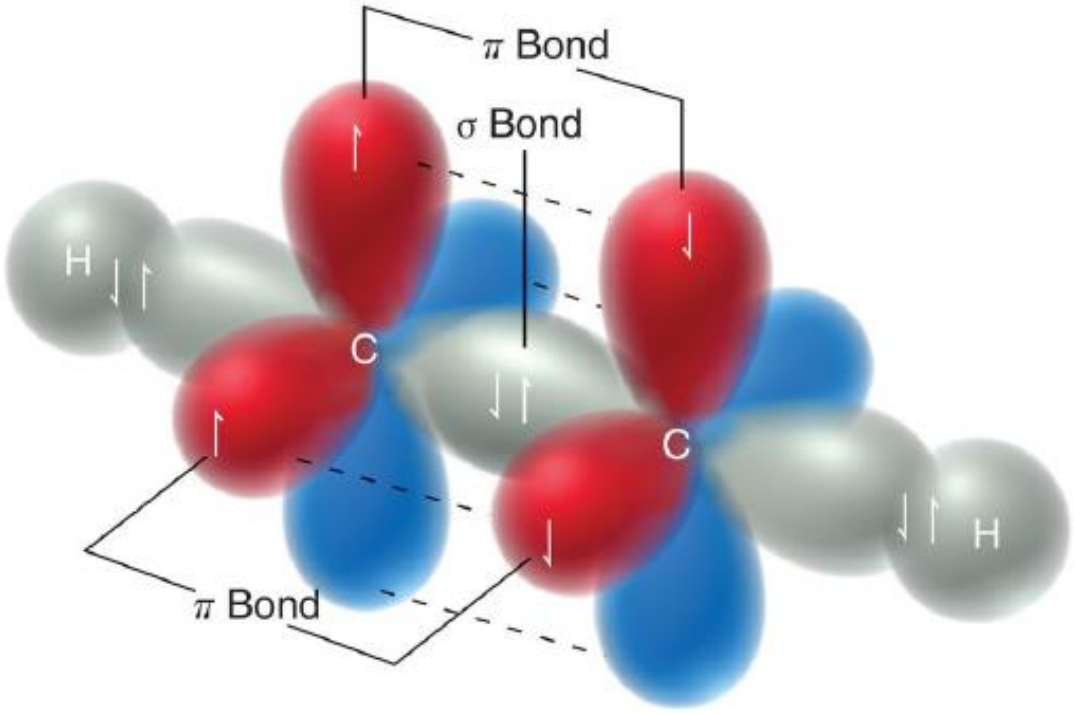
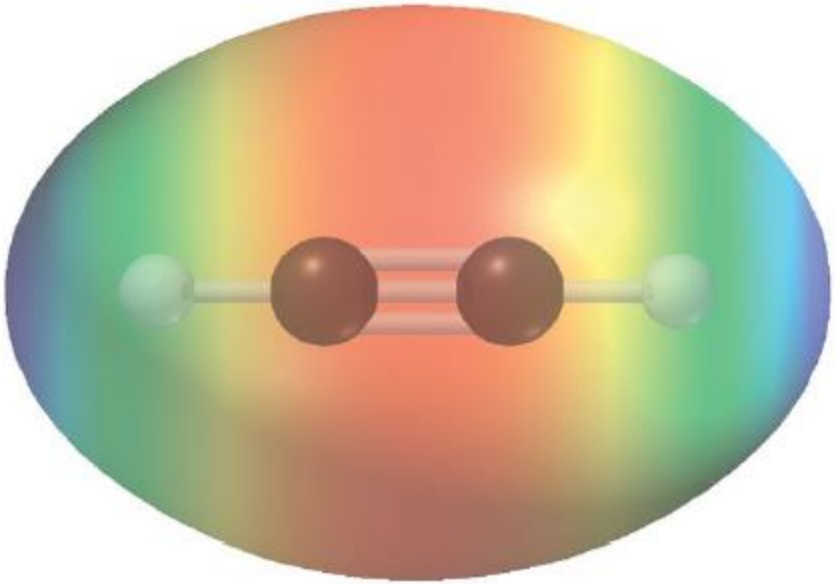
Alkynes

- Alkynes are molecules that possess a C≡C triple bond



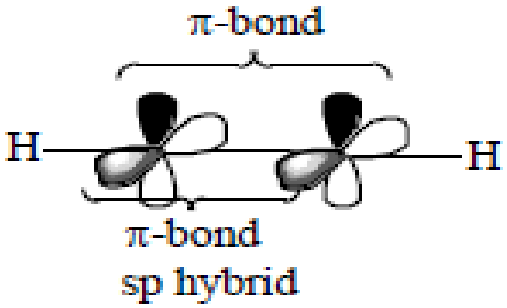
Alkynes

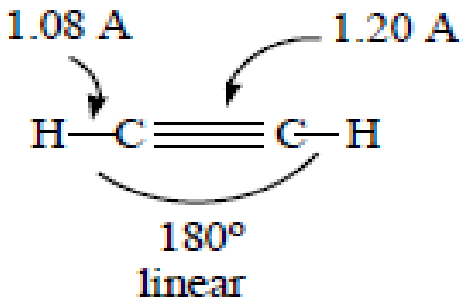
- Given the presence of pi bonds, alkynes are similar to alkenes in their ability to act as a nucleophile



- Many of the addition reactions of alkenes also work on alkynes

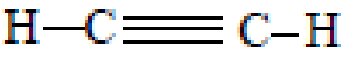
- Alkynes, also called acetylenes ,contain a structural unit in which carbon is bonded to another carbon with three bonds ,C≡C. The double unsaturation gives rise to the general formula of CnH2n-2 for alkynes. The carbon atoms in an alkyne are sp hybridized. The single bonds are made of sp hybridized carbon atoms overlapped with hydrogen or carbon. The remaining two unhybridized p-orbitals join inside-to-side overlap to make two orthogonal p-bonds. The overall alkyne structure is linear with a C-C bond length of 1.20 Å and C-H bond length of 1.08Å.





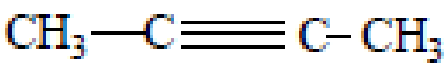
Nomenclature of Alkynes

- Unbranched alkynes are named by replacing-ane with-yne
- The chain is numbered to give the carbon atoms of the triple bond the lower possible numbers
- The lower number of the two carbon atoms of the triple bond is used to designate the location of the triple bond
- The locations of substituent groups of branched alkynes and substituted alkynes are also indicated with numbers
- Mono substituted acetylenes or 1-alkynes are called terminal alkynes, and the hydrogen attached to the carbon of the triple bond is called the acetylenic hydrogen atom

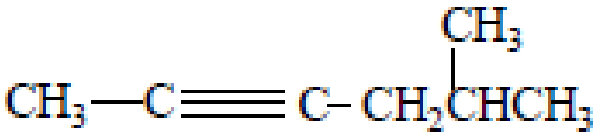


ethyne
acetylene

propyne



2-butyne



5-methyl-2-hexyne

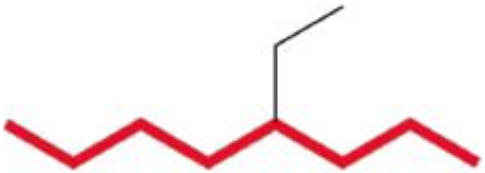
Nomenclature of Alkynes

1. Identify the parent chain, **which should include the C≡C triple bond**

Pentane

Pentene

Pentyne



Parent = octane

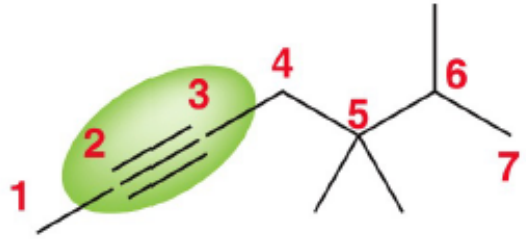
Parent = heptyne

2. **Identify and name the substituents.**

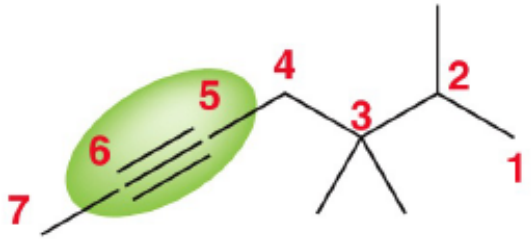
Nomenclature of Alkynes

3. Assign a locant (and prefix if necessary) to each substituent **giving the C≡C triple bond the lowest number possible**

Correct



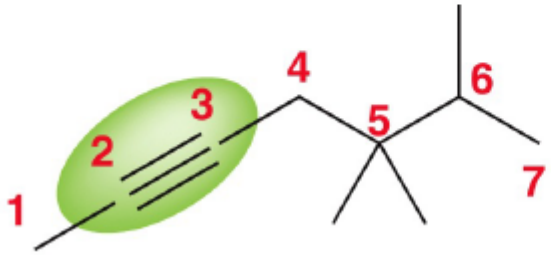
Incorrect



– The locant is ONE number, NOT two. Although the triple bond bridges carbons 2 and 3, the locant is the lower of those two numbers

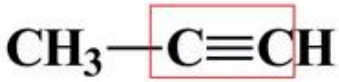
Nomenclature of Alkynes

4. List the numbered substituents before the parent name in alphabetical order. Ignore prefixes (except iso) when ordering alphabetically
5. **The C≡C triple bond locant is placed either just before the parent name or just before the -yne suffix**

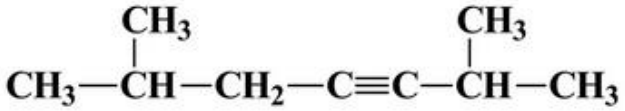


5,5,6-Trimethyl-2-heptyne
or
5,5,6-Trimethylhept-2-yne

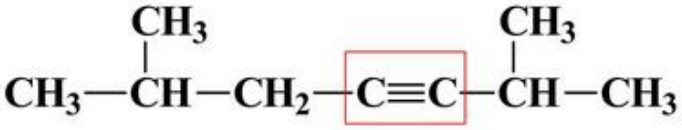
5-bromo-2-pentyne



methylacetylene

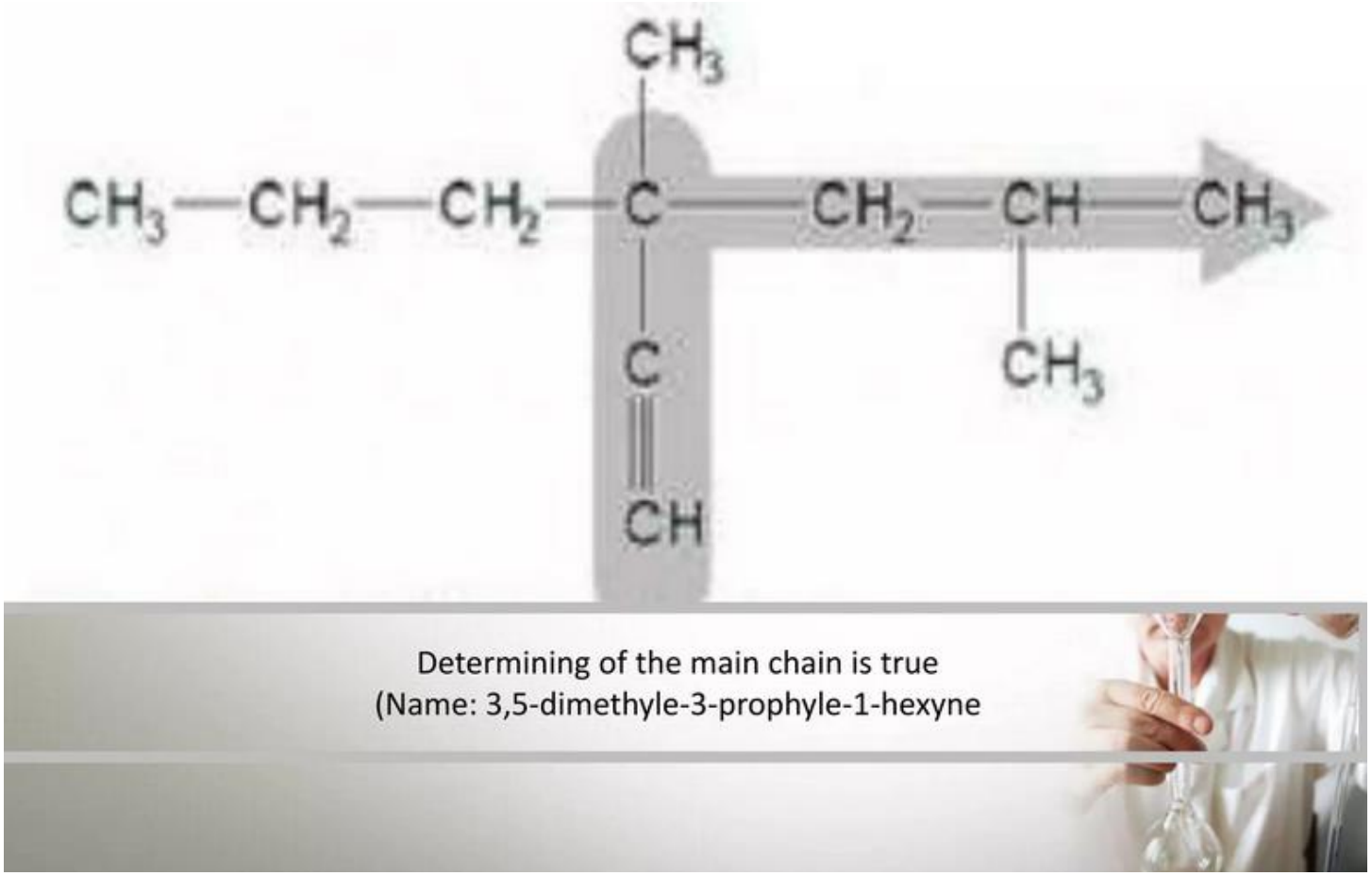


2,6-dimethyl-3-heptyn

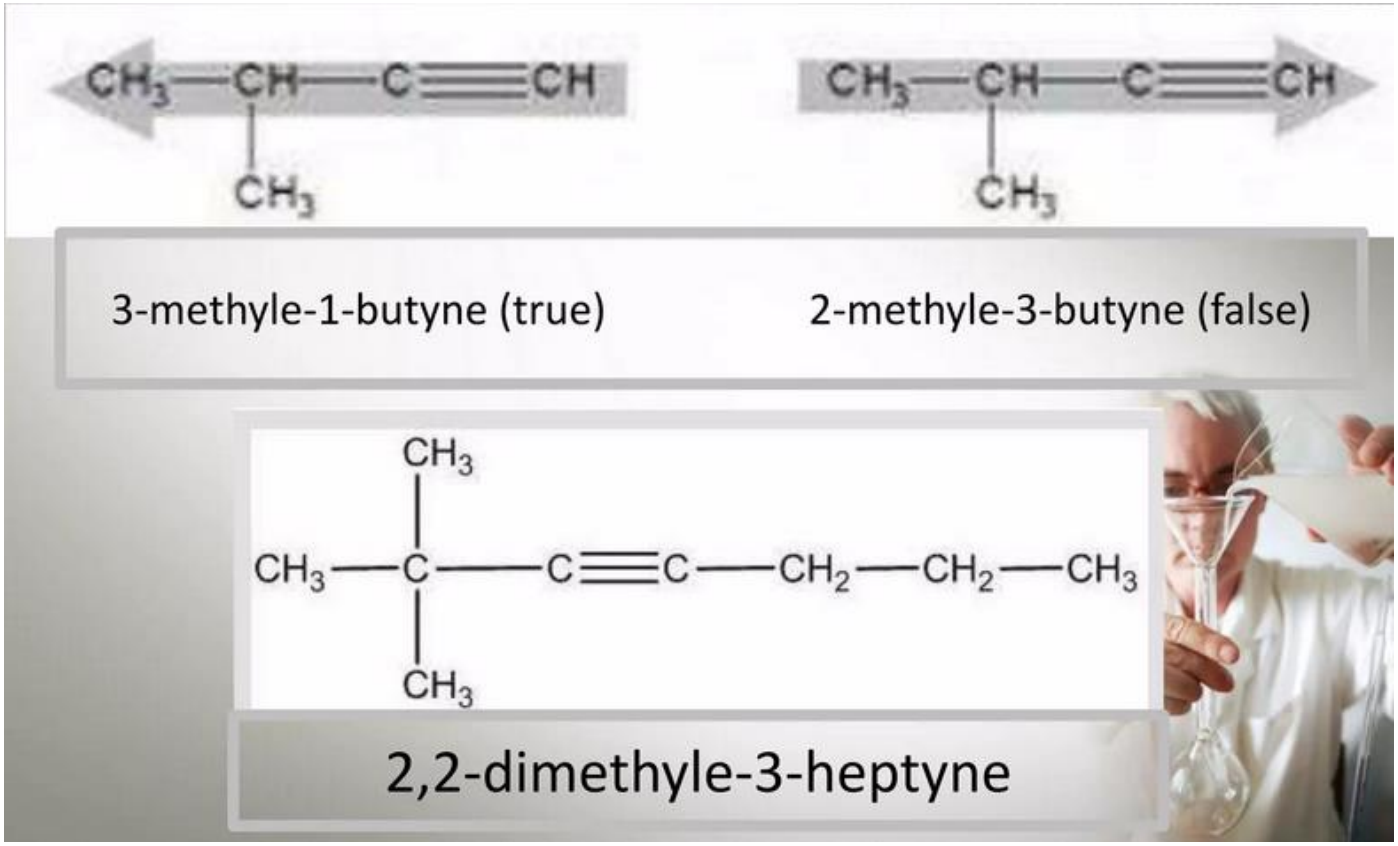


isobutylisopropylacetylene

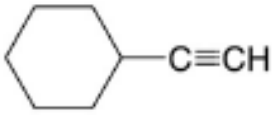
Nomenclature of Alkynes



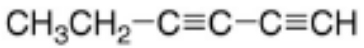
Nomenclature of Alkynes



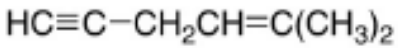
2,5-dimethyl-3-heptyne



ethynylcyclohexane



1,3-hexadiyne



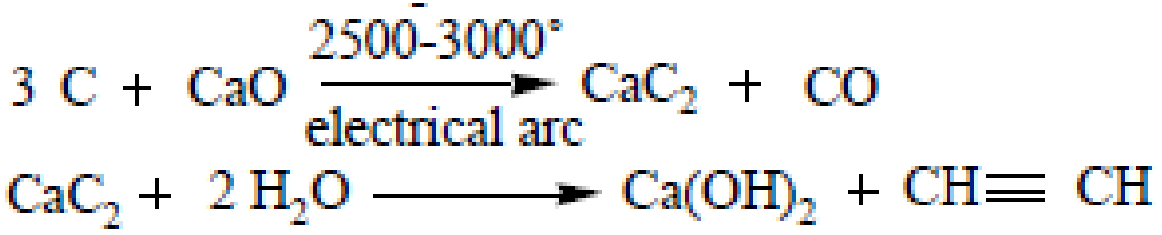
5-methyl-4-hexen-1-yne

Physical Properties of Alkynes

- Alkynes are low boiling materials that possess a high heat content. Thus a major use for alkynes , especially acetylene, is as a fuel for high temperature flames.
- Acetylene is fairly unstable and detonates under pressure. Pure acetylene is not stored as a liquid or a gas under pressure. It is adsorbed on to carbon and kept in steel container sat about 10 atm of pressure.
- The boiling points of alkynes are some what higher than the boiling points of alkenes.

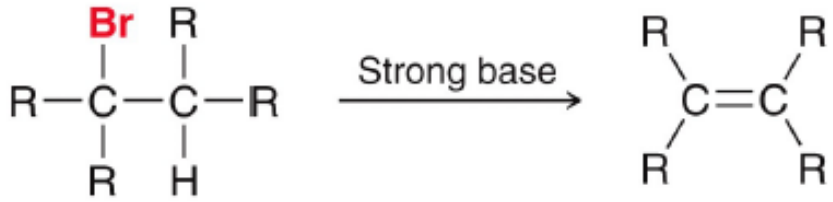
Preparation of alkynes

- Most alkynes are synthesized from acetylene . Pure acetylene is obtained from calcium carbide , a substance produced from carbon and calcium oxide.

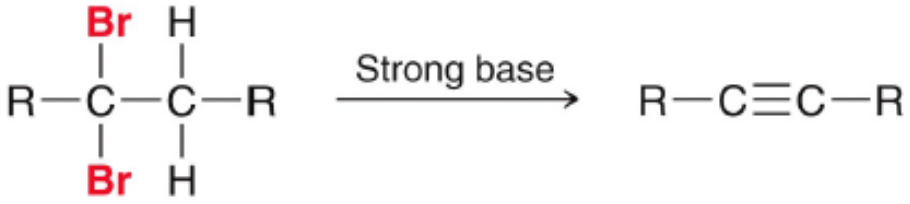


Preparation of Alkynes

- Like alkenes, alkynes can also be prepared by elimination
- Need a **dihalide** to make an alkyne



An alkyl halide

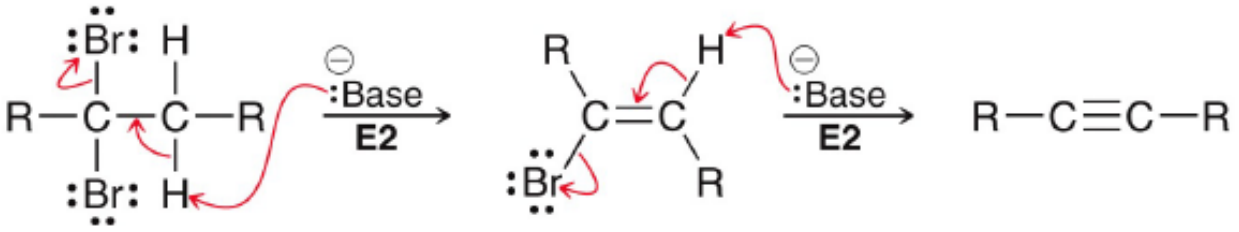


An alkyl dihalide

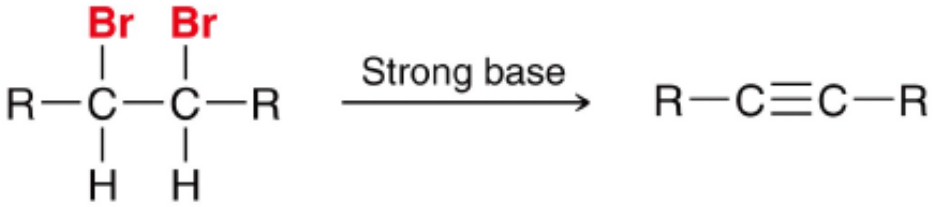
Preparation of Alkynes

- Such eliminations usually occur via an E2 mechanism
- **Geminal** or **vicinal** **dihalides** can be used

geminal dihalide

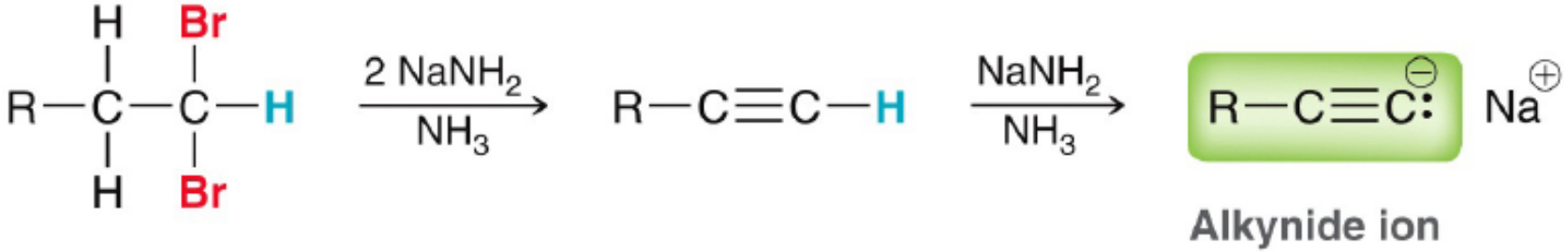


vicinal dihalide

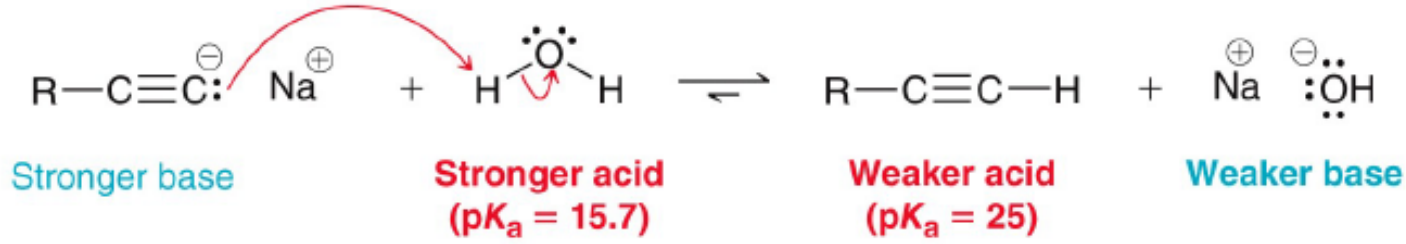


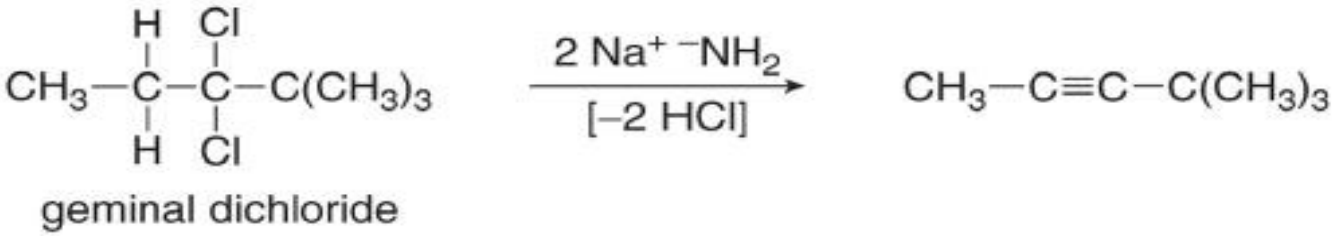
Preparation of Alkynes

- excess equivalents of $NaNH_2$ are used to shift the equilibrium toward the elimination products

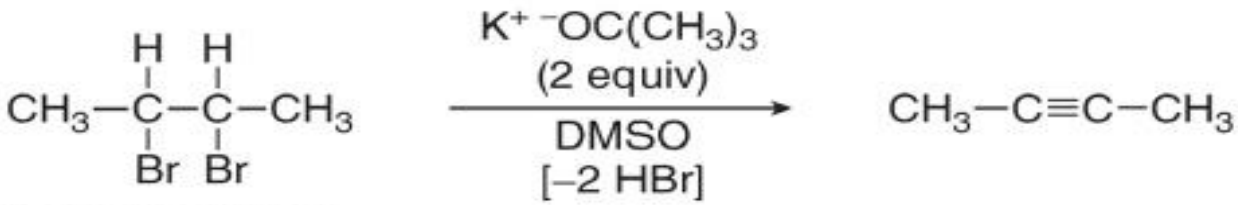


- Aqueous workup is then needed to produce the neutral alkyne:





geminal dichloride



vicinal dibromide

- IMPORTANT NOTE: Synthesis of a terminal alkyne by dehydrohalogenation requires 3 equivalents of the base, due to the acidity of the terminal alkyne H