Alkynes

1-Nomenclature and Synthesis

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Alkynes – Introduction and Nomenclature

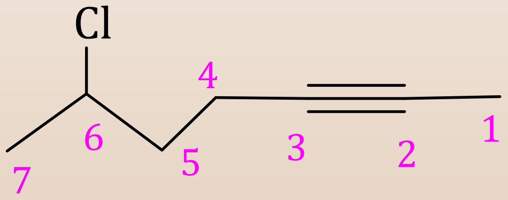
Alkynes have a triple bond in the structure. The triple bond is sp hybridized, has a 180^{o} bond angle, and is linear in shape. Alkynes have 2^{o} of unsaturation, i.e., they have 4 H less than the corresponding alkanes.

Alkynes names will end in "-*yne*" as the suffix. The first three alkynes are given below. As you can see with butyne there are 2 isomers possible. In this case the location of the triple bond is to be noted. The general name is given in italics.

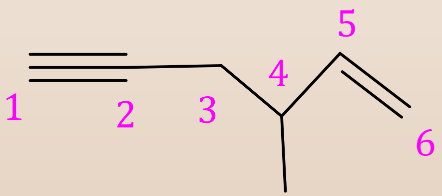
$HC \equiv CH$	ethyne (*acetylene*)
$CH_3C \equiv CH$	propyne
$CH_3CH_2C \equiv CH$	but-1-yne
$CH_3C \equiv CCH_3$	but-2-yne

Nomenclature

- Numbering of chain with triple bond is such that the first carbon of the triple bond gets assigned the smallest number.
- In case of alkene and alkynes, alkynes get priority for naming and numbering, i.e., name should end in yne.



6-chlorohept-2-yne



4-methylhex-5-ene-1-yne

Alkynes rarely exist in cyclic compounds since the triple bond has a bond angle of 180^{o} and it needs a really large ring to exist in a stable state.

Physical Properties and Applications

Physical Properties are similar to alkenes and alkynes.

1. Boiling points - Small molecular weight alkynes are gases and then become liquid as the molecular weight increases (more van der Waal and internal dipole forces).
2. Solubility in water - They are insoluble in water due to difference in IMF.
3. Density - They have lower density than water.
4. Odor – Variable and generally not pleasant.

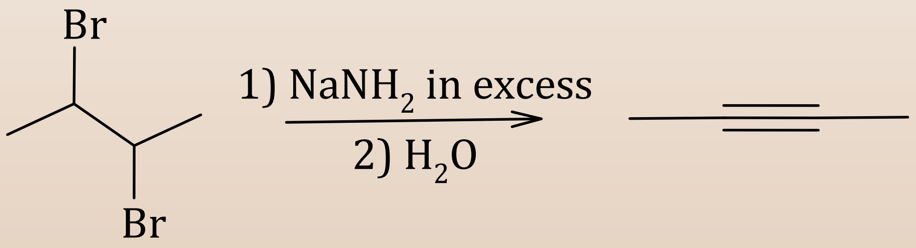
Applications

- Acetylene (ethyne) torch – used in welding. Burns to give a very high temperature flame.
- Used primarily as starting materials for alkenes or alkanes.
- Functional group can be found in molecules – but not common.

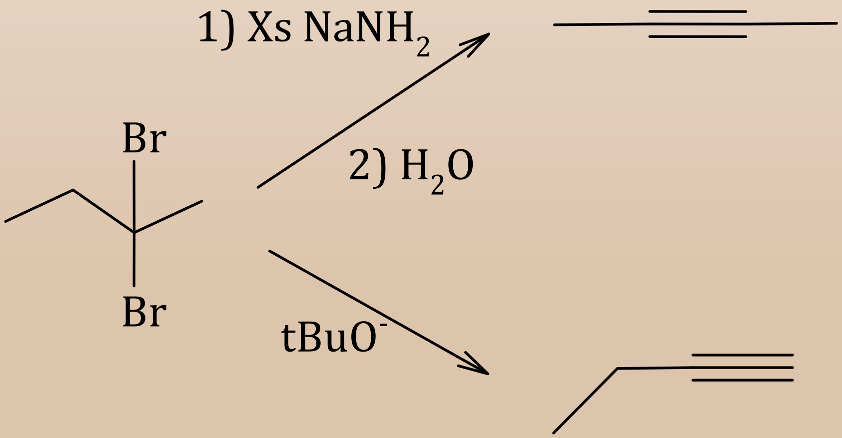
Synthesis – From Alkyl Halides

Elimination using alkyl halides as substrate is the best way to make alkynes. The mechanism is E2.

We can use any halide, bromo or chloro to make an alkene and then convert it to alkyne.

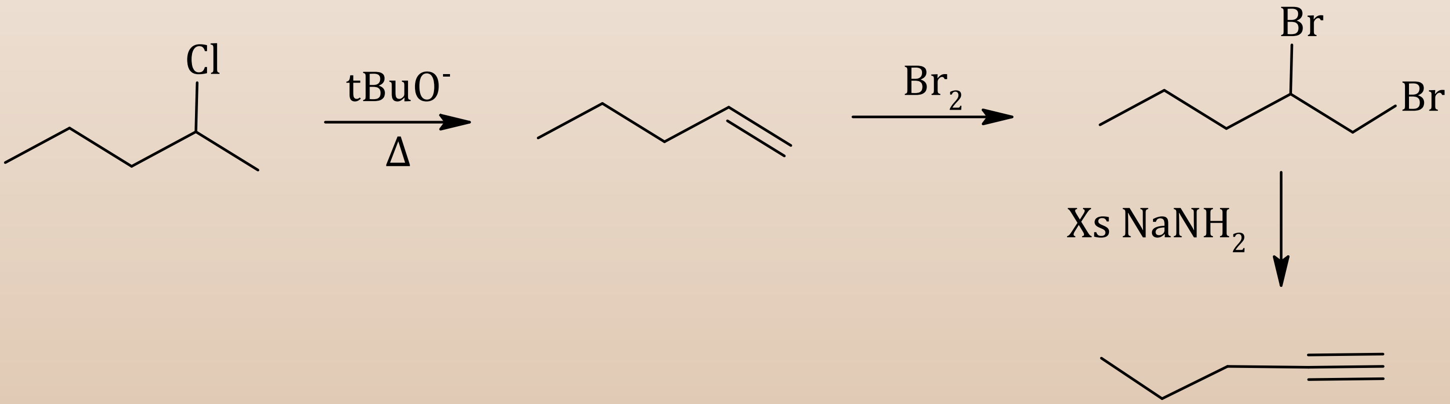


A terminal or internal alkyne can be synthesized by the choice of the base used for elimination. A bulky base will give terminal alkyne by picking up the less sterically hindered terminal protons and small base will give an internal alkyne.



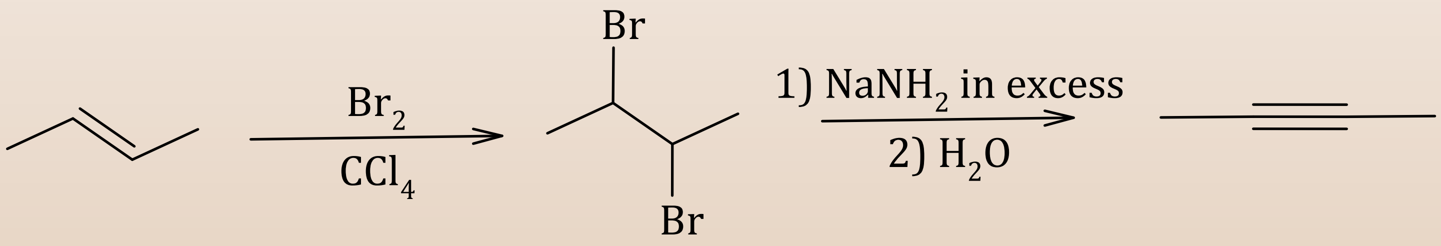
Synthesis – From Alkyl Halides

If a there is only one halide on an alkane, an elimination reaction is done first make an alkene which is then treated with halogen to make dihalogenated alkane and then treatment with excess sodium amide will lead to an alkyne.



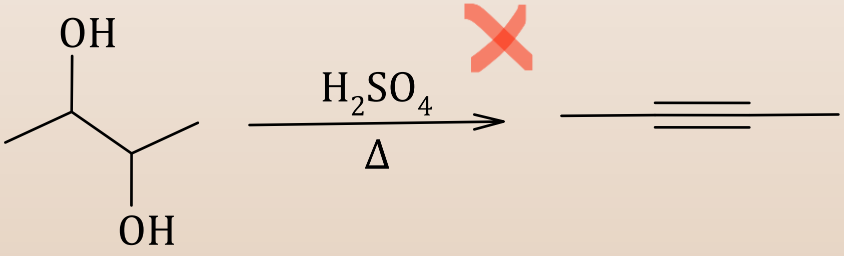
Synthesis – From Alkenes

To make an alkyne from an alkene, one has to halogenate it to get the two halides as the leaving groups and then carry out elimination with a strong base.

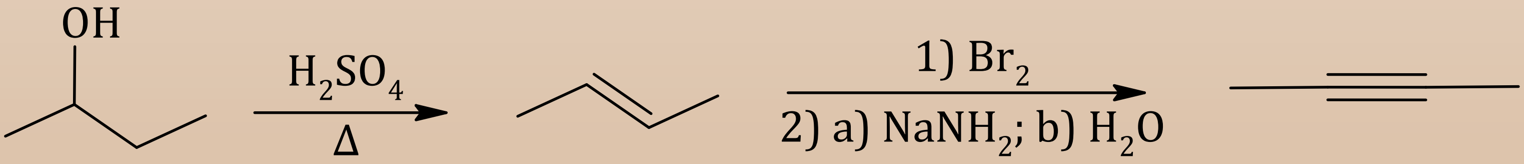


Synthesis – From Alcohols

We might think that if dihalides can do two eliminations to give alkynes then diols should be dehydrated twice to give alkynes. But that does not happen. Diols cannot be used to synthesize alkynes.



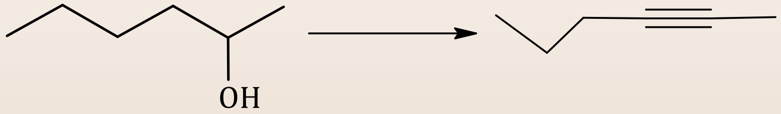
Alcohols are dehydrated to give an alkene and then alkynes can be synthesized as they are from alkenes.



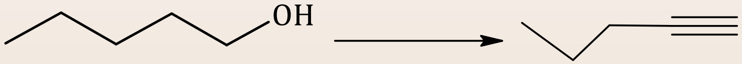
Solved Problem: Synthesizing alkynes

Show how you will carry out the synthesis of the alkynes below from the starting material given.

a)

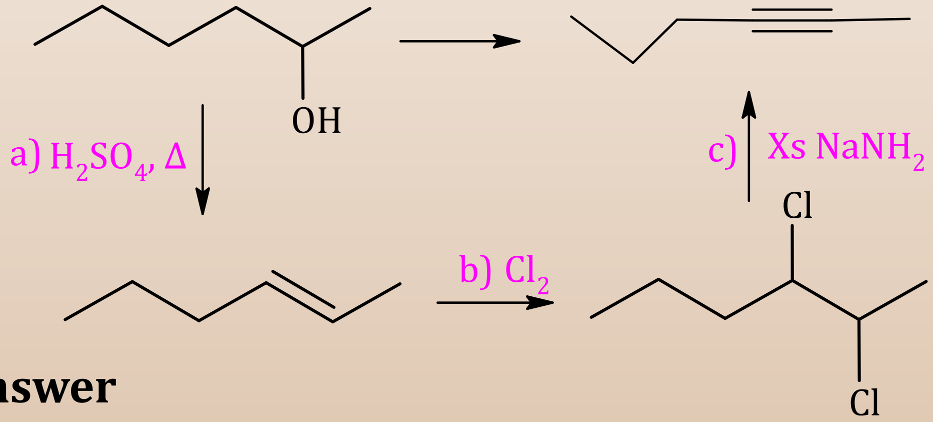


b)



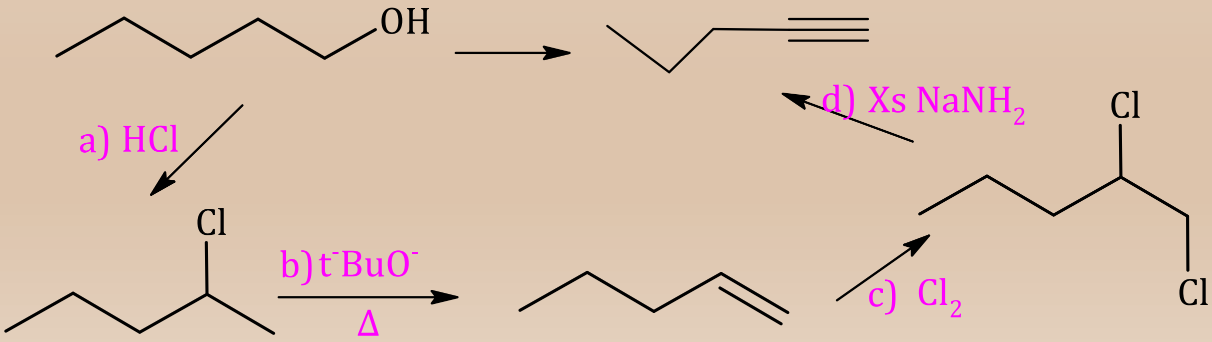
ANSWER

a)



Notes: Step **a** is done to make the alkene which will be Zaitsev's product because this is acidic dehydration. Step **c** needs a small base to get internal alkyne.

Answer b)



Notes: Step **a** carbocation mechanism so will give a 2° halide. Step **b** will give Hoffman product which is needed to get the terminal alkyne. Step **d** needs a small base to get internal alkyne.

Key Words/Concepts

- Nomenclature
- Synthesis using alkyl halides and alkenes.