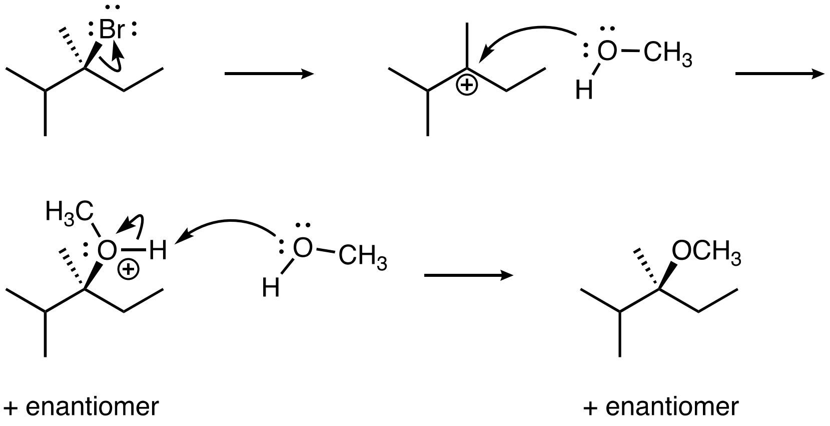
Consider the mechanism for the S_N1 reaction between *t*-butyl chloride and ethanol to form ethyl *t*-butyl ether.



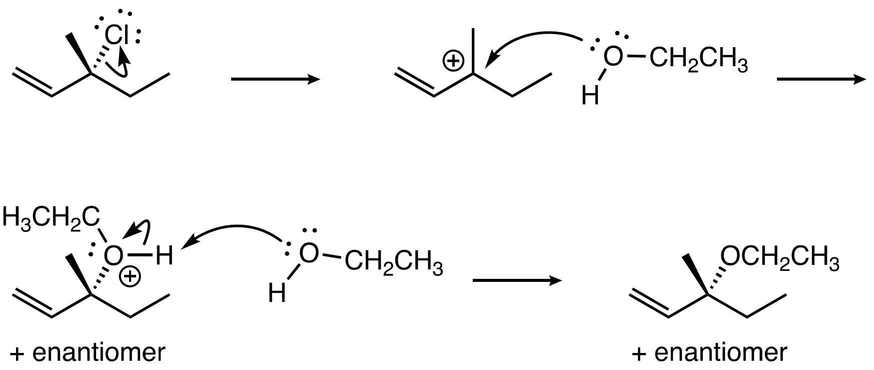
Consider the mechanism for the S_N1 reaction between 1-bromo-1-methylcyclohexane and methanol to form 1-methoxy-1-methylcyclohexane.



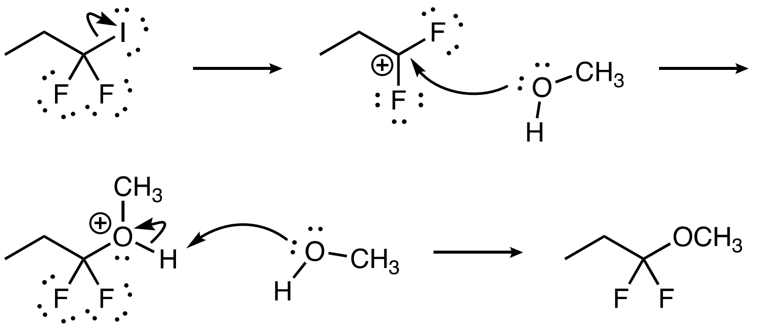
Consider the mechanism for the S_N1 reaction between (S)-3-bromo-2,3-dimethylpentane and methanol to form (S)-3-methoxy-2,3-dimethylpentane.



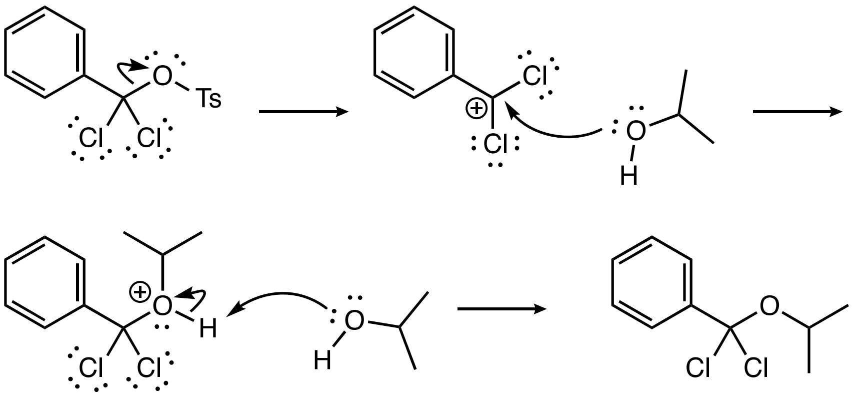
Consider the mechanism for the S_N1 reaction between (*R*)-3-chloro-3-methyl-1-pentene and ethanol to form (*R*)-3-ethoxy-3-methyl-1-pentene.



Consider the mechanism for the S_N1 reaction between 1,1-difluoro-1-iodoproane and methanol to form 1,1-difluoro-1-methoxypropane.



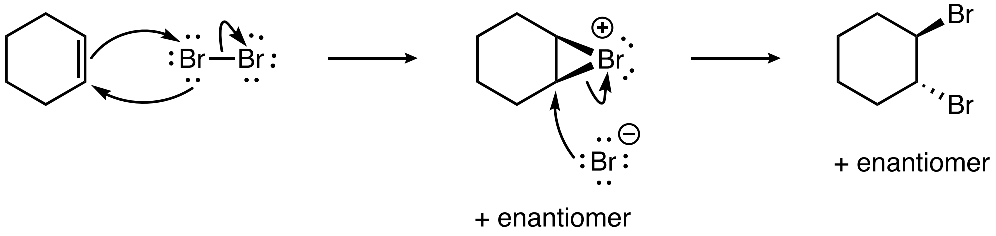
Consider the mechanism for the S_N1 reaction between dichloro(phenyl)methyl 4-methylbenzenesulfonate and isopropanol to form (dichloro(isopropoxy)methyl)benzene.



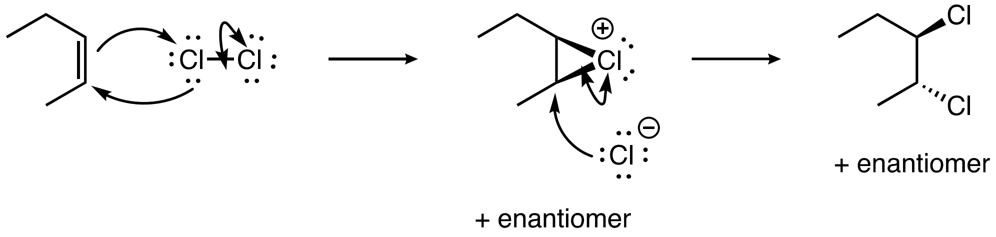
ALKENE

HALOGENATION / HYDROHALOGENATION

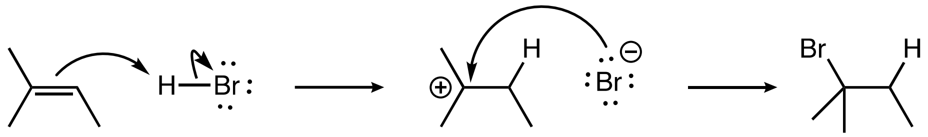
Consider the mechanism for the halogenation of cyclohexene with bromine to form (1*R*,2*R*)-1,2-dibromocyclohexane.



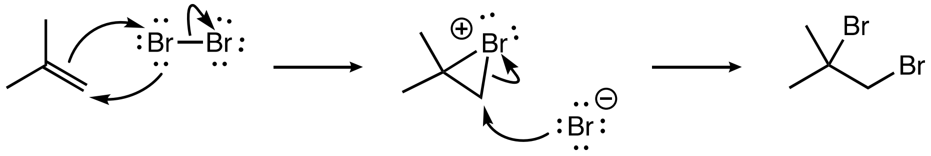
Consider the mechanism for the halogenation of (*Z*)-2-pentene with chlorine to form (2*R*,3*R*)-2,3-dichloropentane.



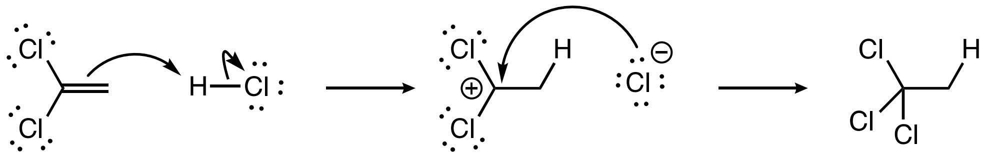
Consider the mechanism for the hydrohalogenation of 2-methyl-2-butene with hydrobromic acid to form 2-bromo-2-methylbutane.



Consider the mechanism for the halogenation of 2-methylpropene with bromine to form 1,2-dibromo-2-methylpropane.

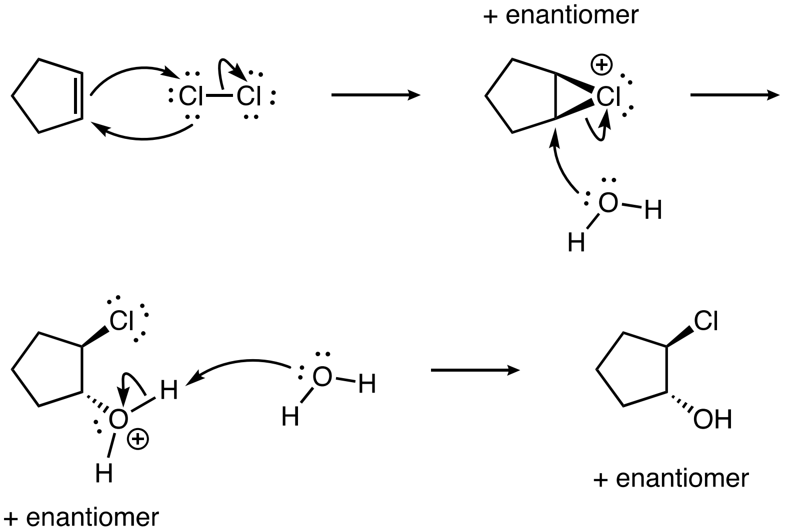


Consider the mechanism for the hydrohalogenation of 1,1-dichloroethane with hydrochloric acid to form 1,1,1-trichloroethane.

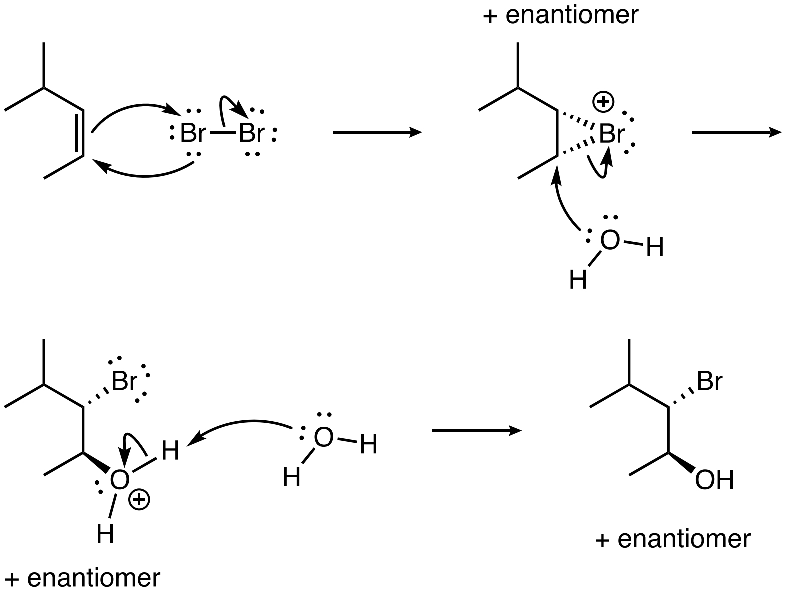


HALOHYDRIN FORMATION

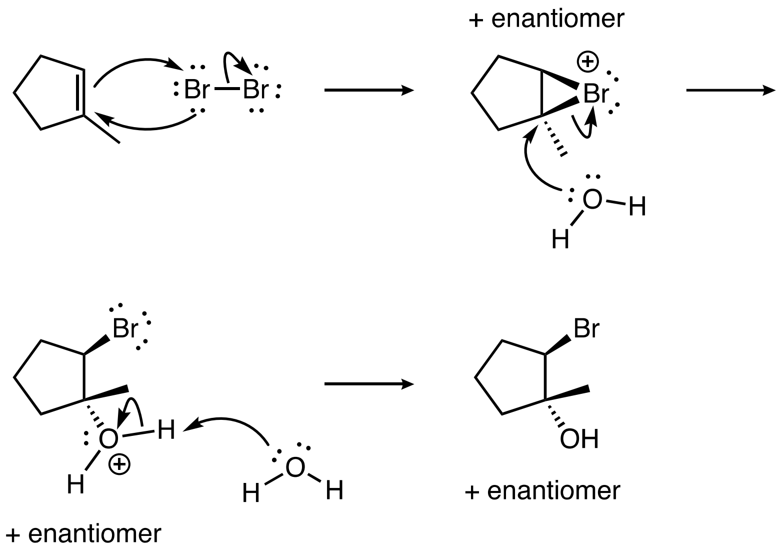
Consider the mechanism for the formation of a halohydrin from cyclopentene and chlorine in the presence of water to form (1*R*,2*R*)-2-chlorocyclopentanol.



Consider the mechanism for the formation of a halohydrin from (*Z*)-4-methyl-2-pentene and bromine in the presence of water to form (2*S*,3*S*)-3-bromo-4-methyl-2-pentanol.

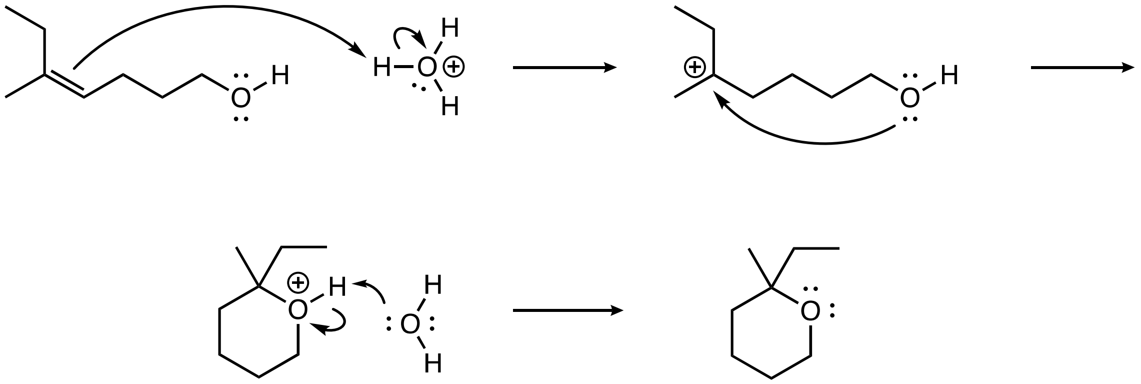


Consider the mechanism for the formation of a halohydrin from methylcyclopentene and bromine in the presence of water to form (1*R*,2*R*)-2-bromo-1-methylcyclo-1-pentanol.

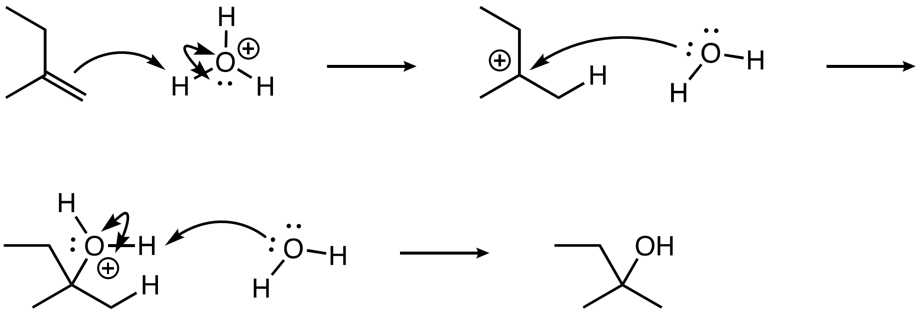


HYDRATION / DEHYDRATION

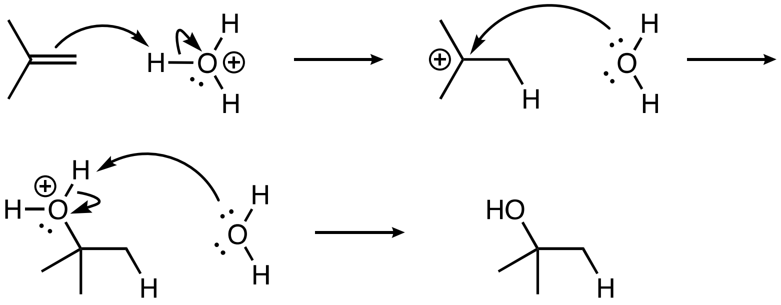
Consider the mechanism between (*Z*)-5-methyl-4-heptenol and hydronium ion to form the cyclic ether product.



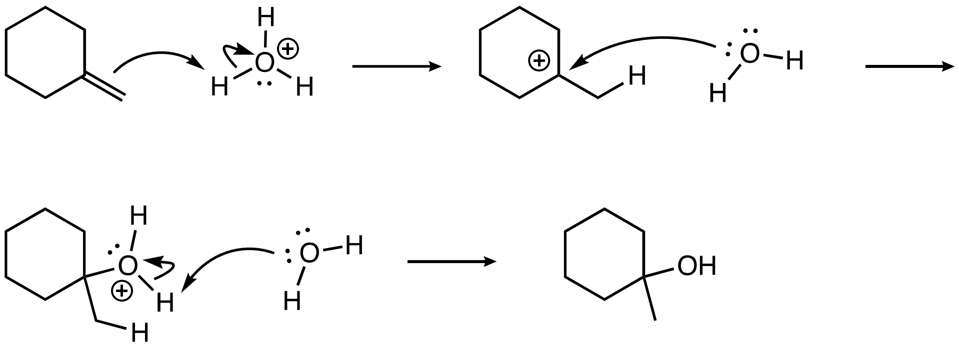
Consider the mechanism for the acid-catalyzed hydration of 2-methylbutene to form 2-methyl-2-butanol.



Consider the mechanism for the acid-catalyzed hydration of 2-methylpropene with hydronium to form *tert*-butanol.



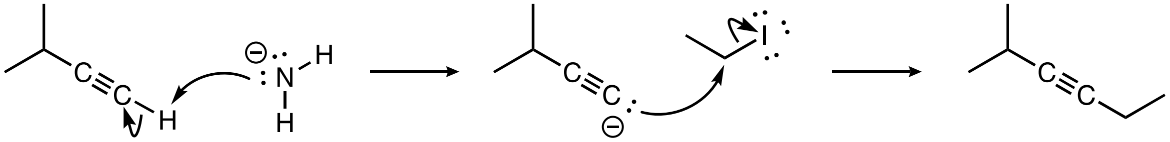
Consider the mechanism for the acid-catalyzed hydration of methylenecyclohexane to form 1-methylcyclo-1-hexanol.



ALKYNE

ALKYLATION

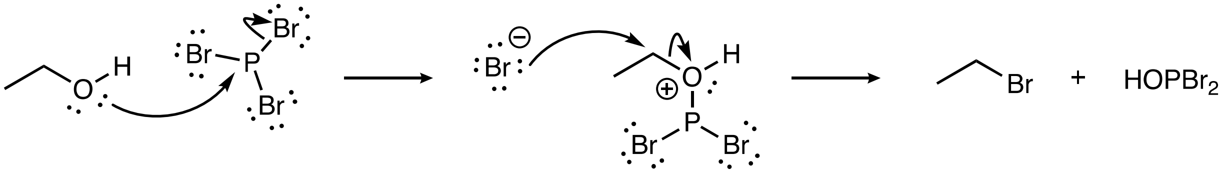
Consider the mechanism for the reaction of 3-methyl-1-butyne with amide and then iodoethane to form 2-methyl-3-hexyne.



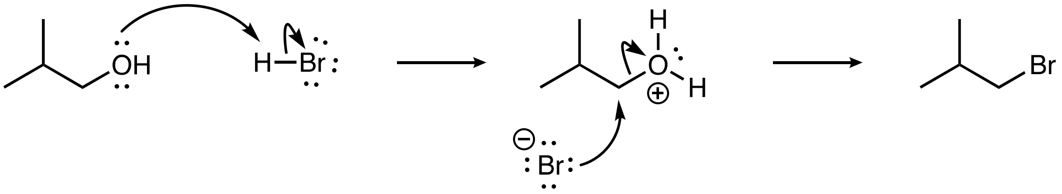
ALCOHOL

FORMATION OF A GOOD LEAVING GROUP THEN S$_N$2

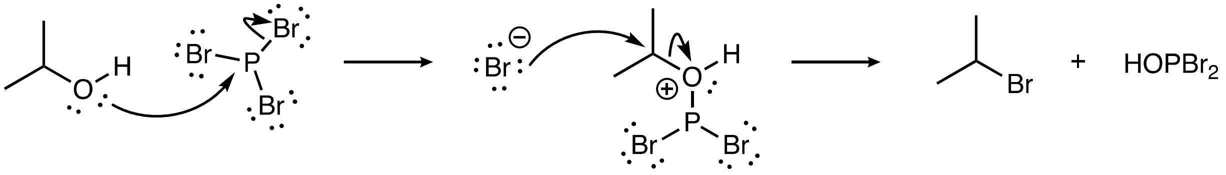
Consider the mechanism for the reaction of ethanol and phosphorus tribromide to form bromoethane.



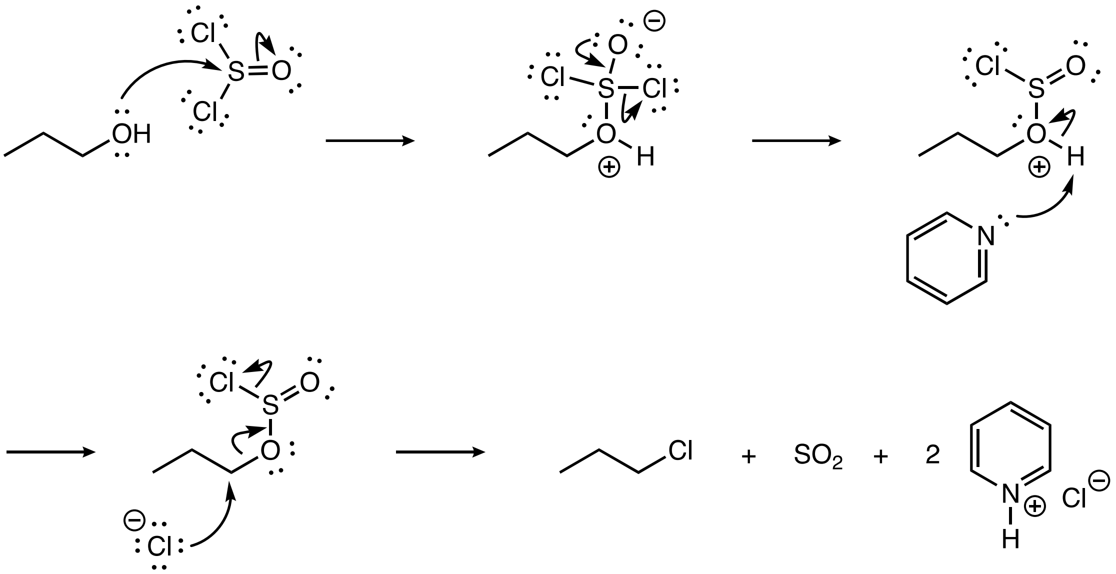
Consider the mechanism for the reaction between 2-methylpropanol and hydrobromic acid to form 1-bromo-2-methylpropane.



Consider the mechanism for the reaction between 2-propanol and phosphorus tribromide to form 2-bromopropane.



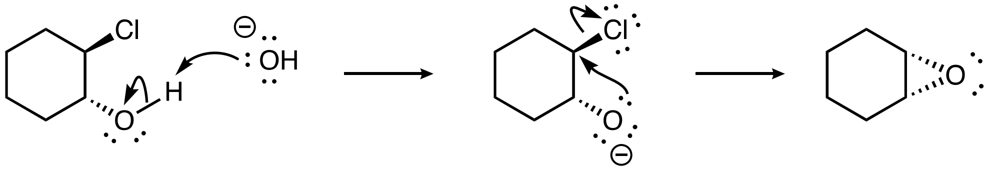
Consider the mechanism for the reaction between 1-propanol and thionyl chloride to form 1-chloropropane.



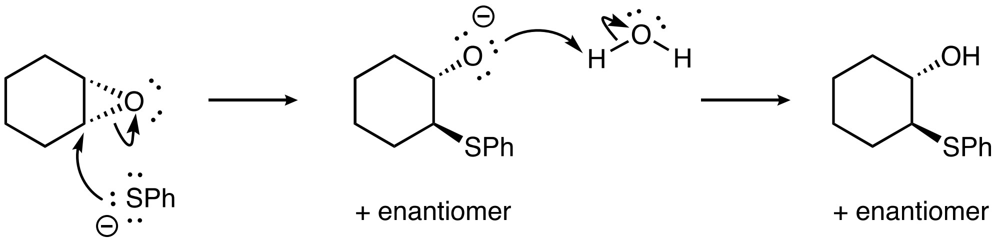
EPOXIDATION / RING-OPENING

Consider the mechanism for the epoxidation of (1*R*,2*R*)-2-chlorocyclohexanol with hydroxide and its subsequent reaction with thiophenolate to form (1*S*,2*S*)-2-(phenylthiol)cyclohexanol.

Step 1:

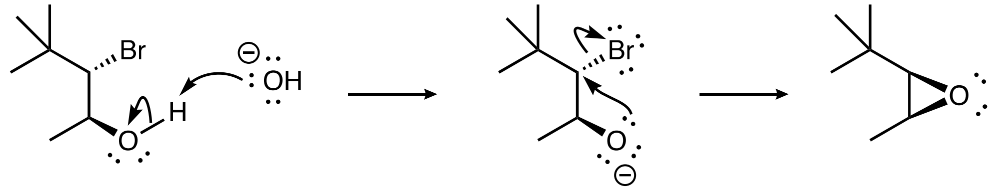


Step 2:

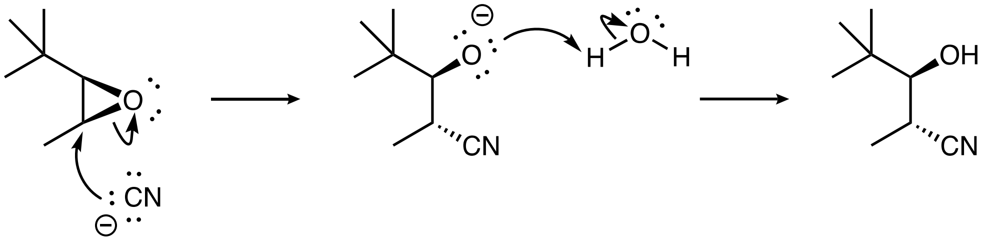


Consider the mechanism for the epoxidation of (2*S*,3*S*)-3-bromo-4,4-dimethyl-2-pentanol with hydroxide and its subsequent reaction with cyanide to form (2*S*,3*S*)-3-hydroxy-2,4,4-trimethylpentanenitrile.

Step 1:

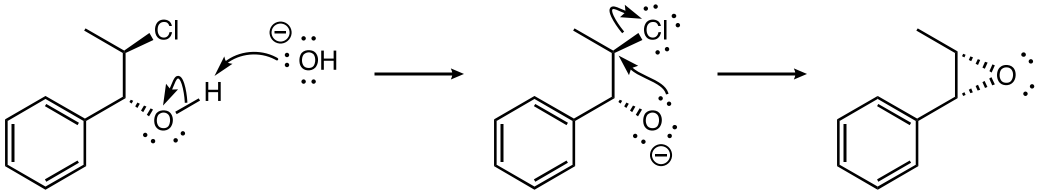


Step 2:

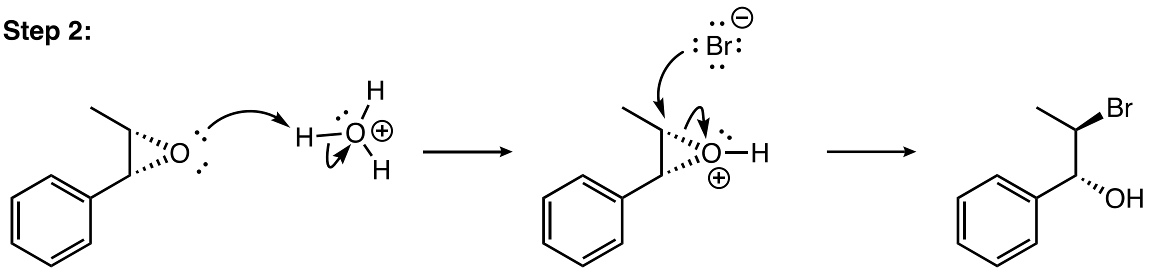


Consider the mechanism for the epoxidation of (1*R*,2*R*)-2-chlorophenylpropanol with hydroxide and its subsequent reaction with hydrobromic acid to form (1*R*,2*R*)-2-bromophenylpropanol.

Step 1:

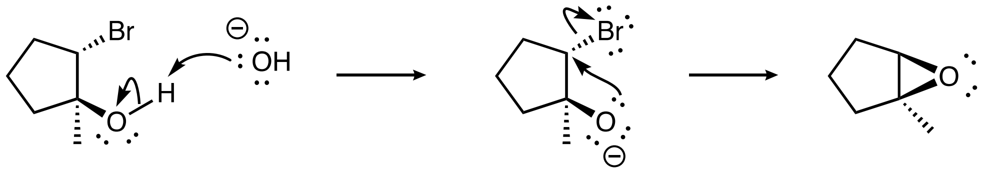


Step 2:

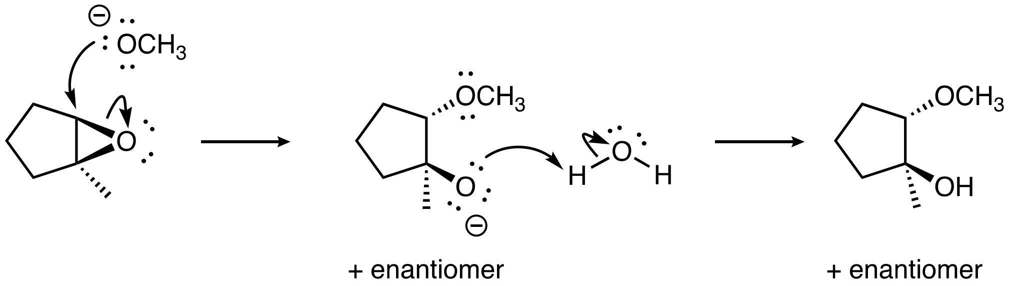


Consider the mechanism for the epoxidation of (1*S*,2*S*)-2-bromo-1-methyl-1-cyclopentanol and its subsequent reaction with methoxide to form (1*S*,2*S*)-2-methoxy-1-methyl-1-cyclopentanol.

Step 1:

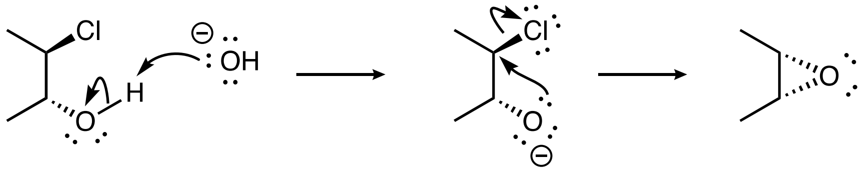


Step 2:

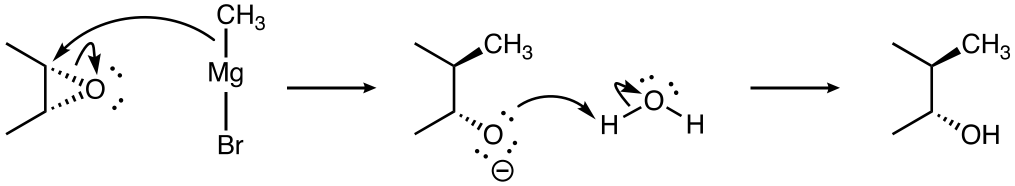


Consider the mechanism for the epoxidation of (2*R*,3*R*)-3-chloro-2-butanol and its subsequent reaction with methylmagnesium bromide to form (*R*)-3-methyl-2-butanol.

Step 1:

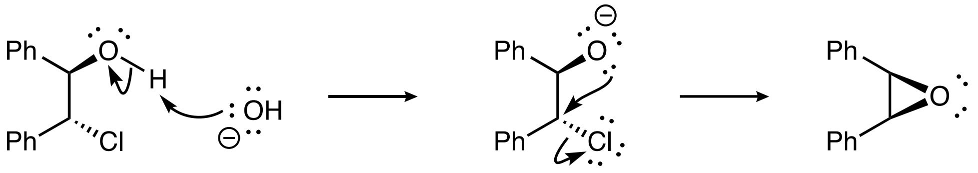


Step 2:

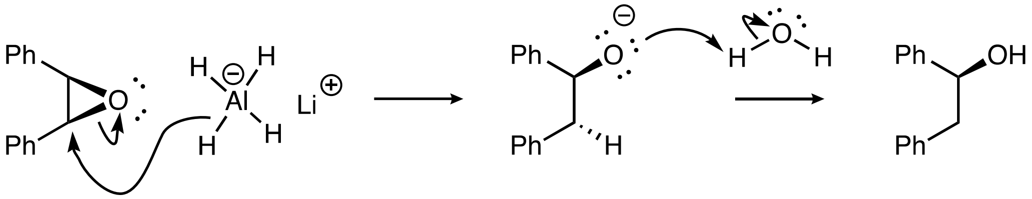


Consider the mechanism for the epoxidation of (1*R*,2*R*)-2-chloro-1,2-diphenyl-1-ethanol and its subsequent reaction with lithium aluminum hydride to form (*S*)-1,2-diphenyl-1-ethanol.

Step 1:



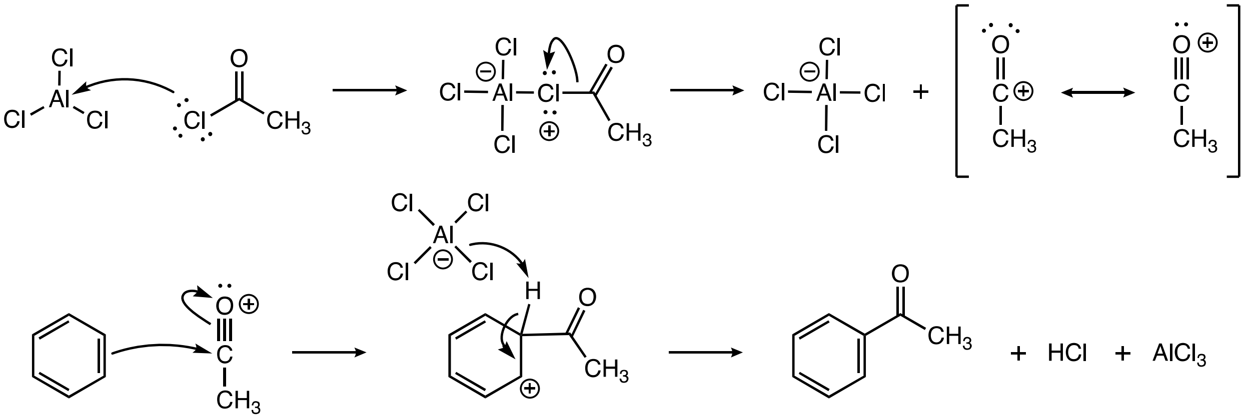
Step 2:



AROMATIC RING

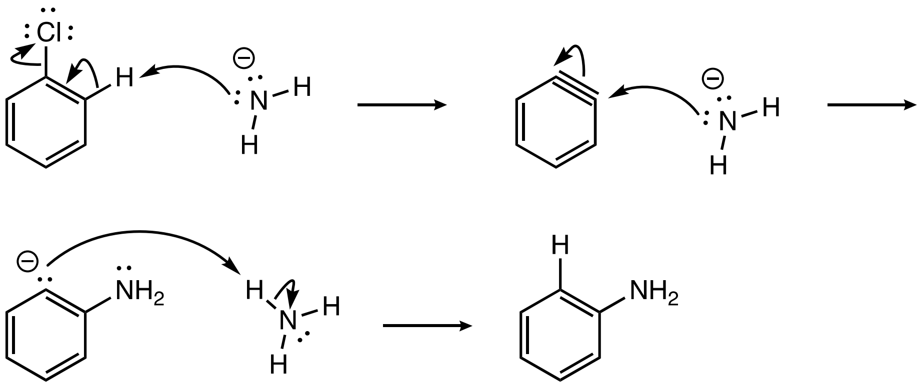
ACYLATION

Consider the mechanism for the Friedel-Crafts acylation of benzene to form acetophenone.



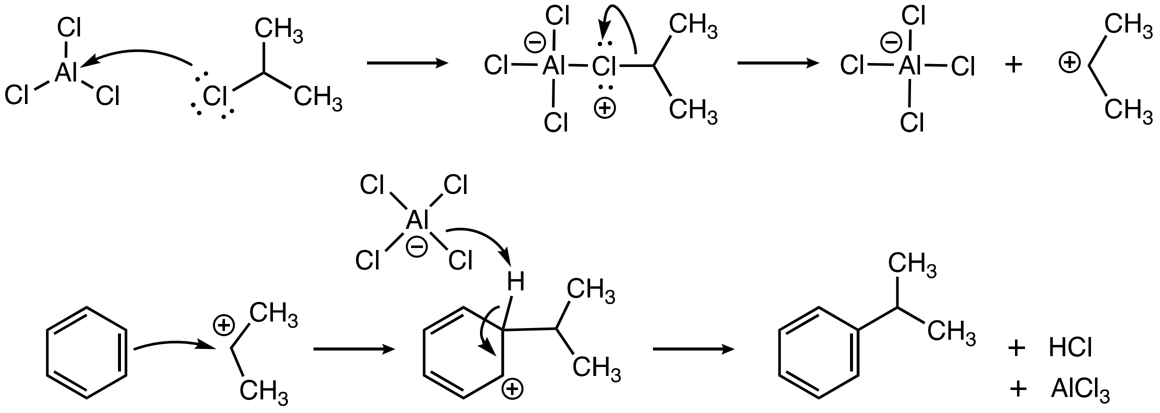
ADDITION–ELIMINATION

Consider the mechanism for the addition–elimination reaction of chlorobenzene with amide to form aniline.



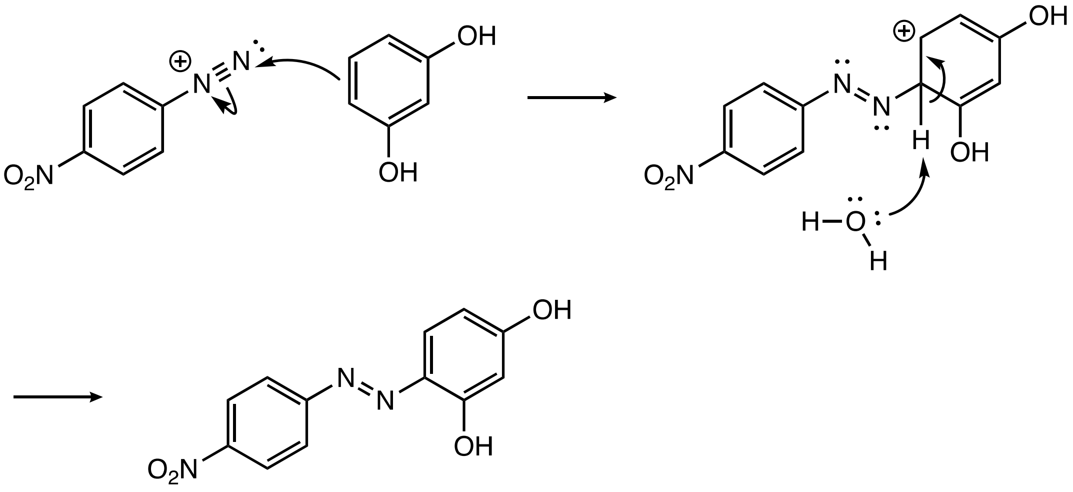
ALKYLATION

Consider the mechanism for the Friedel-Crafts alkylation of benzene to form isopropylbenzene.



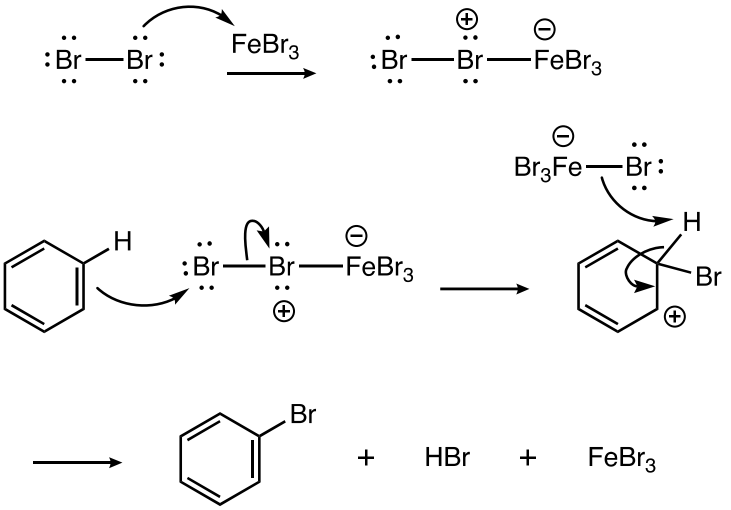
AZO COUPLING

Consider the mechanism for the azo coupling reaction between 4-nitrobenzenediazonium and resorcinol to form azo violet.

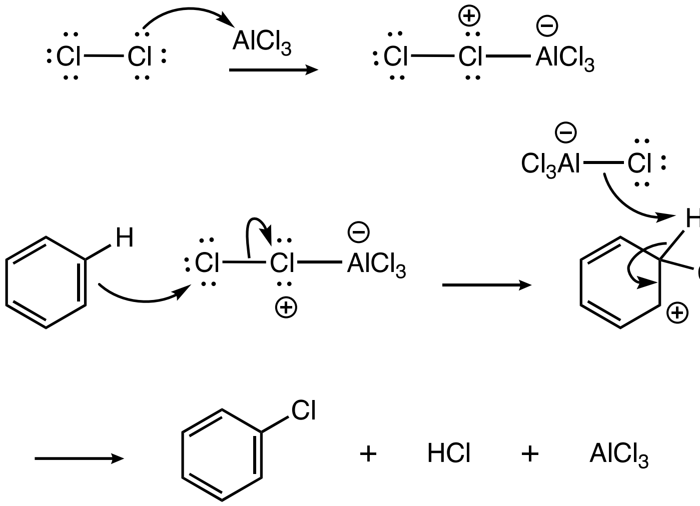


ELECTROPHILIC AROMATIC SUBSTITUTION

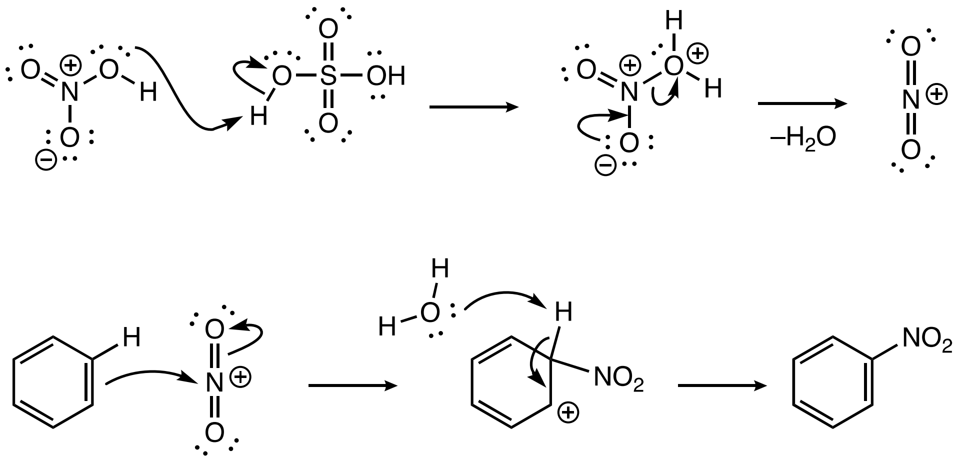
Consider the mechanism for the electrophilic aromatic bromination of benzene to form bromobenzene.



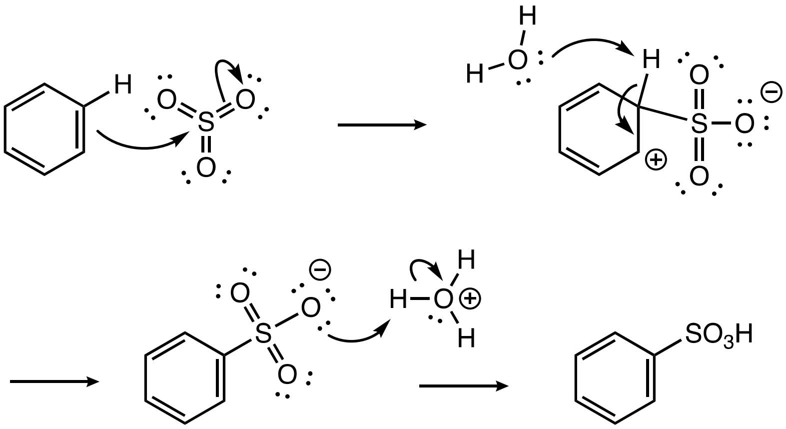
Consider the mechanism for the electrophilic aromatic chlorination of benzene to form chlorobenzene.



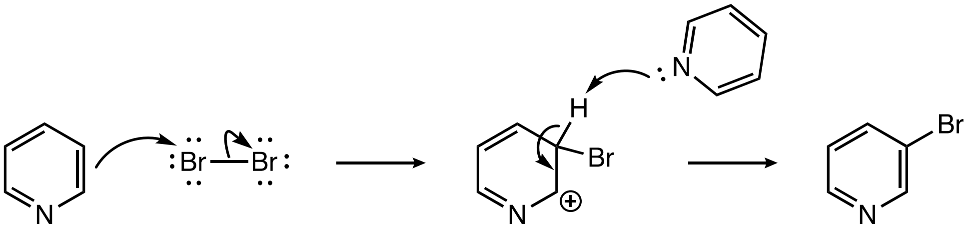
Consider the mechanism for the electrophilic aromatic nitration of benzene to form nitrobenzene.



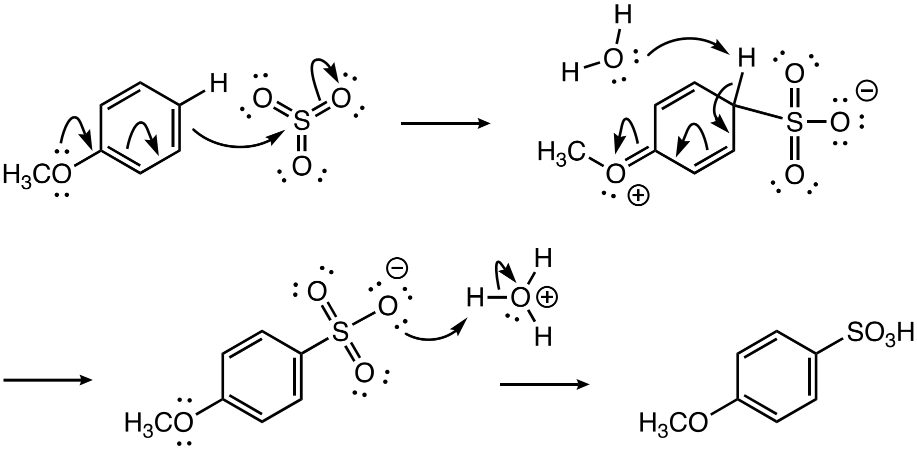
Consider the mechanism for the electrophilic aromatic sulfonation of benzene to form benzenesulfonic acid.



Consider the mechanism for electrophilic aromatic bromination of pyridine to form 3-bromopyridine.

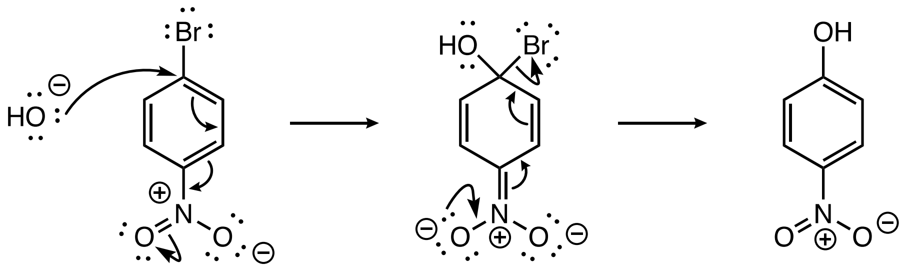


Consider the mechanism for the electrophilic aromatic sulfonation of anisole with hydroxide to form 4-methoxybenzenesulfonic acid.

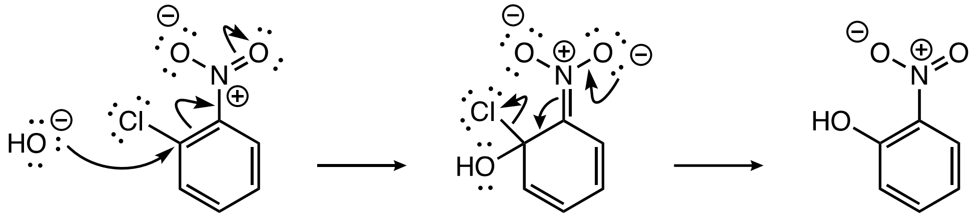


NUCLEOPHILIC AROMATIC SUBSTITUTION

Consider the mechanism for the nucleophilic aromatic substitution of 1-bromo-4-nitrobenzene with hydroxide to form 4-nitrophenol.



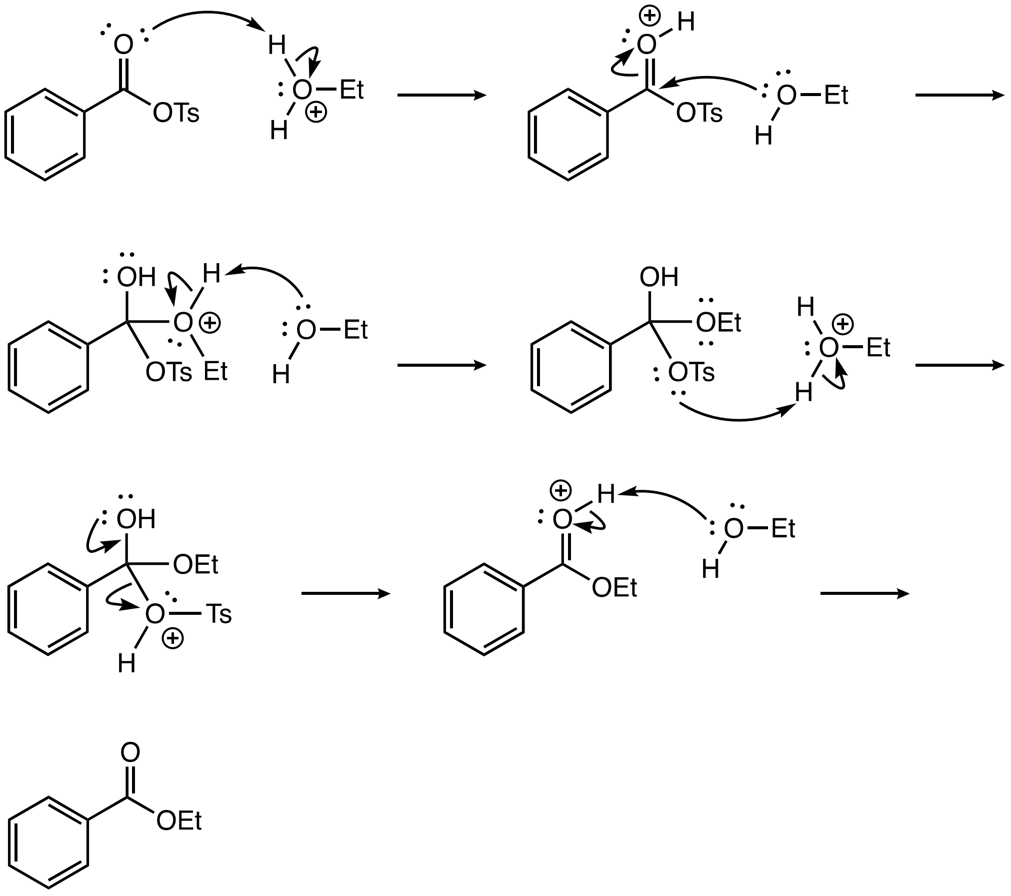
Consider the mechanism for the nucleophilic aromatic substitution of 1-choloro-2-nitrobenzene with hydroxide to form 2-nitrophenol.



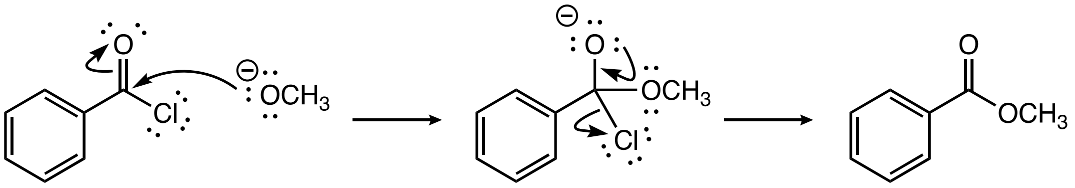
CARBONYL

ACYL SUBSTITUTION

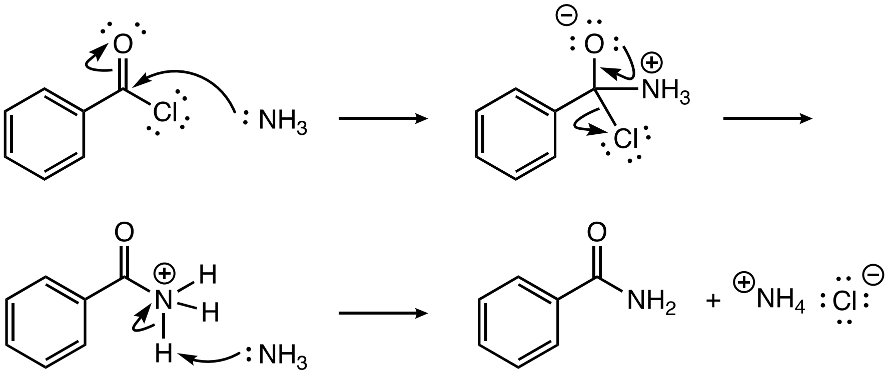
Consider the mechanism for the acid-catalyzed nucleophilic acyl substitution of benzoic 4-methylbenzenesulfonic anhydride with ethanol to form ethyl benzoate.



Consider the mechanism for the base-catalyzed nucleophilic acyl substitution of benzoyl chloride with methoxide to form methyl benzoate.

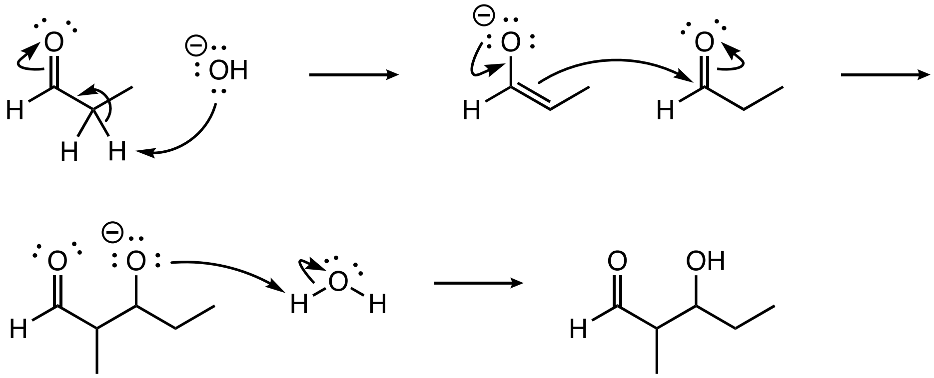


Consider the mechanism for the nucleophilic acyl substitution of benzoyl chloride with ammonia to form benzamide.

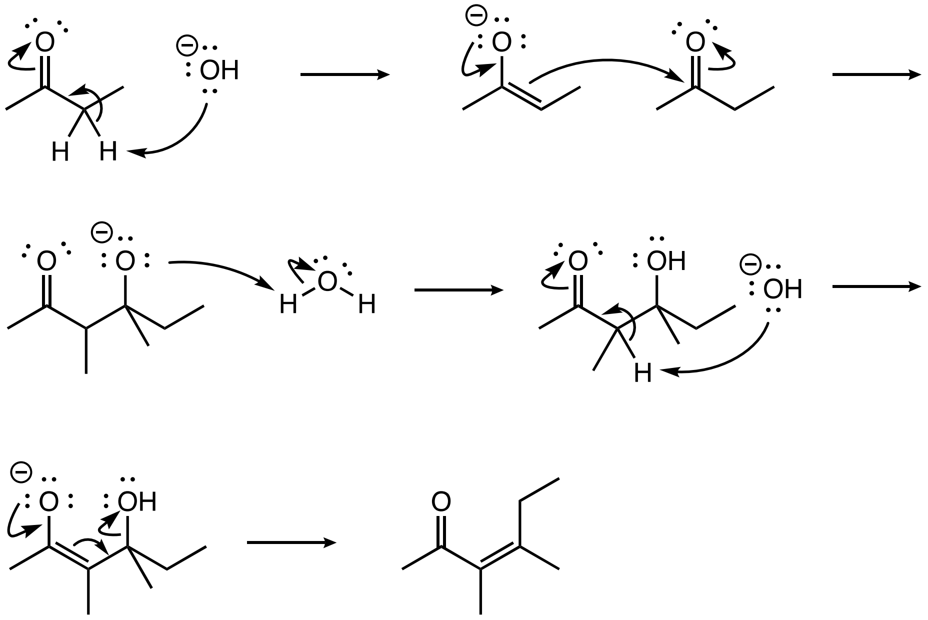


ALDOL ADDITION / SUBSTITUTION

Consider the mechanism for the aldol addition of propanal to itself to form 3-hydroxy-2-methylpentanal.

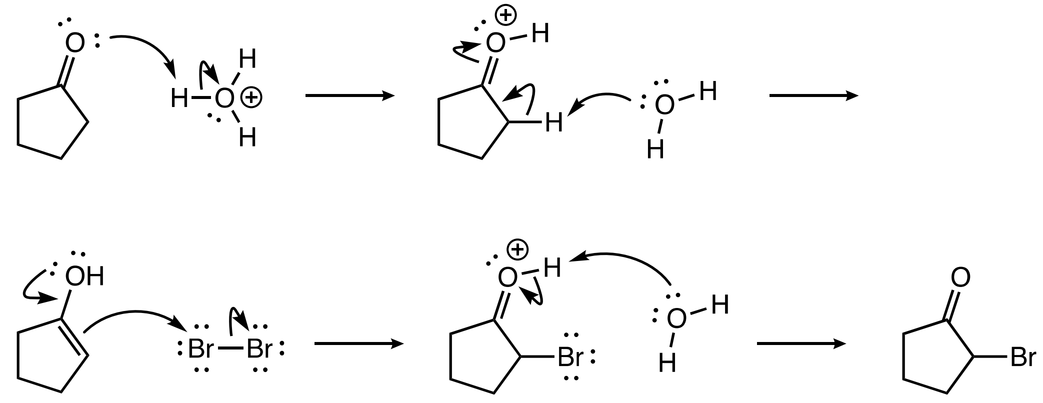


Consider the mechanism for the aldol condensation of 2-butanone to form (*Z*)-3,4-dimethyl-3-hexen-2-one.



ALPHA-HALOGENATION

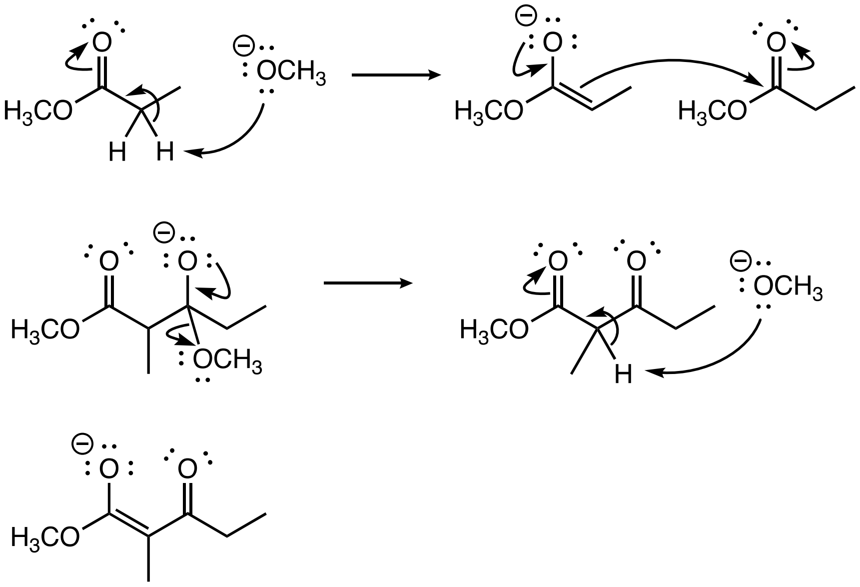
Consider the mechanism for the acid-catalyzed bromination of cyclopentanone to form 2-bromocyclopentanone.



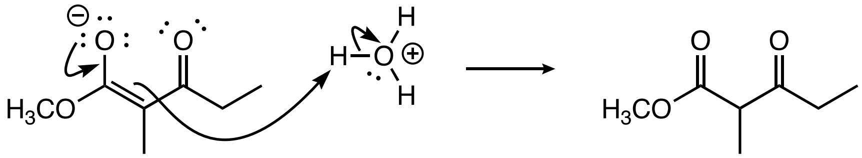
CONDENSATION OF AN ESTER / DIESTER

Consider the mechanism for the Claisen condensation of methyl propanoate to form methyl 2-methyl-3-oxopentanoate.

Step 1:

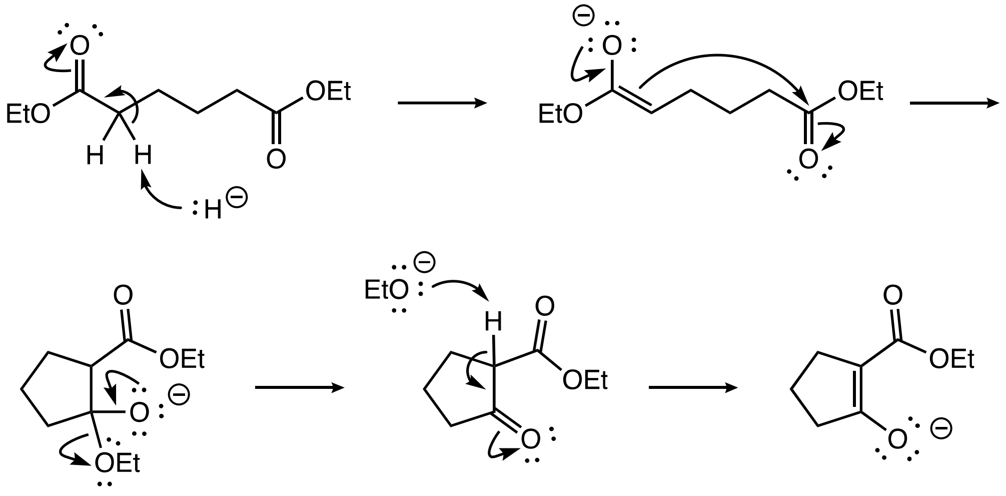


Step 2:

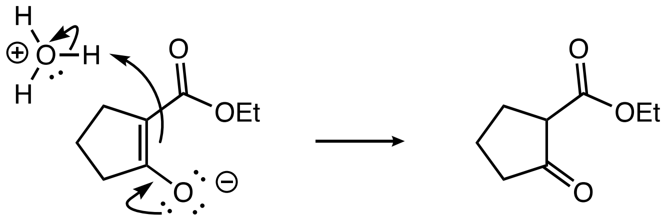


Consider the mechanism for the Dieckmann cyclization of diethyl adipate to form ethyl cyclopentanone-2-carboxylate.

Step 1:



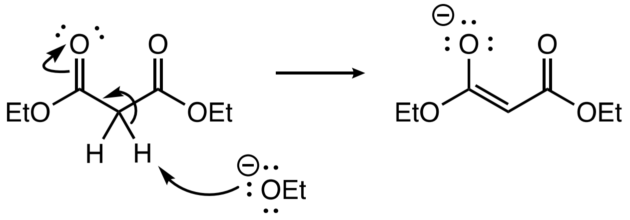
Step 2:



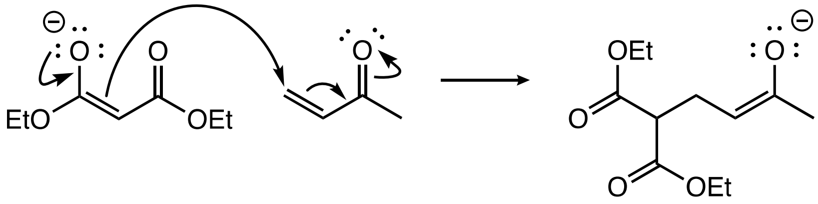
CONJUGATE ADDITION

Consider the mechanism for the conjugate addition of diethyl malonate with methyl vinyl ketone to form diethyl 2-(3-oxobutyl)malonate.

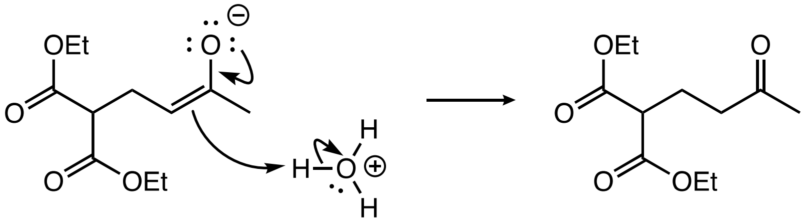
Step 1:



Step 2:

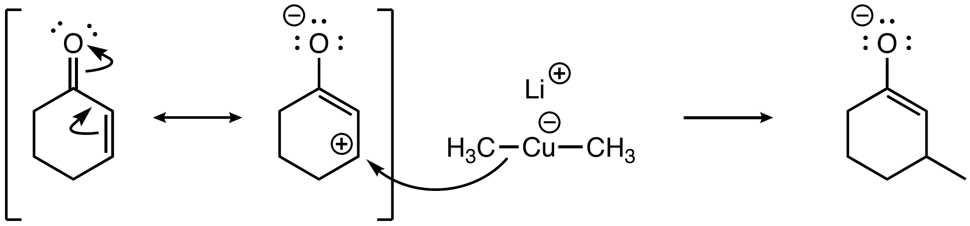


Step 3:

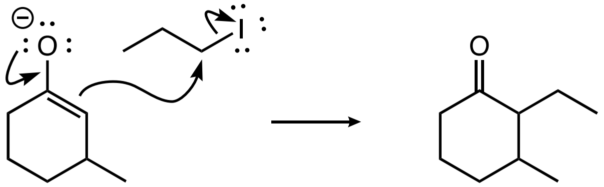


Consider the mechanism for the conjugate addition of cyclo-2-hexen-1-one with lithium dimethylcuprate and subsequently with 1-iodopropane to form 2-ethyl-3-methylcyclo-1-hexanone.

Step 1:

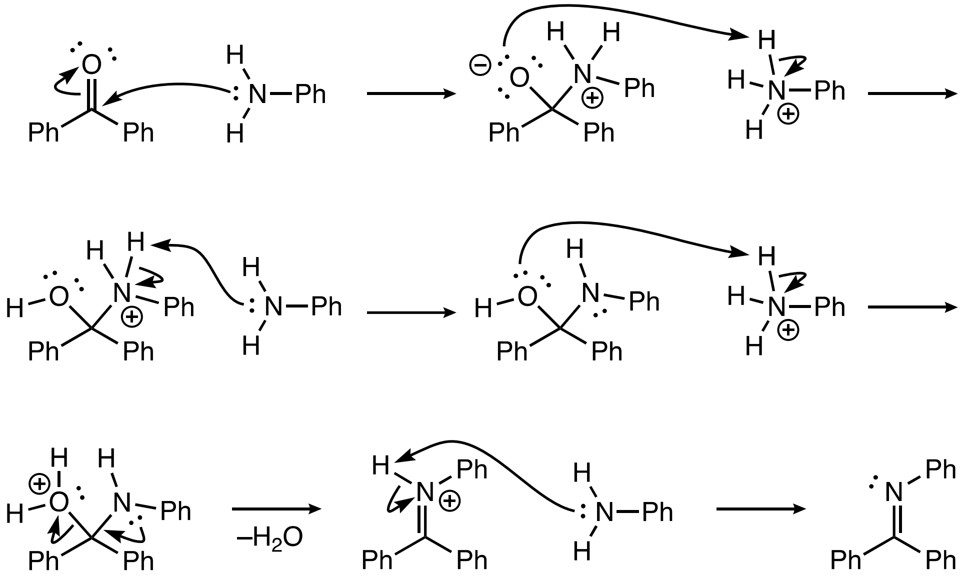


Step 2:

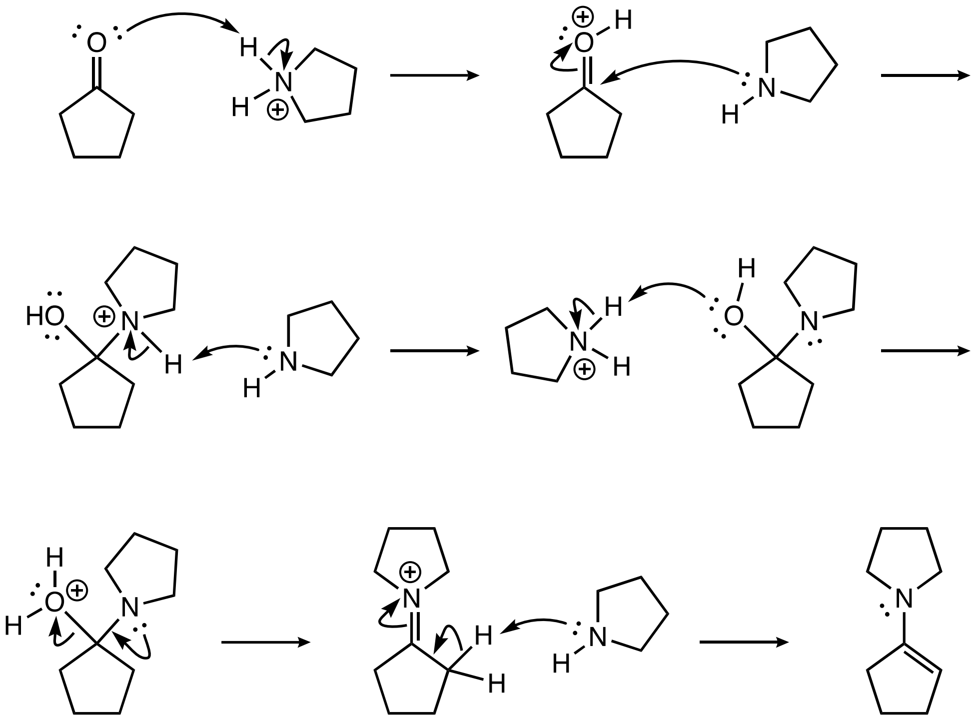


ENAMINE/IMINE SYNTHESIS

Consider the mechanism for the acid-catalyzed nucleophilic addition of phenylamine to benzophenone to form *N*-(diphenylmethylene)phenylamine.

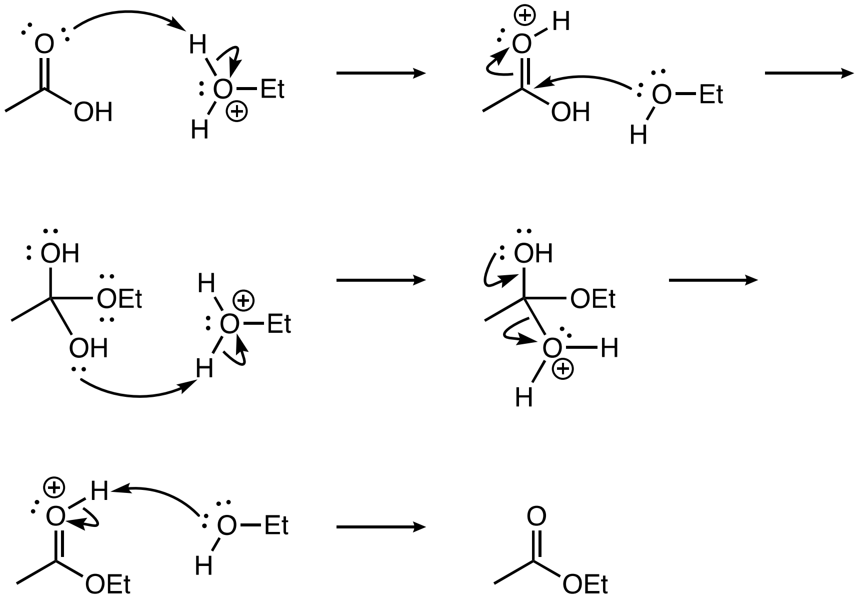


Consider the mechanism for the enamine synthesis between cyclopentanone and pyrrolidine to form 1-(cyclopent-1-en-1-yl)pyrrolidine.



ESTERIFICATION

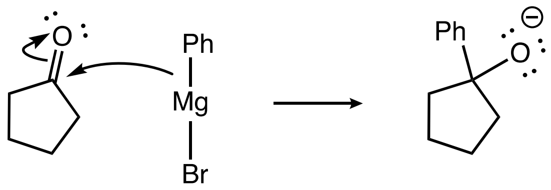
Consider the mechanism for the acid-catalyzed Fischer esterification of acetic acid with ethanol to form ethyl acetate.



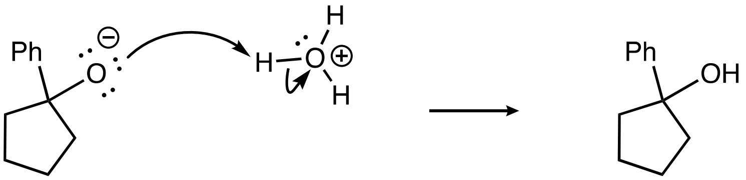
GRIGNARD

Consider the mechanism for the Grignard reaction between phenylmagnesium bromide and cyclopentanone to form phenylcyclopentanol.

Step 1:

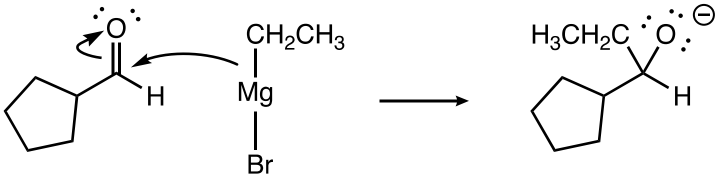


Step 2:

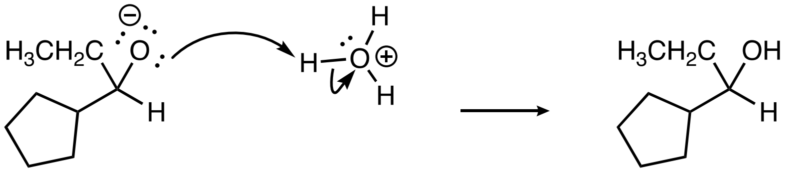


Consider the mechanism for the Grignard reaction between ethylmagnesium bromide and cyclopentanecarbaldehyde to form 1-cyclopentyl-1-propanol.

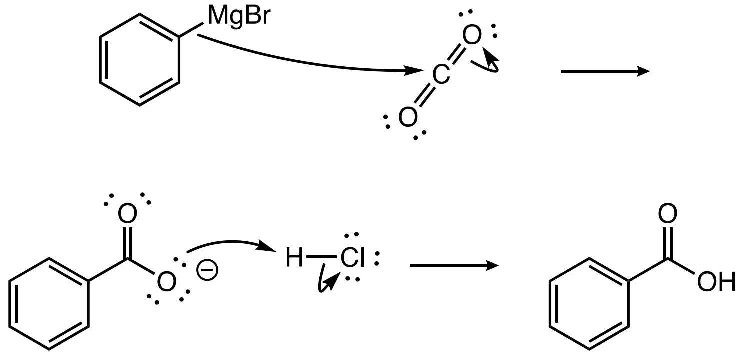
Step 1:



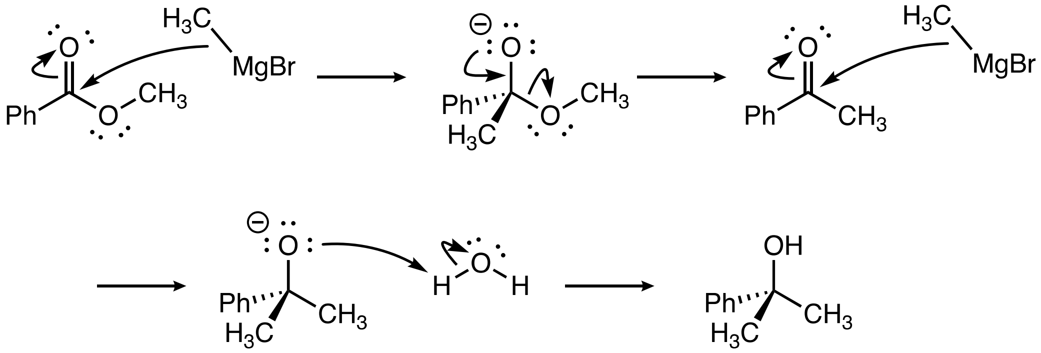
Step 2:



Consider the mechanism for the Grignard reaction between phenylmagnesium bromide and carbon dioxide to form benzoic acid.

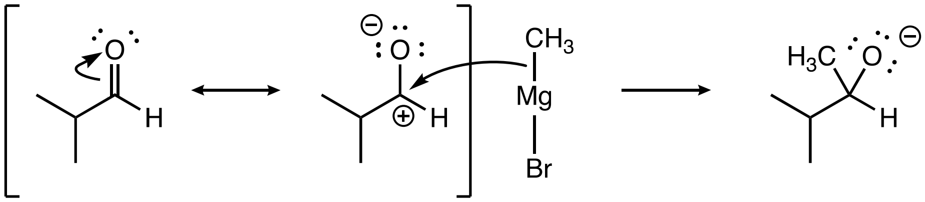


Consider the mechanism for the Grignard reaction between methyl benzoate and methylmagnesium bromide to form 2-phenyl-2-propanol.

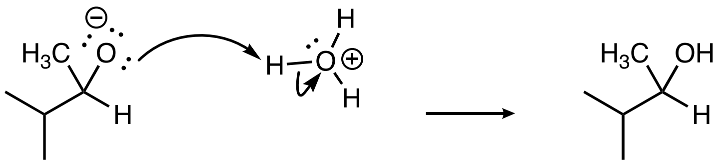


Consider the mechanism for the Grignard reaction between isobutyraldehyde and methylmagnesium bromide to form 3-methyl-2-butanol.

Step 1:

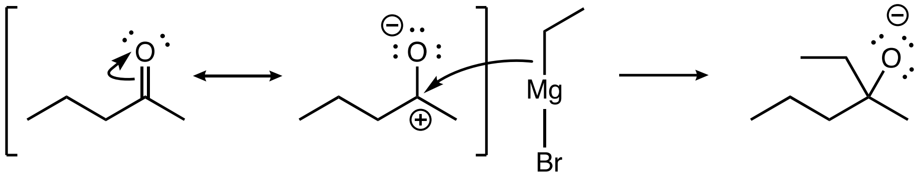


Step 2:

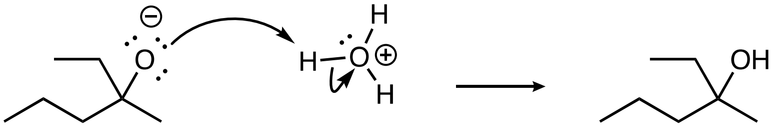


Consider the mechanism for the Grignard reaction between 2-pentanone and ethylmagnesium bromide to form 3-methyl-3-hexanol.

Step 1:

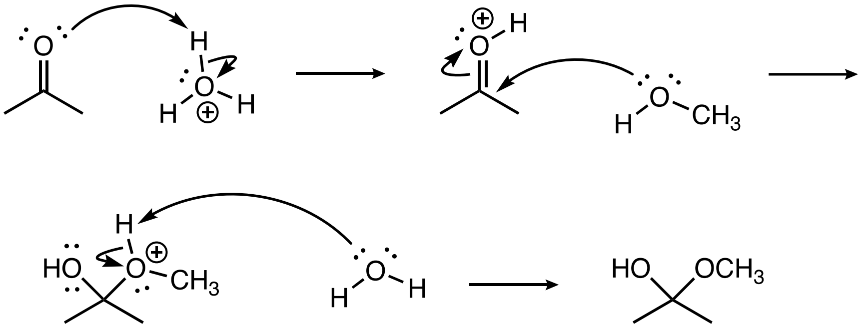


Step 2:

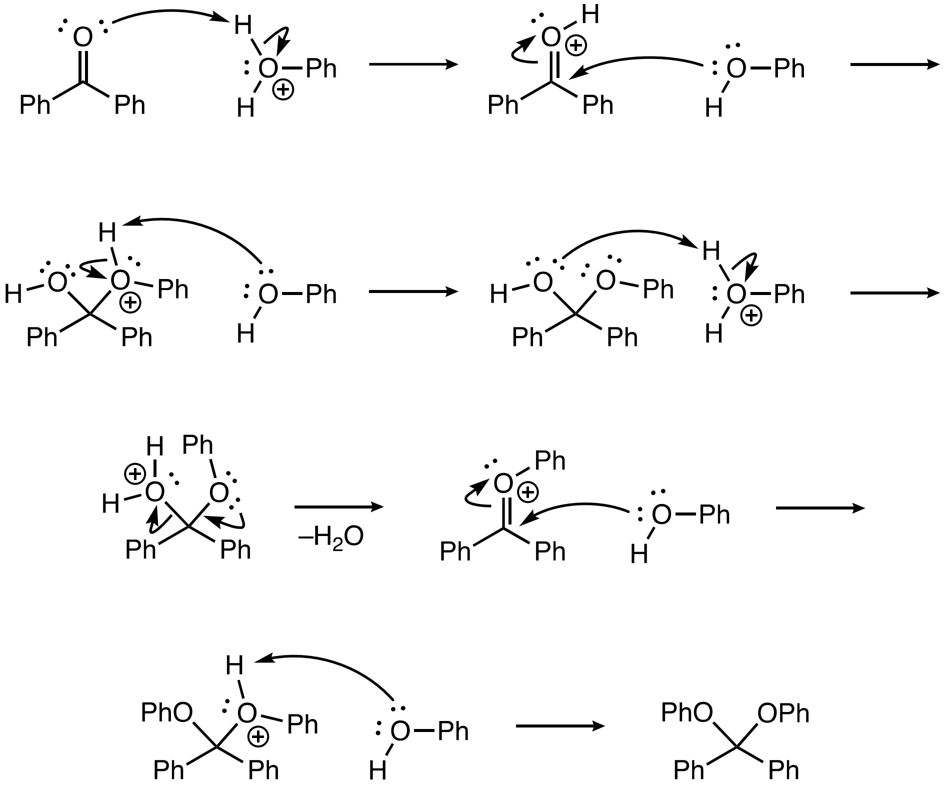


HEMIACETAL / ACETAL FORMATION

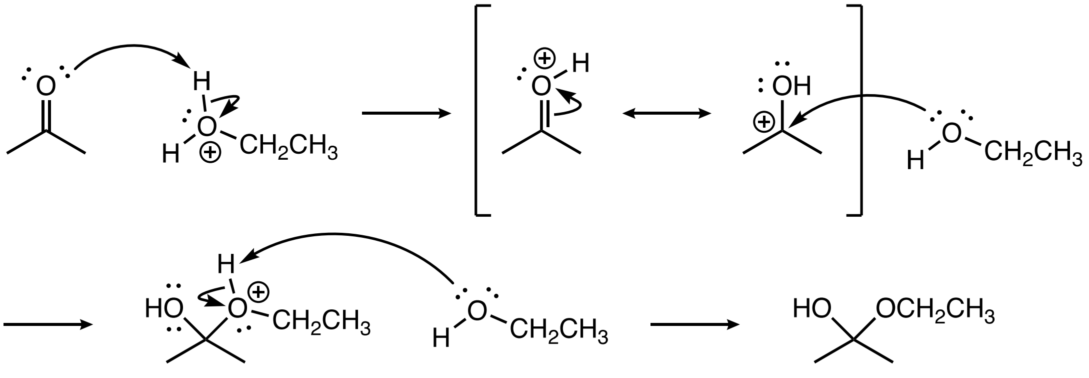
Consider the mechanism for the hemiacetal formation reaction between acetone, hydronium ion, and methanol to form 2-methoxypropan-2-ol.



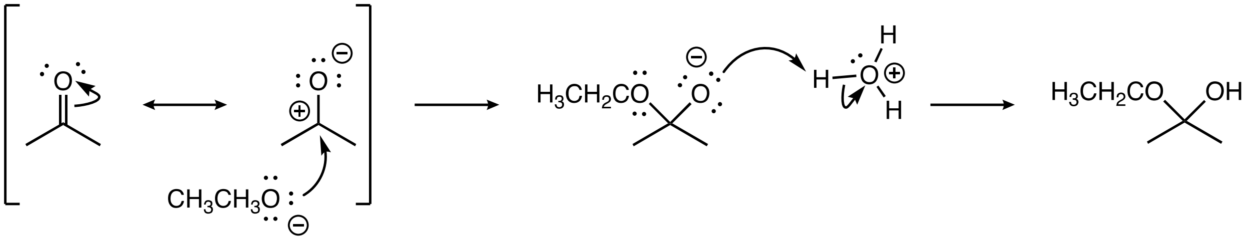
Consider the mechanism for the acid-catalyzed nucleophilic addition of phenol to benzophenone to form diphenoxydiphenylmethane.



Consider the mechanism for the acid-catalyzed hemiacetal formation from acetone and ethanol to form 2-ethoxy-2-propanol.

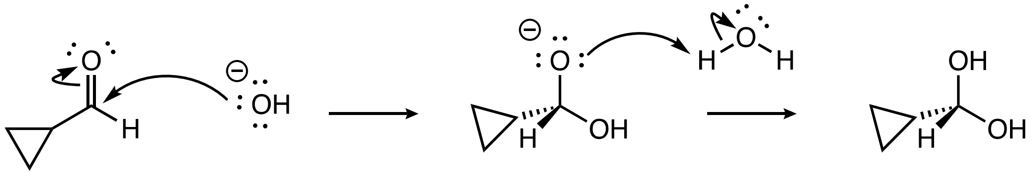


Consider the mechanism for the base-catalyzed hemiacetal formation from acetone and ethoxide to form 2-ethoxy-2-propanol.



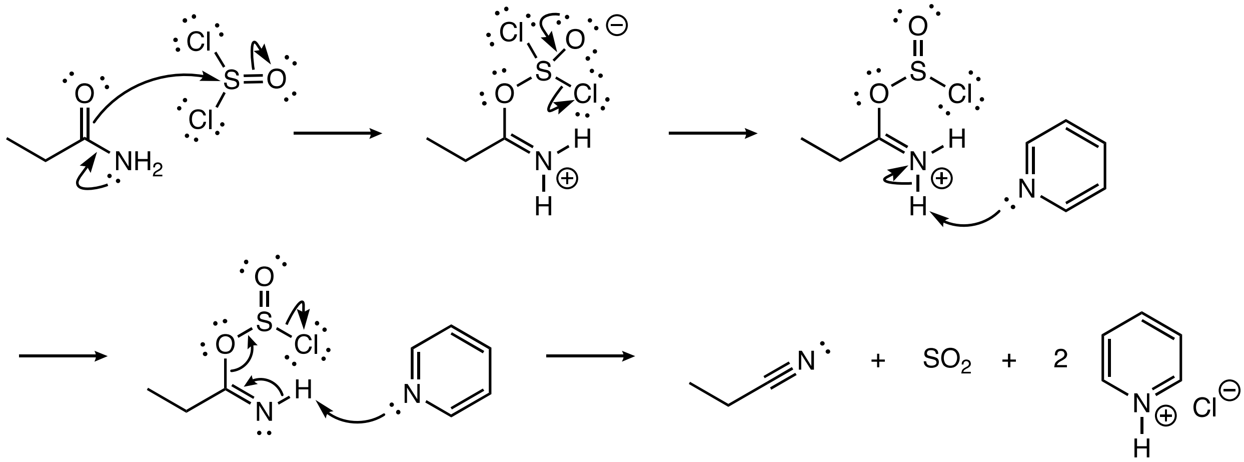
HYDRATION / DEHYDRATION

Consider the mechanism for the base-catalyzed hydration of cyclopropanecarbaldehyde to form cyclopropylmethanediol.



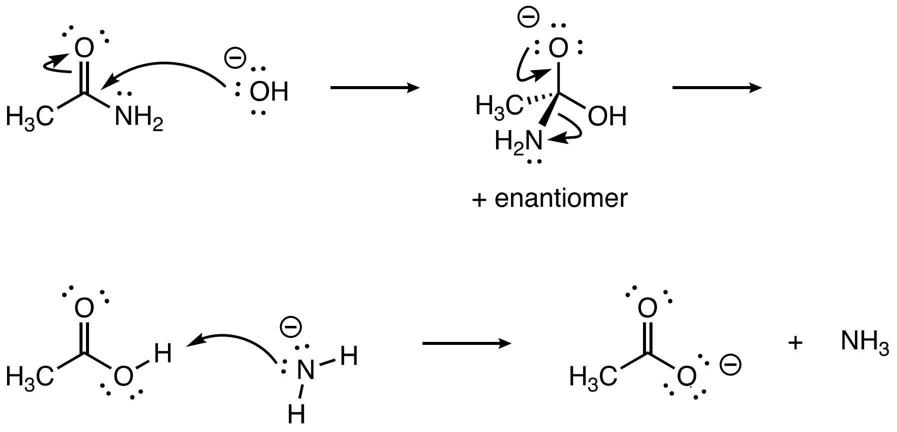
+ enantiomer

Consider the mechanism for the dehydration of propionamide with thionyl chloride to form propionitrile.



HYDROLYSIS

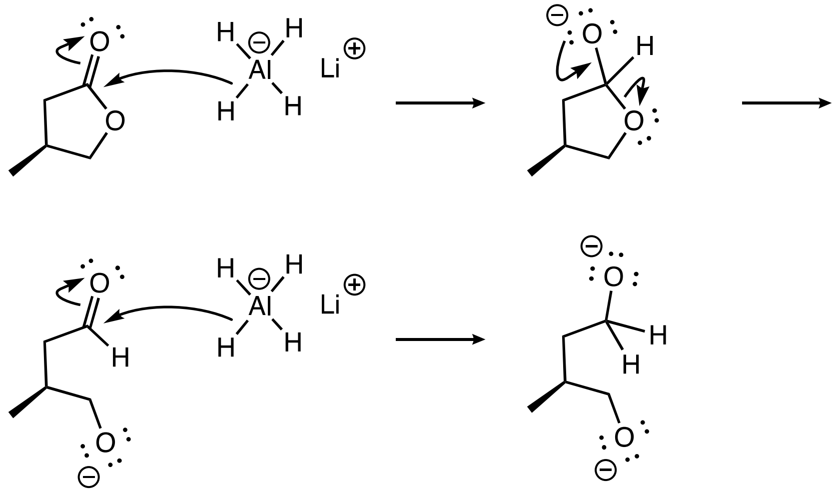
Consider the mechanism for the base-catalyzed hydrolysis of acetamide to give acetate and ammonia.



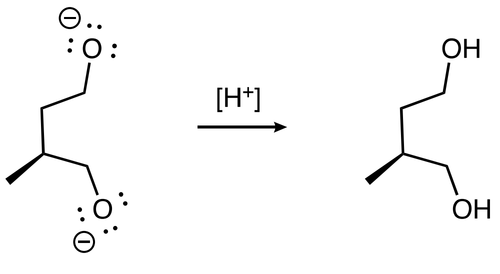
REDUCTION

Consider the mechanism for the reduction of α-methyl-γ-butyrolactone with lithium aluminum hydride to form (*S*)-2-methylbutane-1,4-diol.

Step 1:

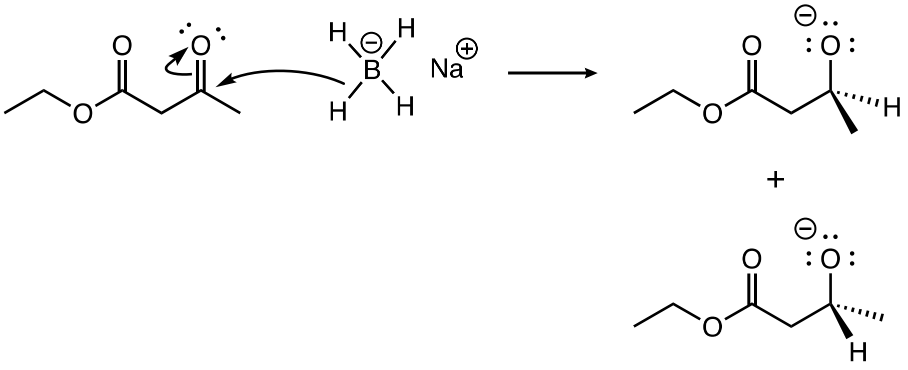


Step 2:

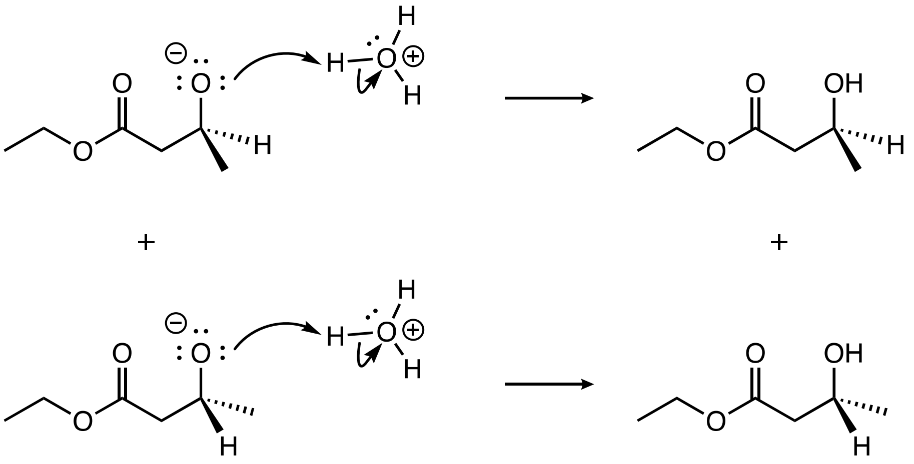


Consider the mechanism for the reduction of ethyl 3-oxobutanoate with sodium borohydride to form ethyl 3-hydroxybutanoate.

Step 1:

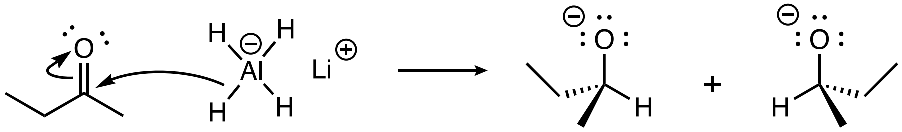


Step 2:

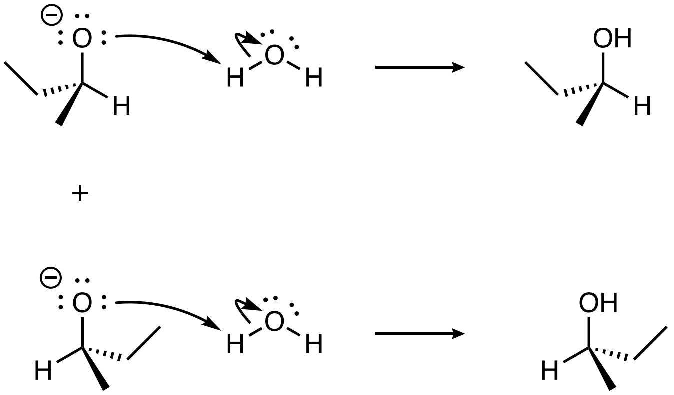


Consider the mechanism for the reduction of 2-butanone with lithium aluminum hydride to form 2-butanol.

Step 1:

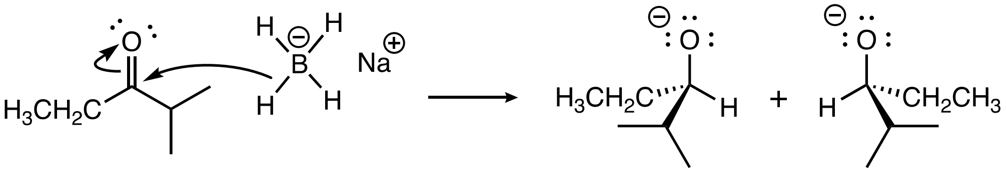


Step 2:

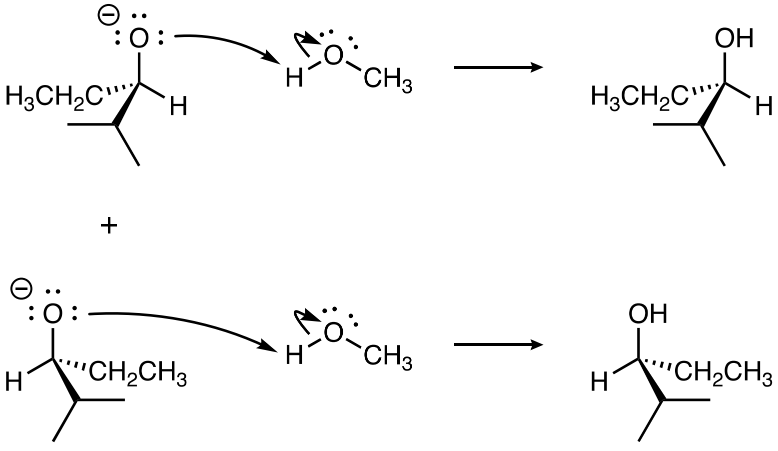


Consider the mechanism for the reduction of 2-methyl-3-pentanone with sodium borohydride to form 2-methyl-3-pentanol.

Step 1:

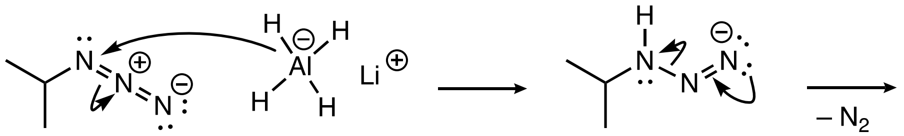


Step 2:

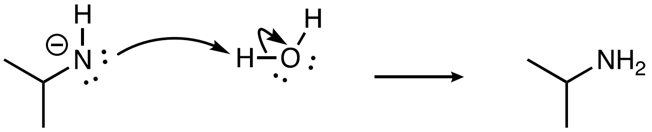


Consider the mechanism for the reduction of 2-azidopropane with lithium aluminum hydride to form isopropylamine.

Step 1:

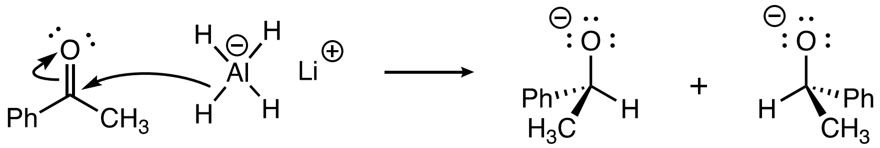


Step 2:

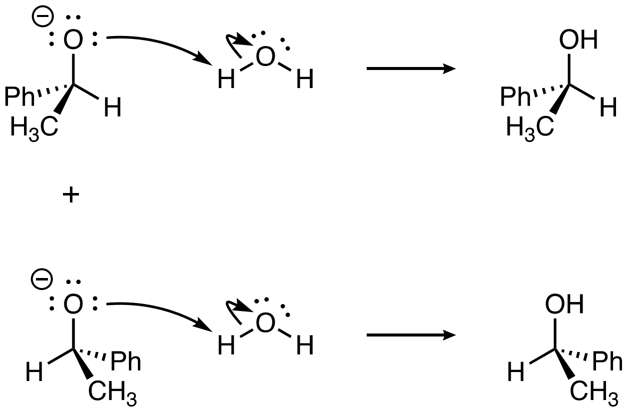


Consider the mechanism for the reduction of acetophenone with lithium aluminum hydride to form 1-phenyl-1-ethanol.

Step 1:

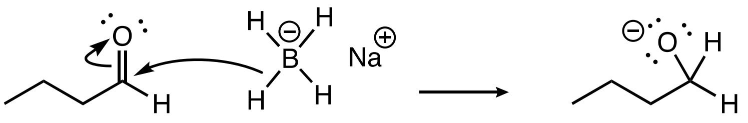


Step 2:

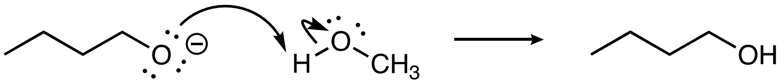


Consider the mechanism for the reduction of butyraldehyde with sodium borohydride to form 1-butanol.

Step 1:

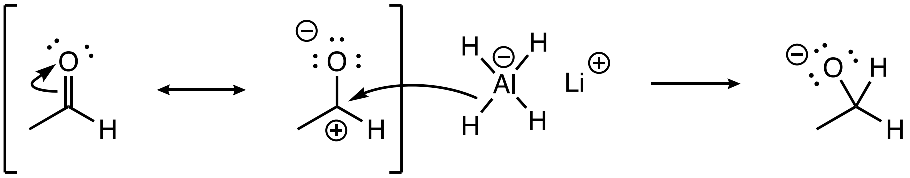


Step 2:

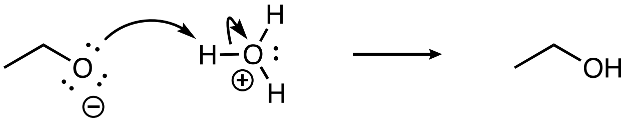


Consider the mechanism for the reduction of acetaldehyde with lithium aluminum hydride to form ethanol.

Step 1:

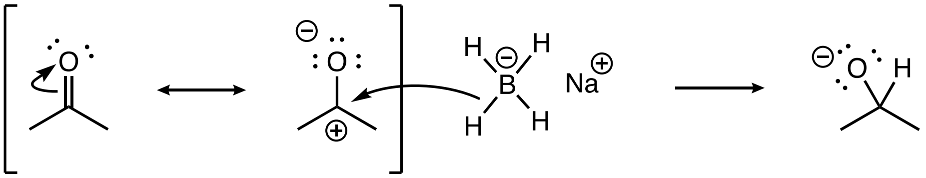


Step 2:

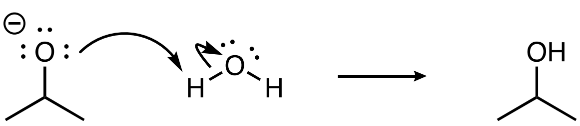


Consider the mechanism for the reduction of acetone with sodium borohydride to form isopropanol.

Step 1:



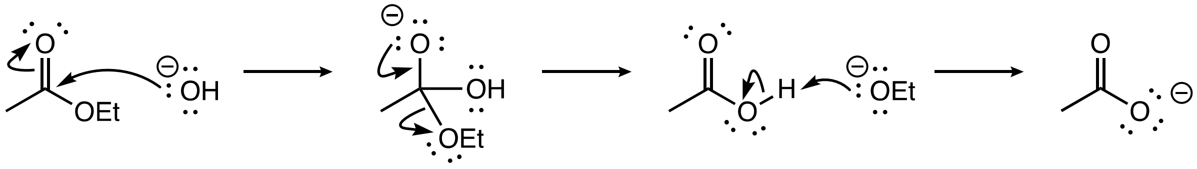
Step 2:



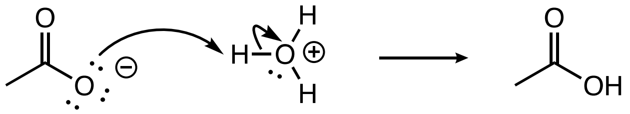
SAPONIFICATION

Consider the mechanism for the saponification of ethyl acetate with hydroxide to form acetic acid.

Step 1:



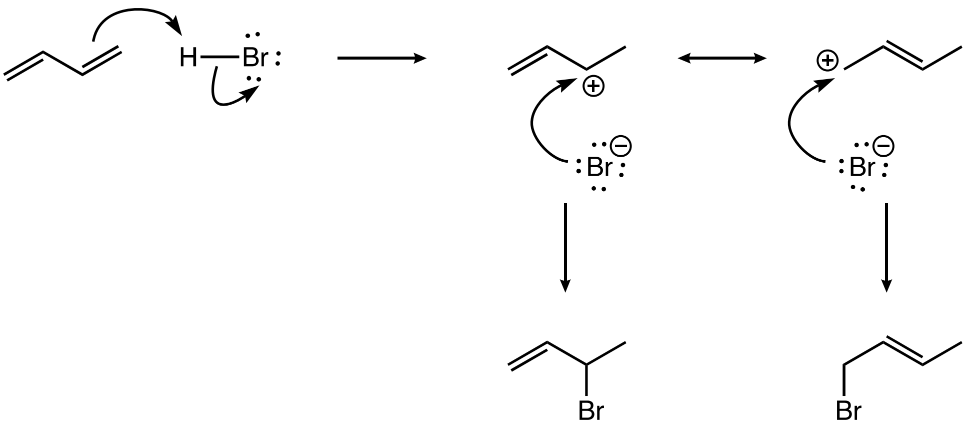
Step 2:



CONJUGATED DIENE

ELECTROPHILIC ADDITION

Consider the mechanism for the addition of a hydrogen halide to a conjugated alkene reaction between 1,3-butadiene and hydrobromic acid to form 3-bromo-1-butene and 1-bromo-2-butene.



Consider the mechanism for the addition of a hydrogen halide to an alkene reaction between 1-methyl-1,3-cyclohexene and hydrobromic acid to form 3-bromo-1-methyl-1-cyclohexene and 3-bromo-3-methyl-1-cyclohexene.