

Unit 3 – Deck 1

Organic Chemistry

The hydrocarbons



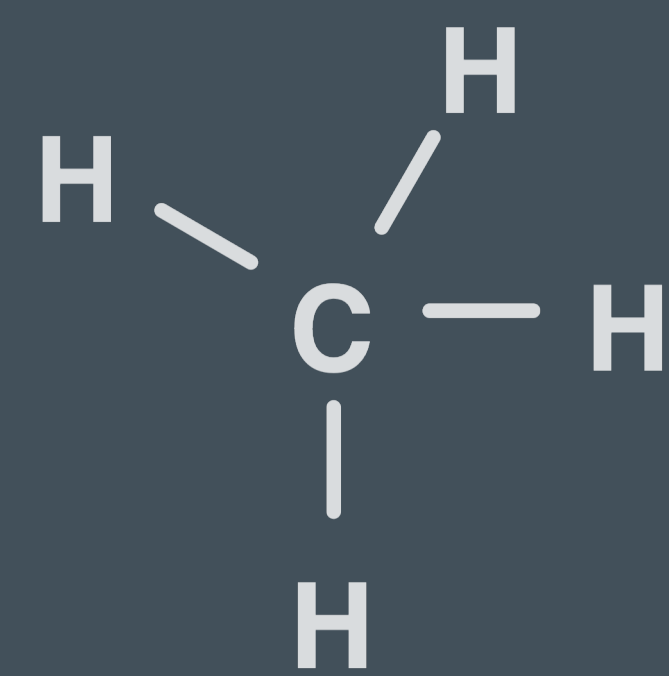
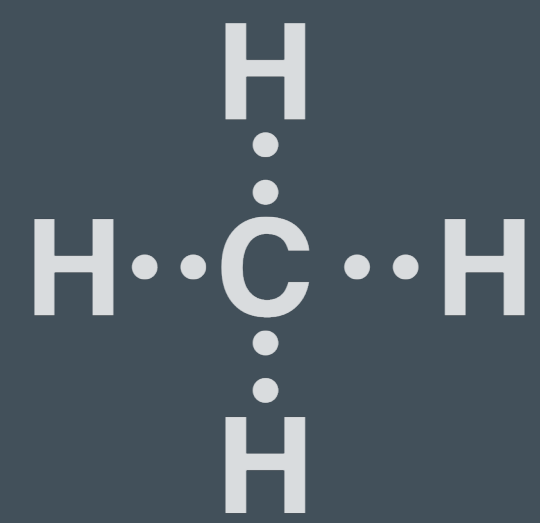
Lecture Topics

- Outline
 - Types of hydrocarbons
 - Basics of nomenclature
 - Isomers
 - Properties of Alkanes
 - Alkane Substitution Reactions
 - Alkenes
 - Properties of Alkenes
 - Reactions of Alkenes (electrophilic addition)
 - Aromatics
 - Electrophilic substitution reactions
 - Resonance

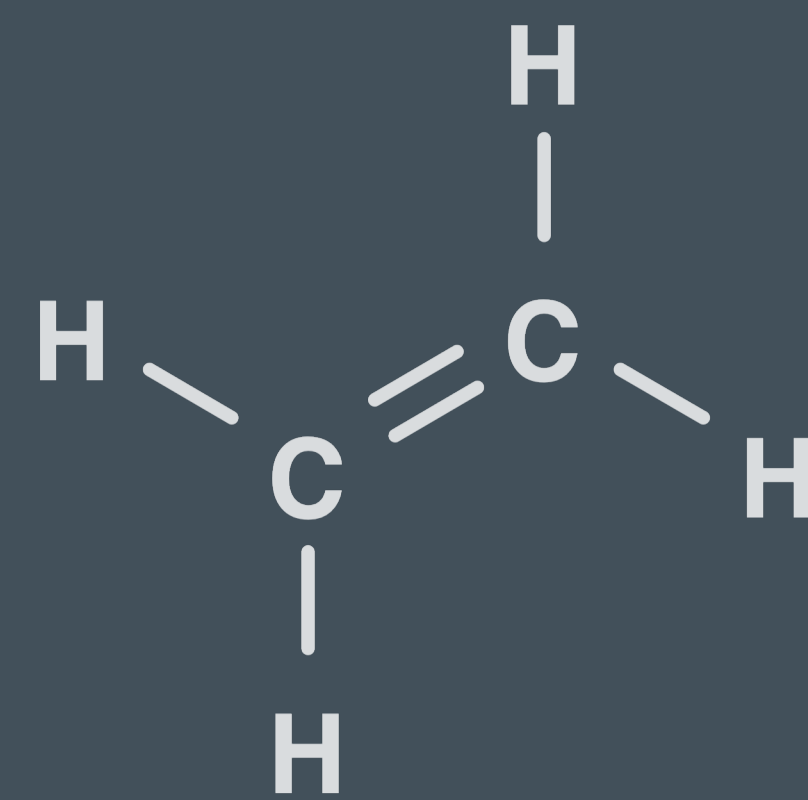
Lewis Structures of Organic Compounds

Carbon almost always makes four bonds to fill octet

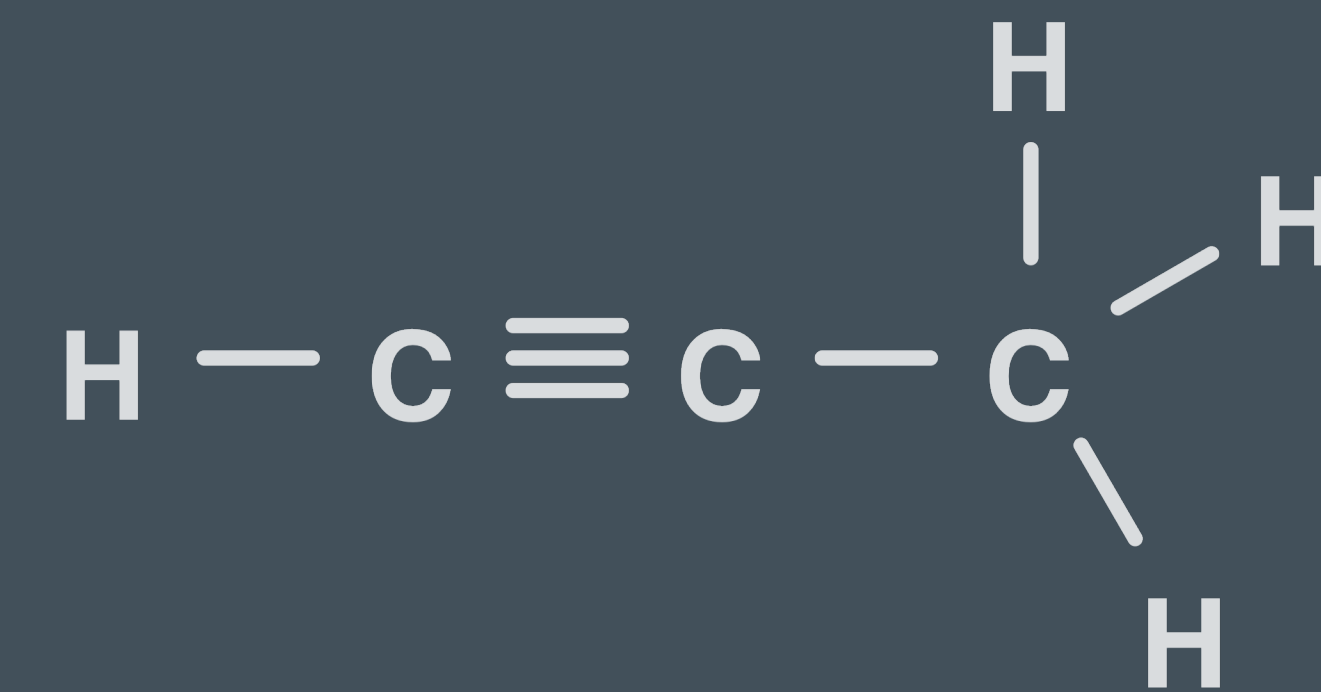
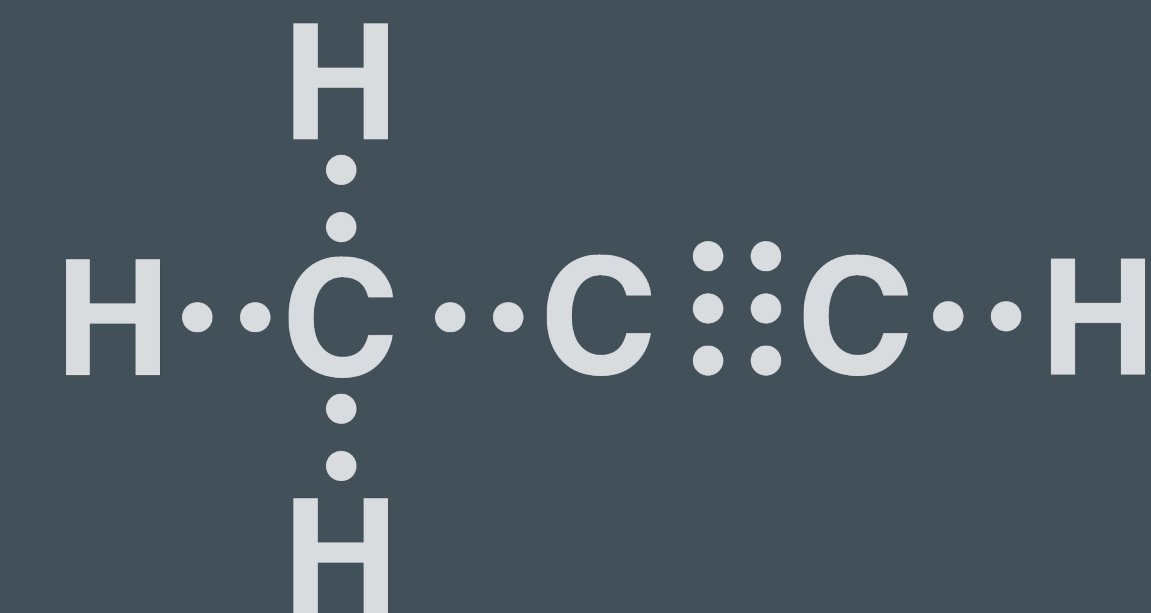
methane



ethene

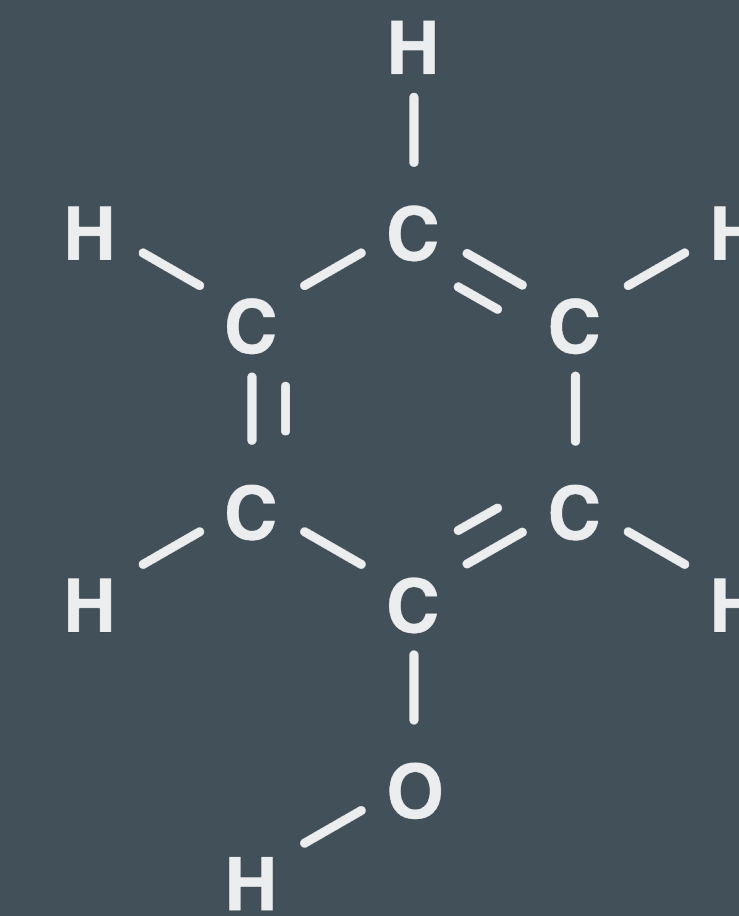
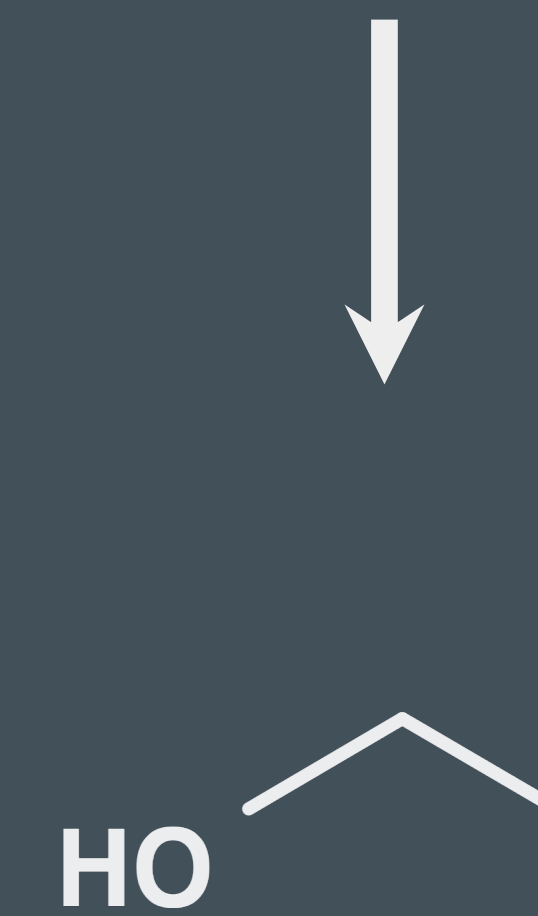
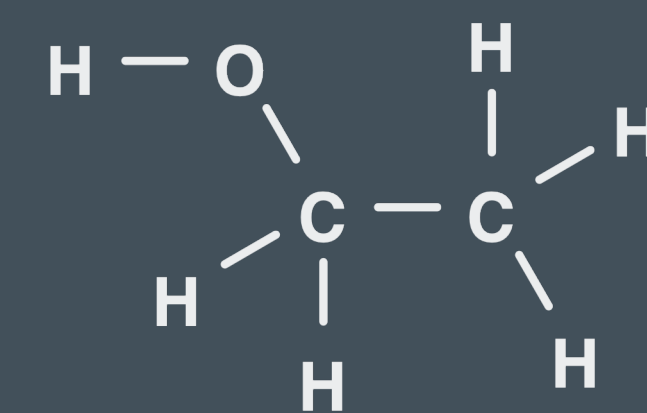
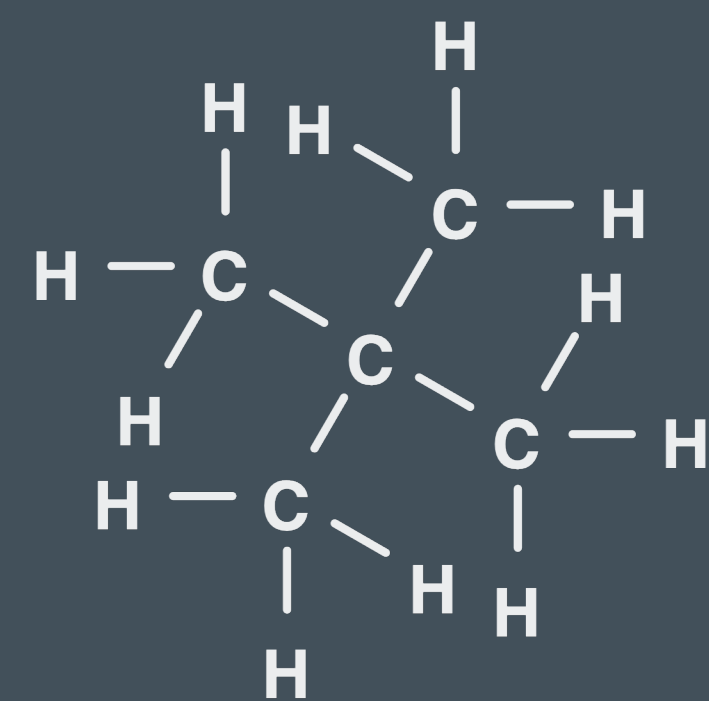
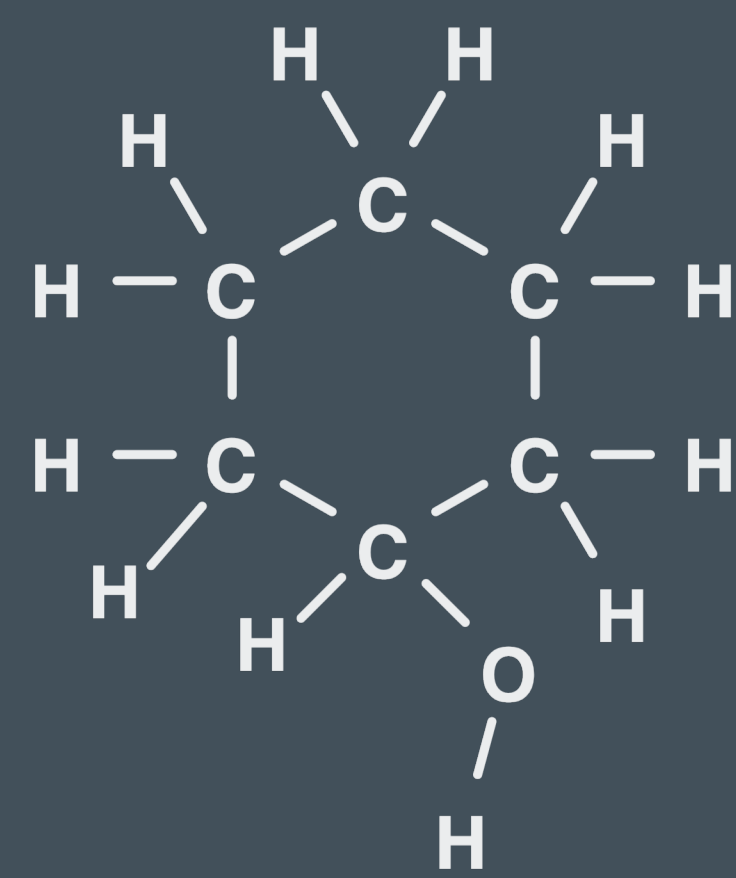


propyne



Abbreviated Organic Structures

The standard representation of organic compounds



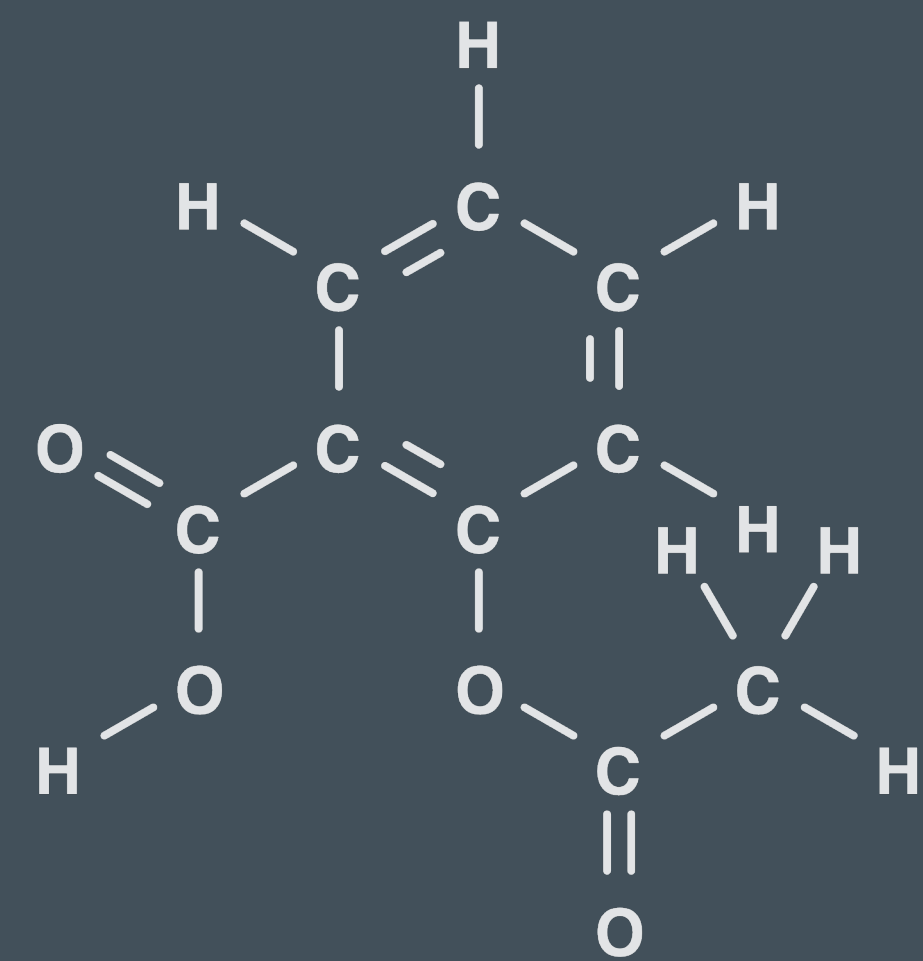
We all know carbon makes 4 bonds. Mentally fill in missing bonds with -H

Practice: Abbreviated Organic Structures

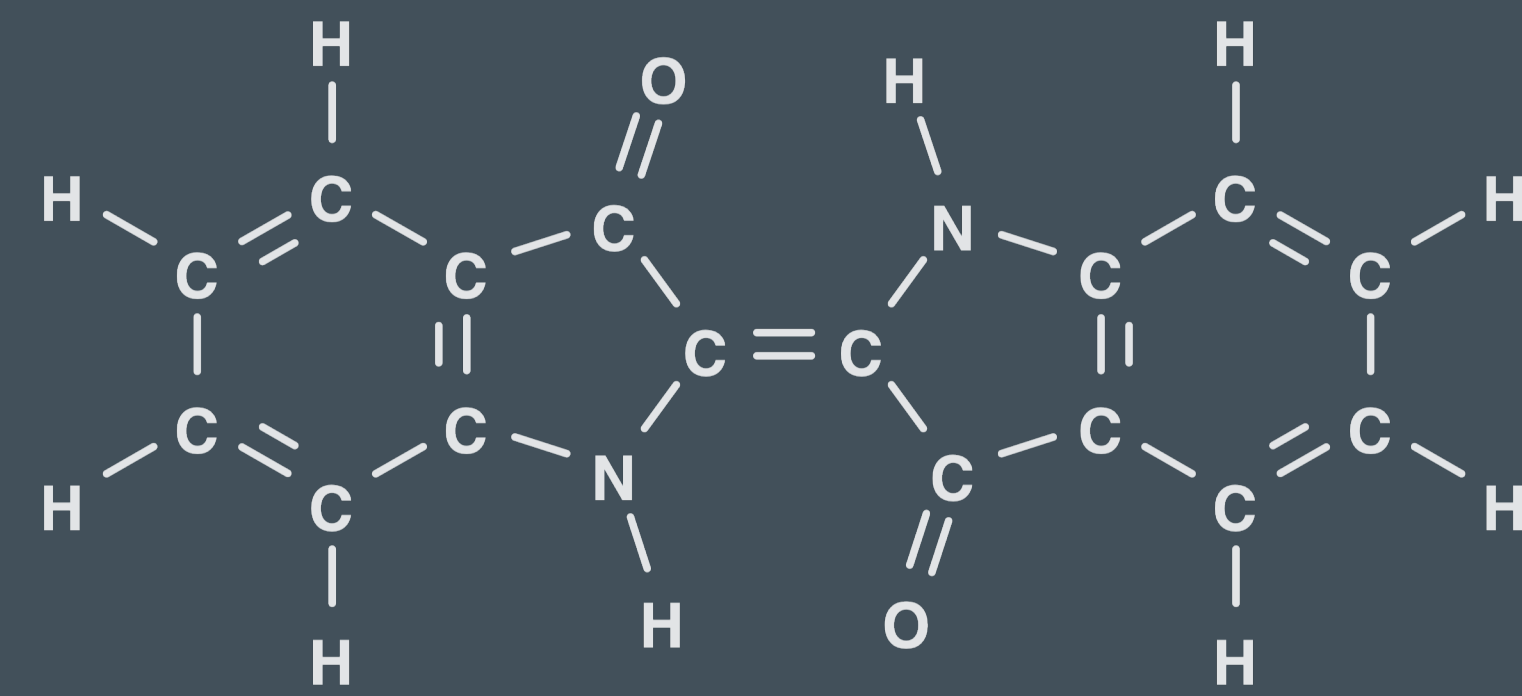


Draw the standard representation of organic compounds

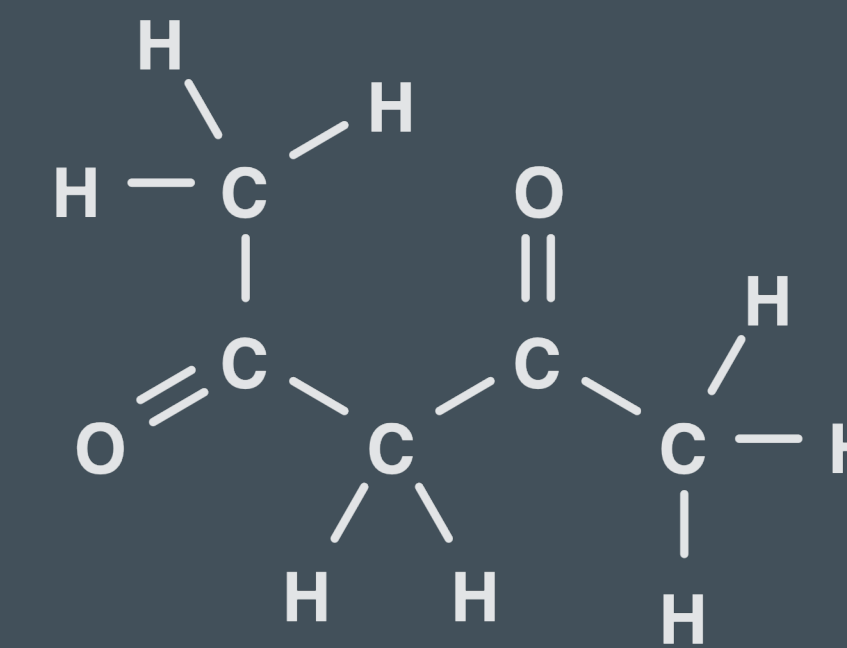
aspirin



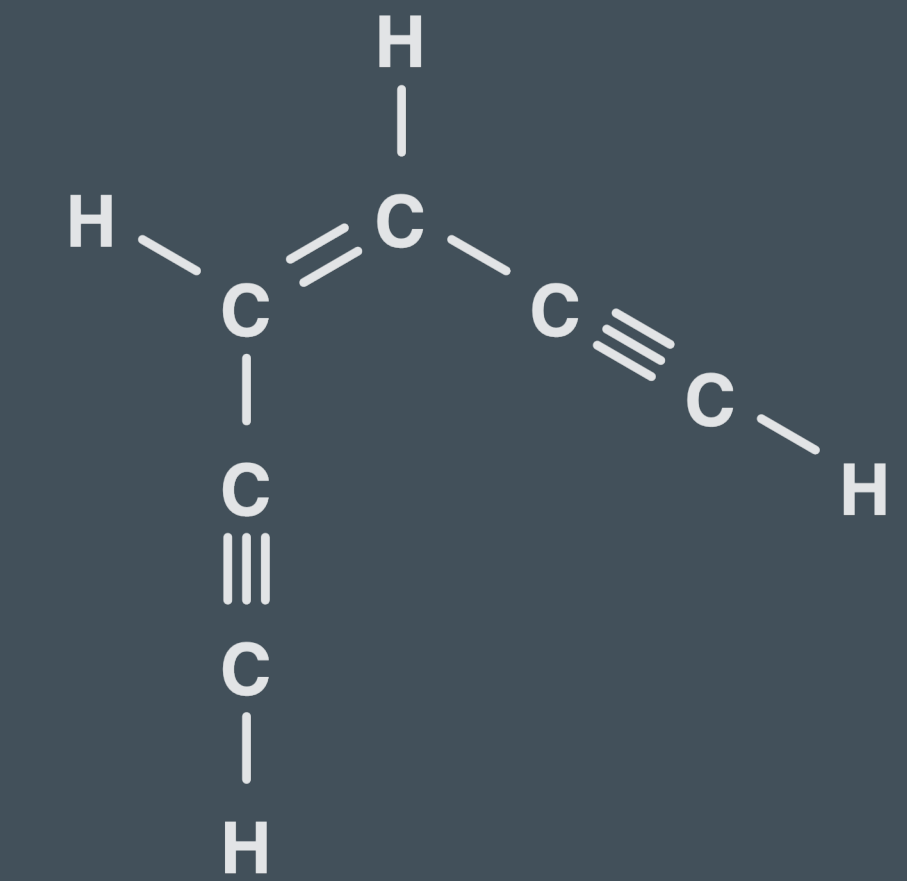
indigo



acetylacetone

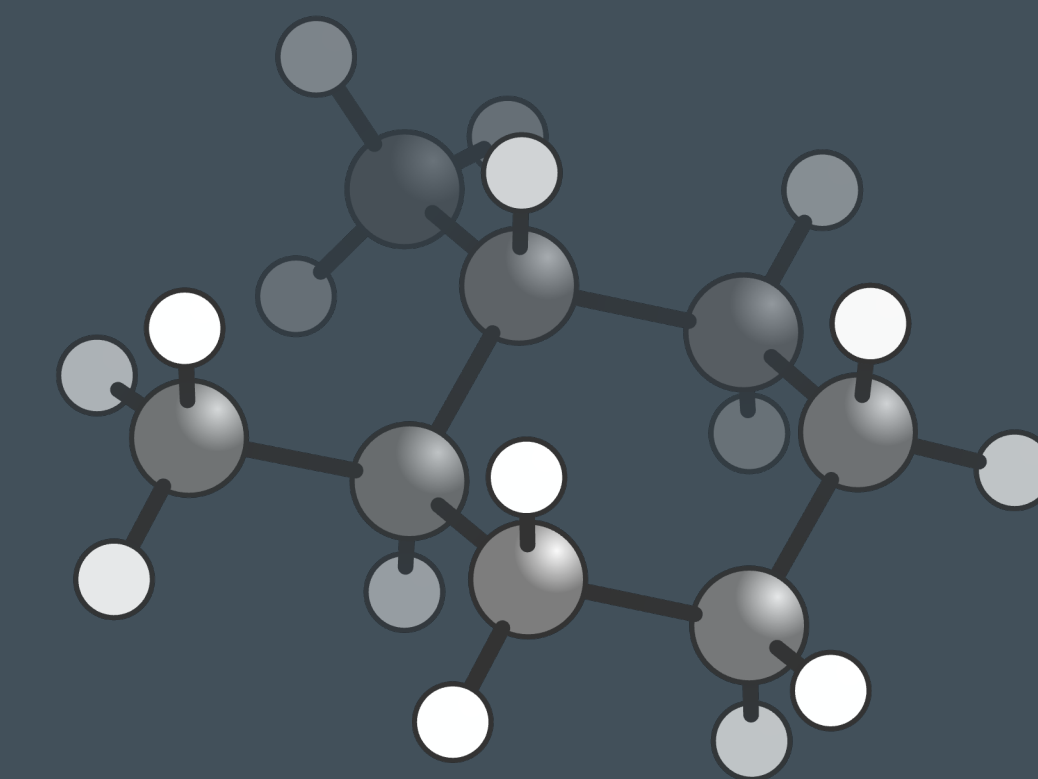
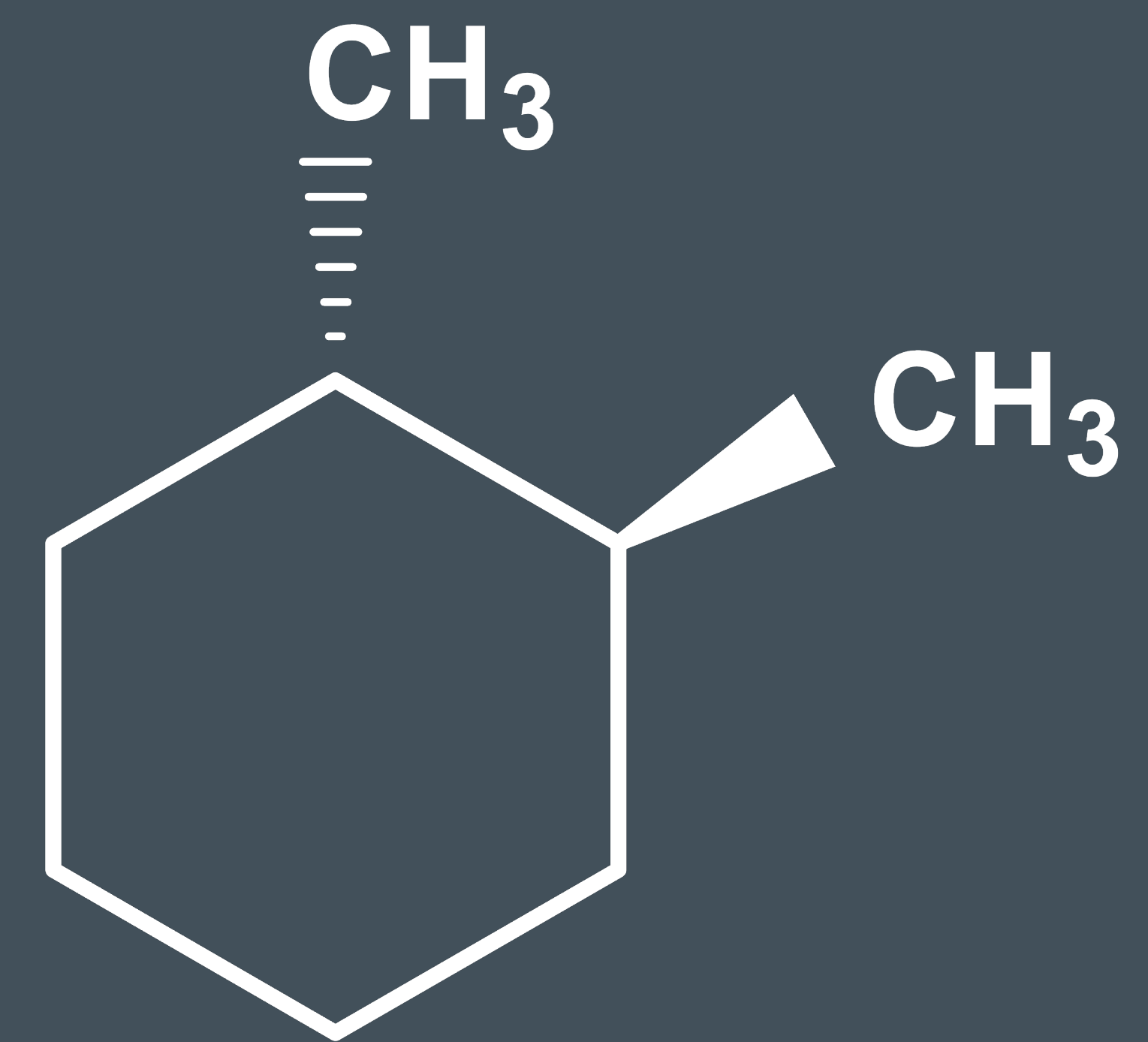
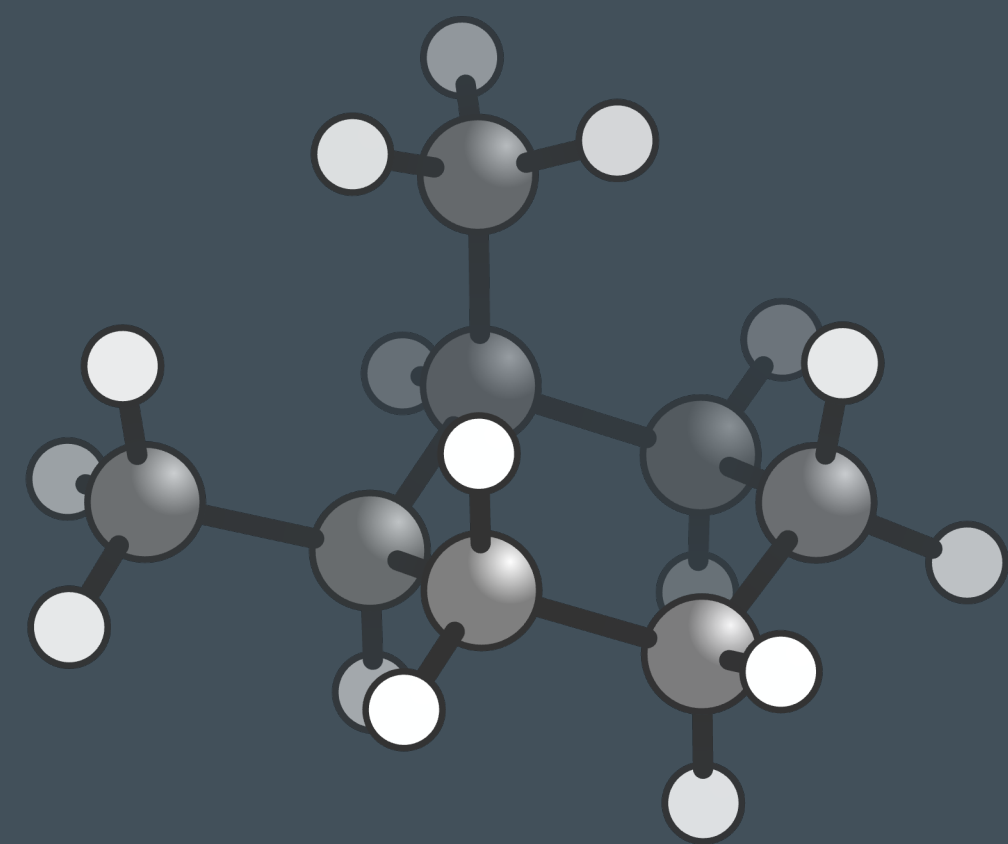
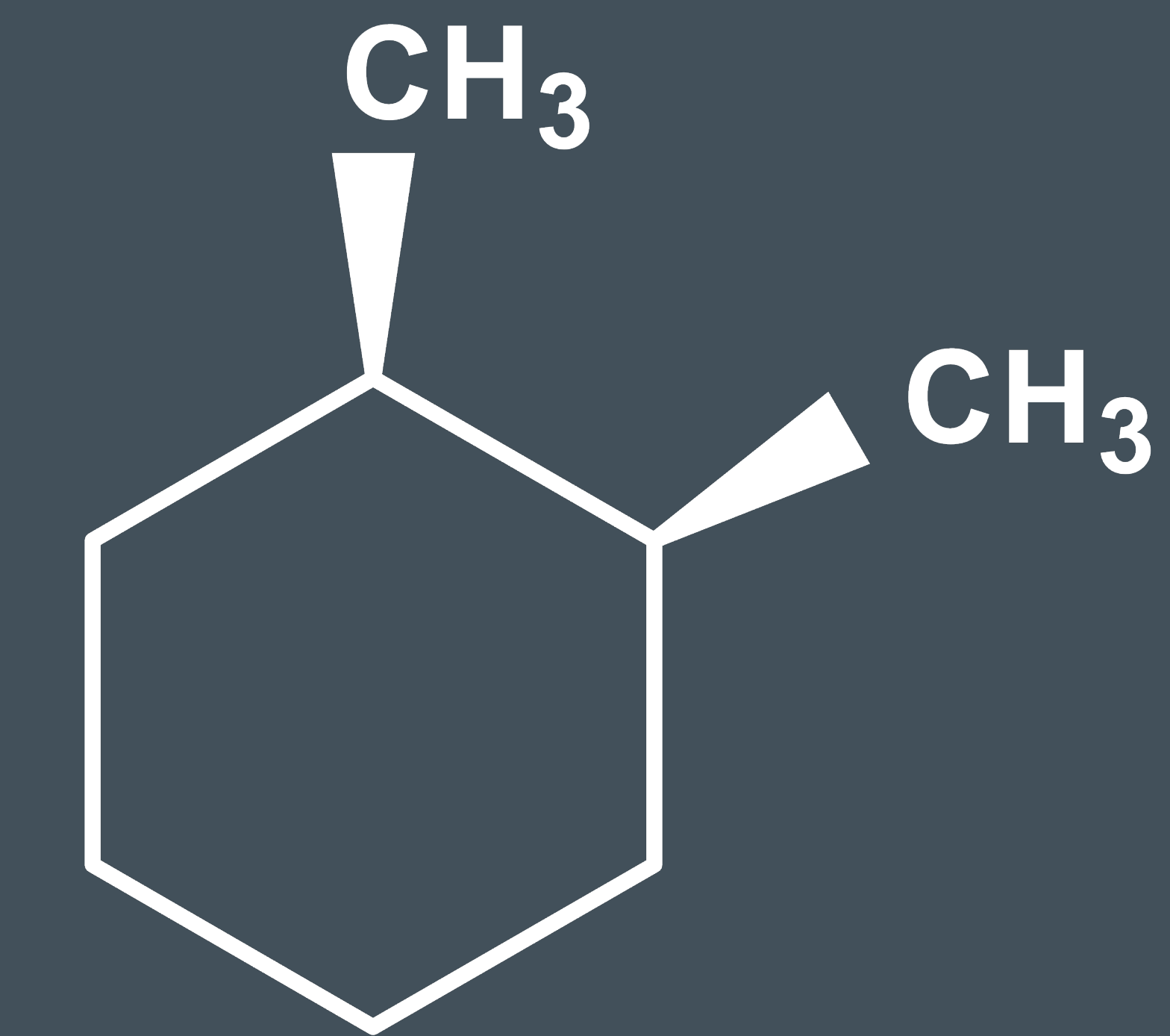


enediyne



We all know carbon makes 4 bonds. Mentally fill in missing bonds with -H

Diagrams Showing 3D Geometry



Naming the Aliphatic Groups

Group Names
(fragments)

Compound Names
(whole compounds)

Methyl-



Methane



Ethyl-



Ethane



Propyl-



Propane



Butyl-



Butane



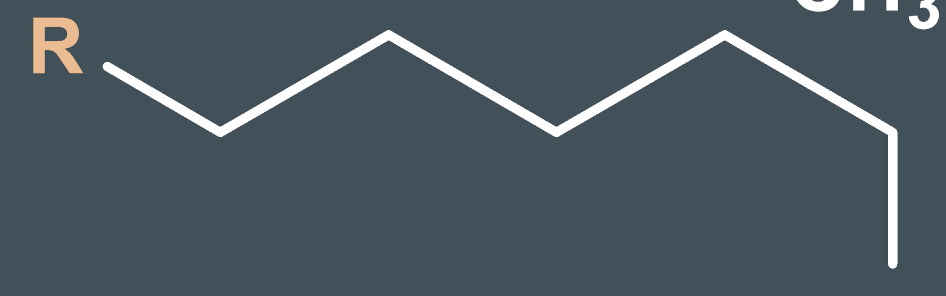
Pentyl-



Pentane



Hexyl-



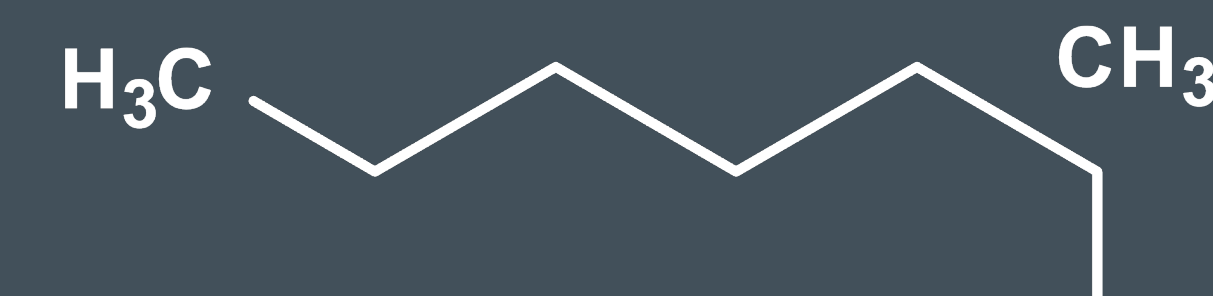
Hexane



Heptyl-



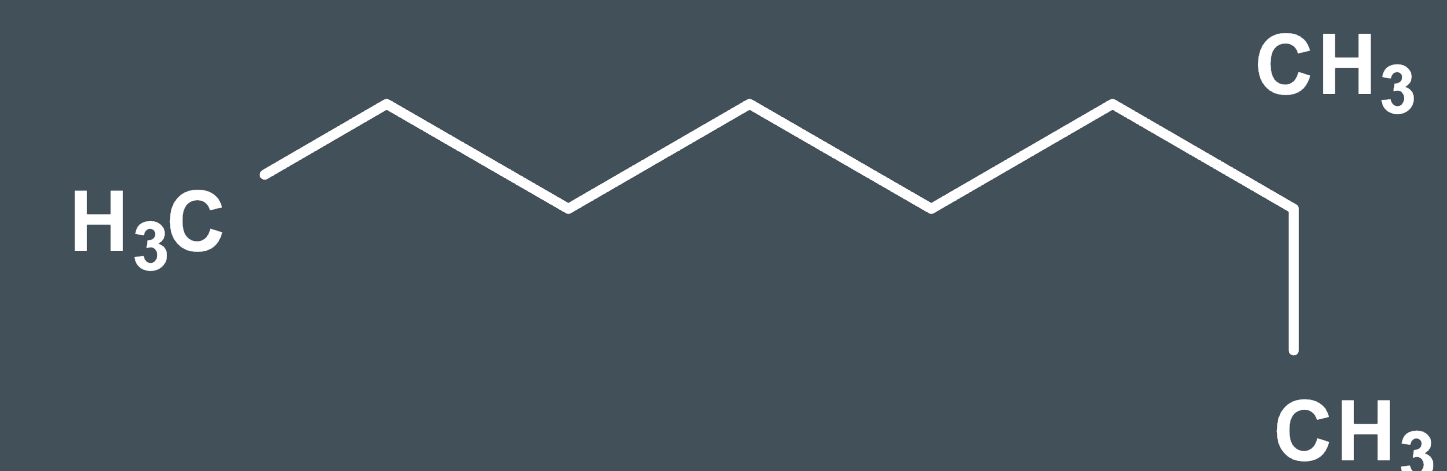
Heptane



Octyl-

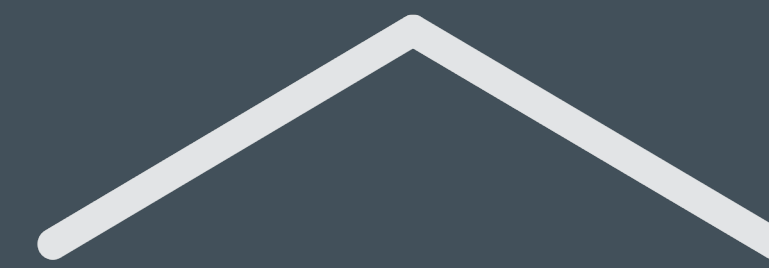


Octane



Saturated vs Unsaturated Hydrocarbons

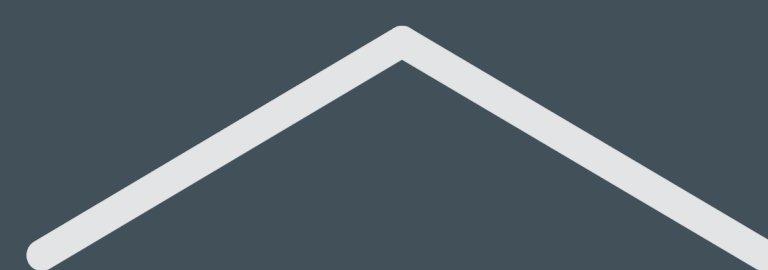
Saturated



propane

Unsaturated

alkane



propane

alkene



propene

alkyne



propyne

Position numbers in chemical names

Saturated (hexane)



Unsaturated (hexene)

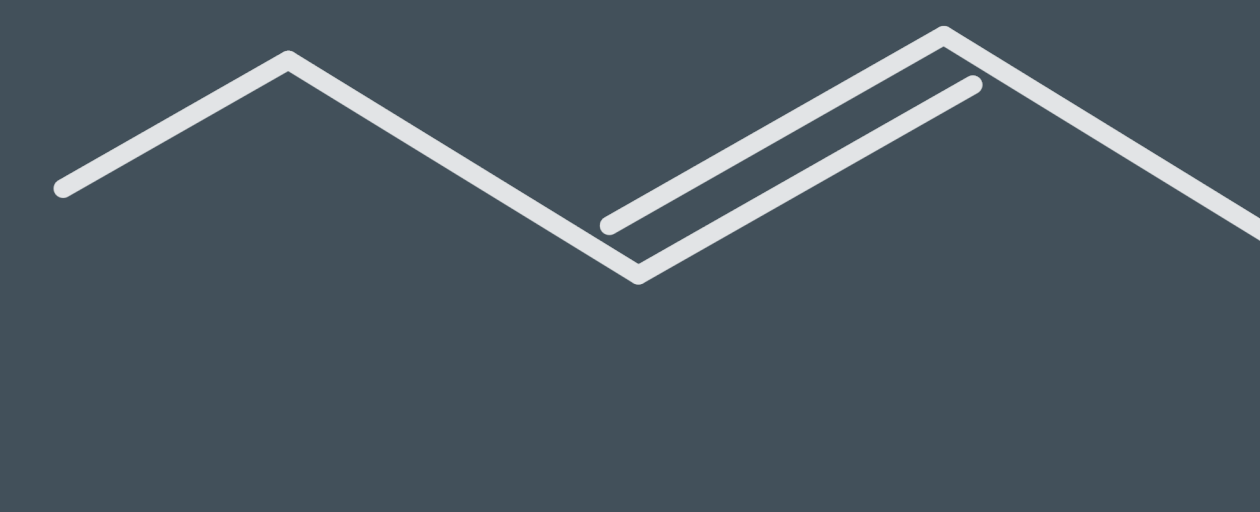
1-hexene



2-hexene

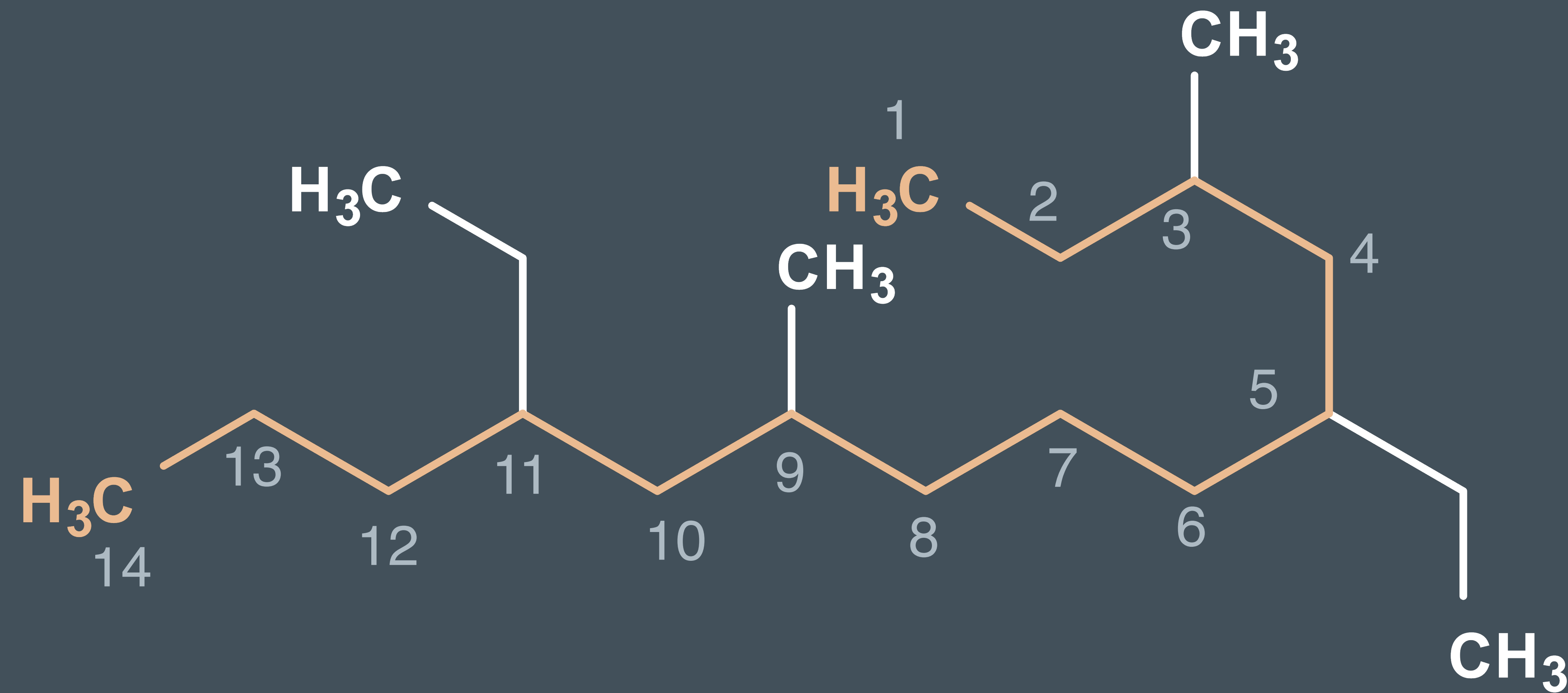


3-hexene



Position numbers for branched hydrocarbons

Number the longest chain first!

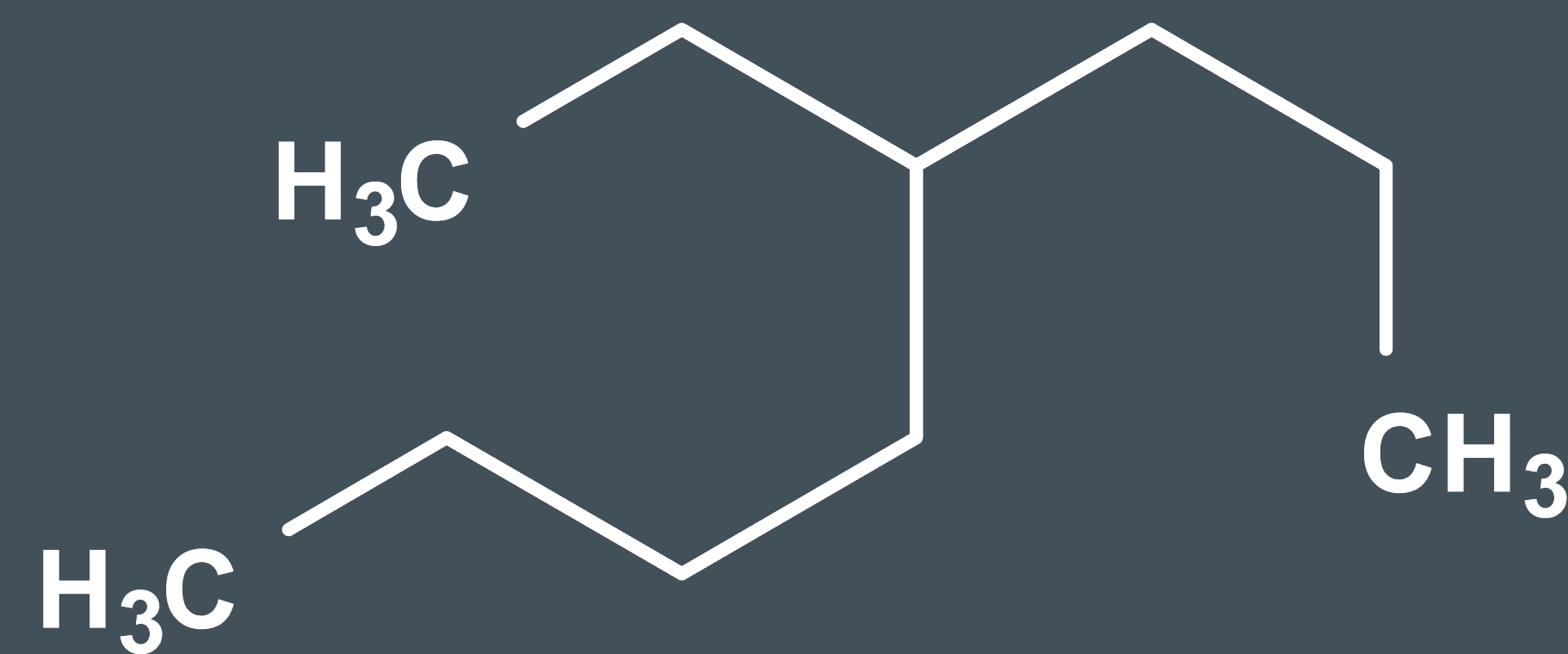


3,9-dimethyl-5,11-diethyl-tetradecane

Position numbers with for branched hydrocarbons



Name the compound



- A. 3-butyl-hexane
- B. 4-ethyl-octane
- C. 5-propyl-heptane
- D. 5-ethyl-octane

Practice: Naming unsaturated hydrocarbons

Draw the following hexyne compounds

1-hexyne

2-hexyne

1,5-hexadiyne

Review: the *degree* of a carbon



Primary (1°)

Secondary (2°)

Tertiary (3°)

Quaternary (4°)

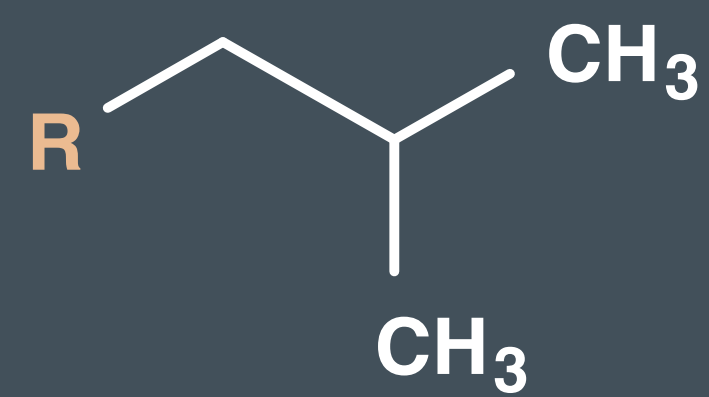
Structural Isomers: Same atoms different *connectivity*

Group Names

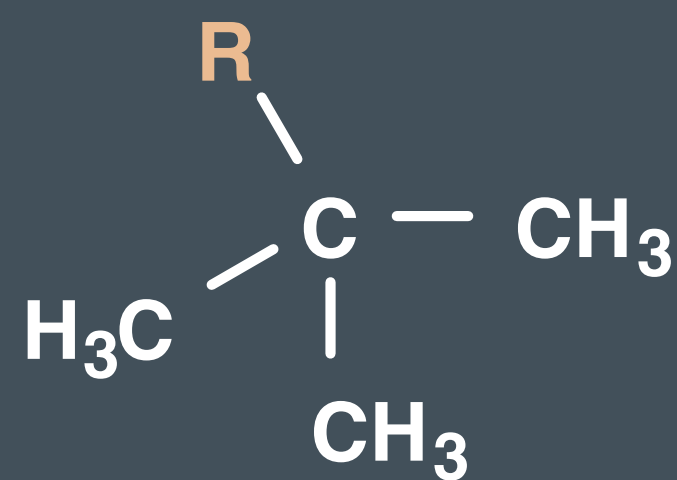
n-butyl



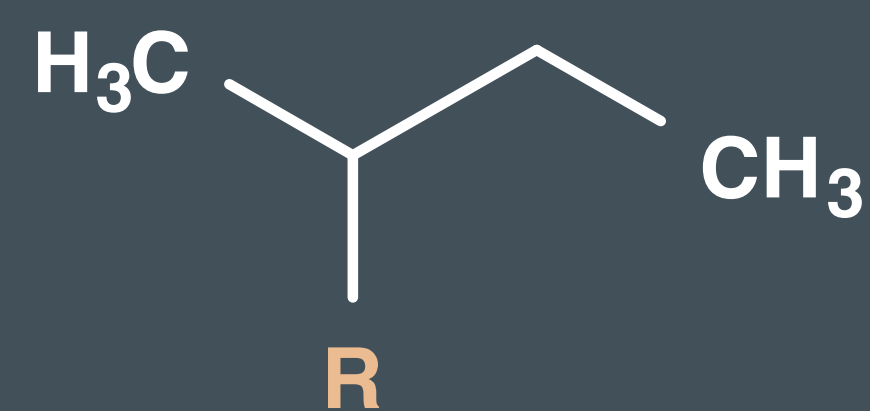
iso-butyl



tert-butyl



sec-butyl

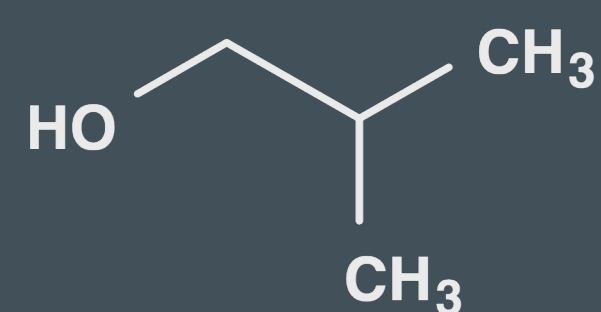


Compound Names

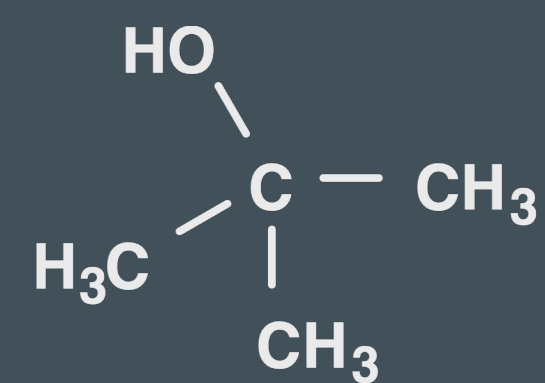
n-butyl alcohol



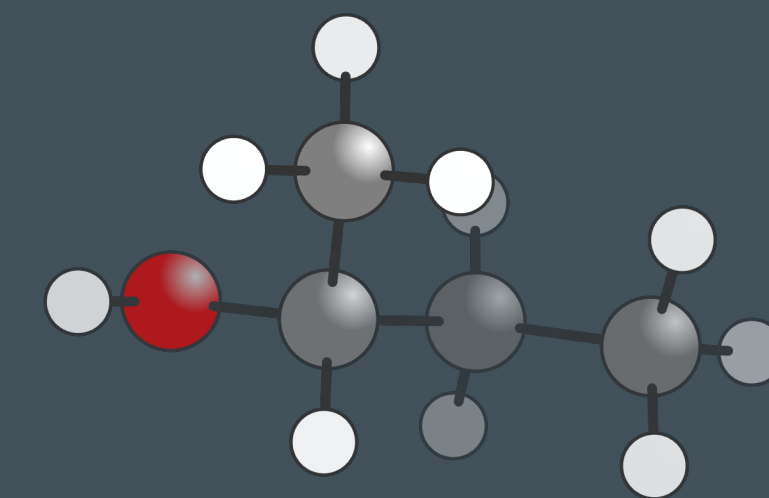
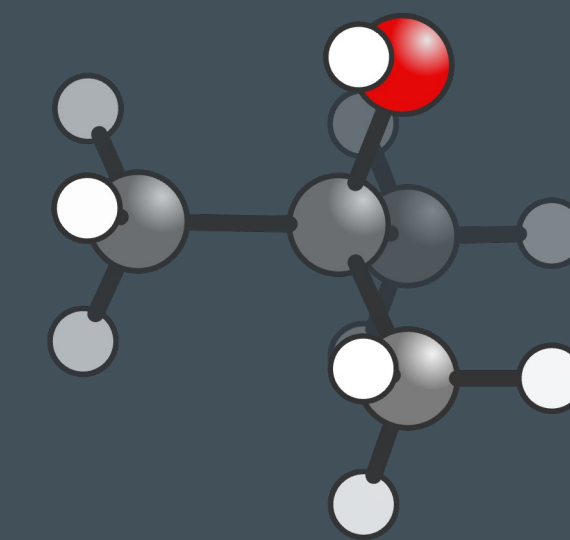
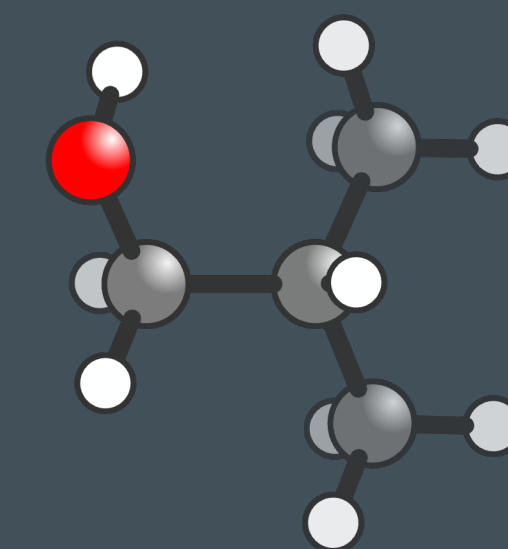
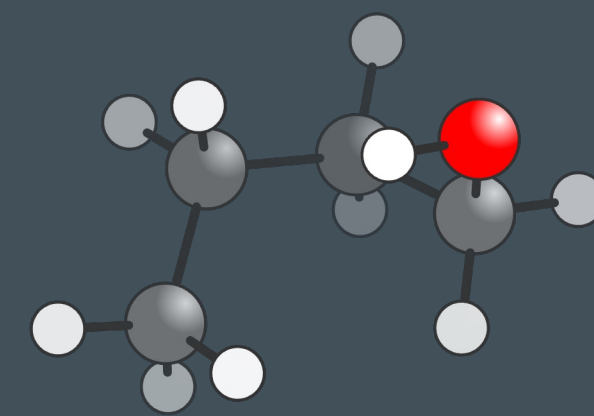
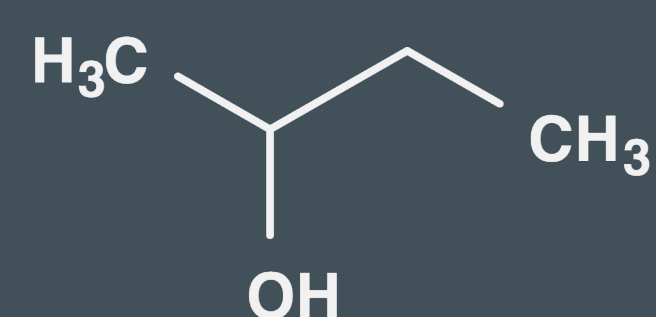
iso-butyl alcohol



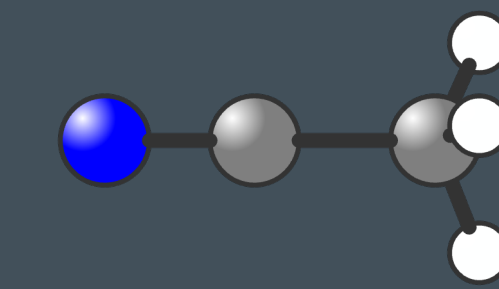
tert-butyl alcohol



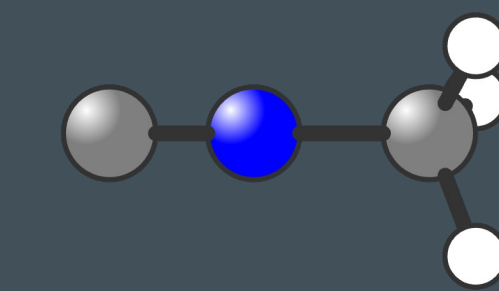
sec-butyl alcohol



Other structural isomers

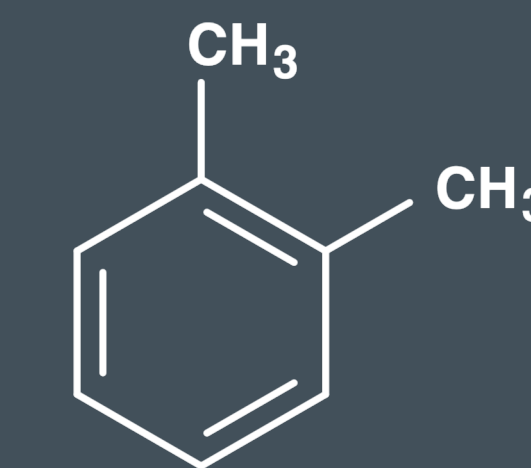


$\text{N} \equiv \text{C} - \text{CH}_3$ Methyl nitrile

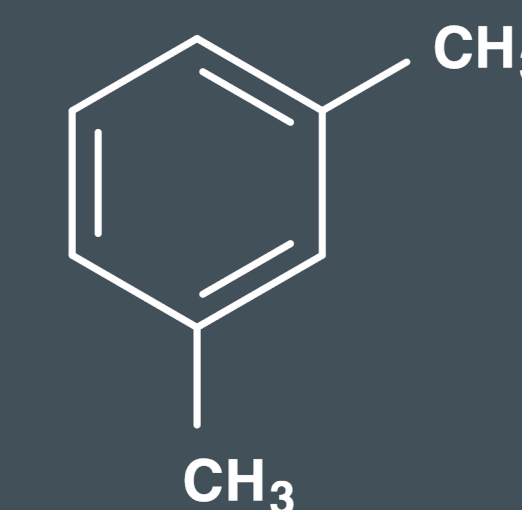


$-\text{C} \equiv \text{N}^+ - \text{CH}_3$ Methyl isonitrile

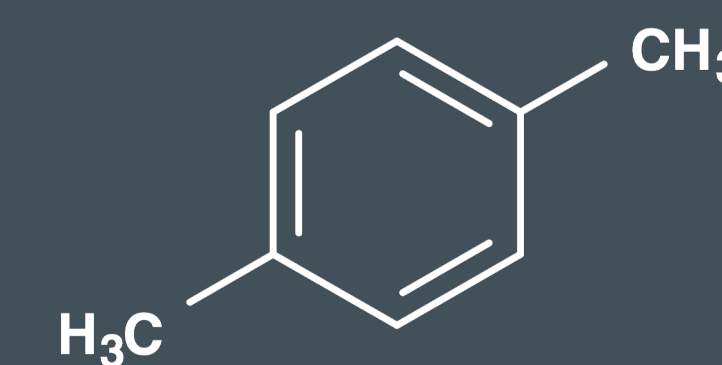
Xylene isomers



ortho-xylene



meta-xylene



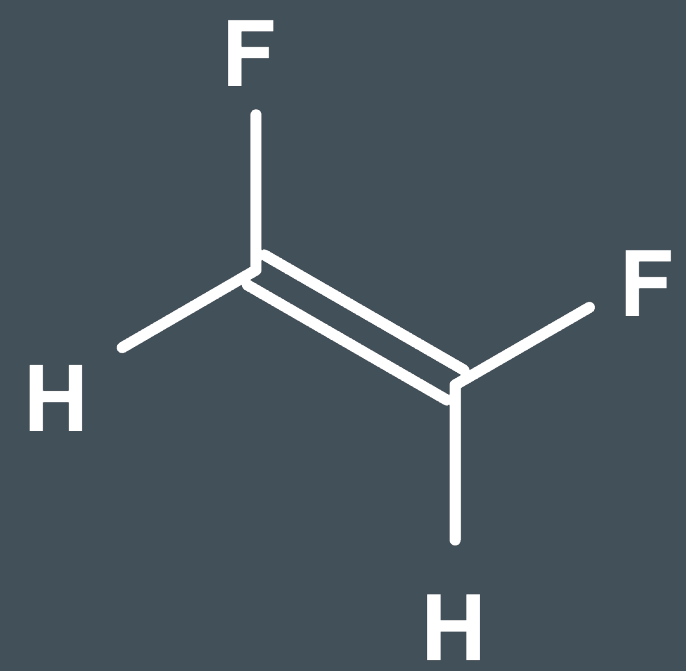
para-xylene

Same composition but different bonding pairs

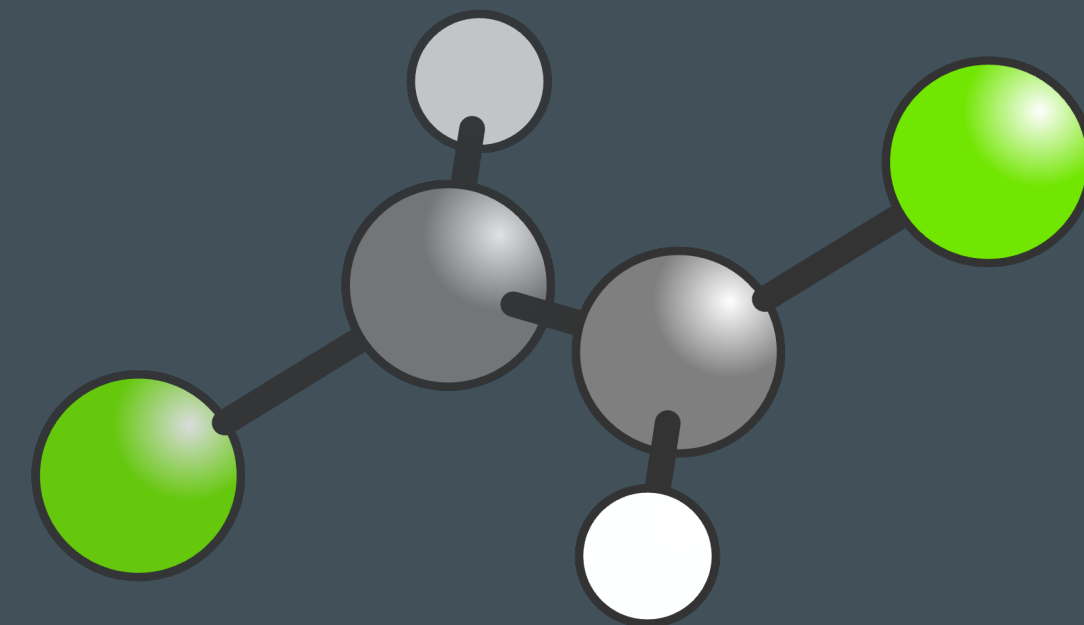
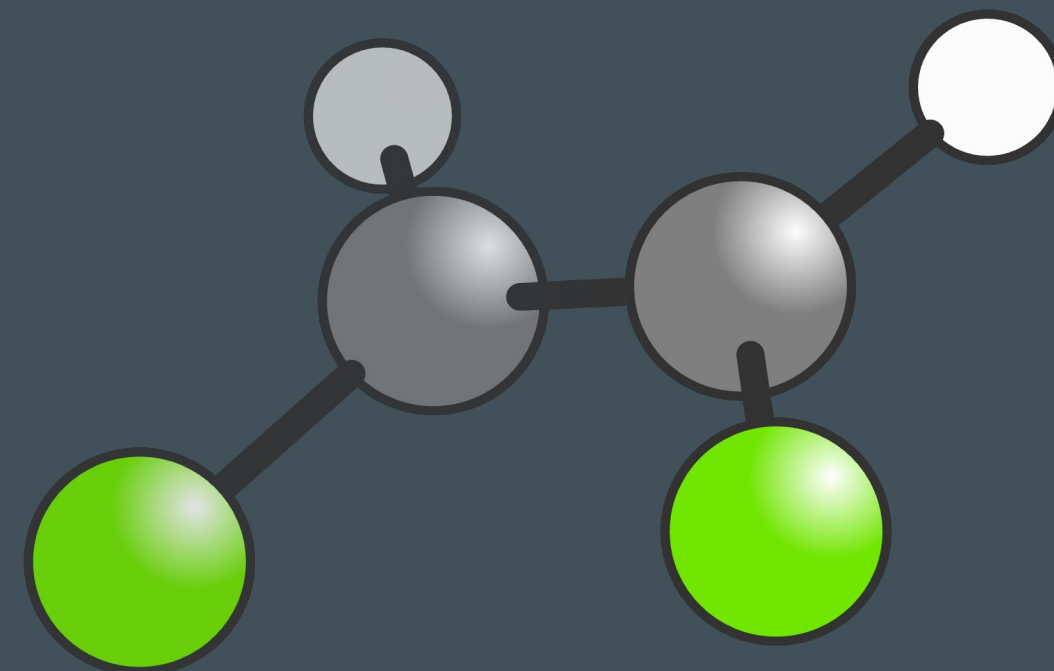
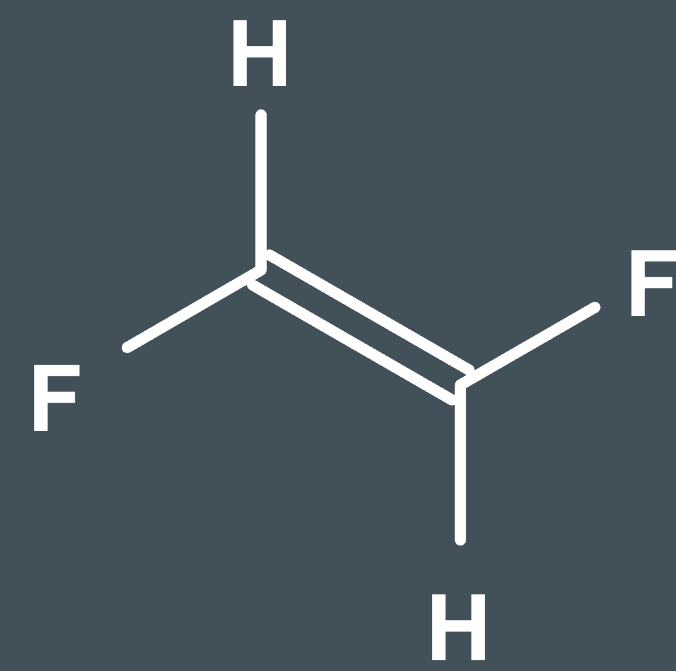
Geometric Isomers: Same atoms, same connectivity different arrangement

Alkenes

cis

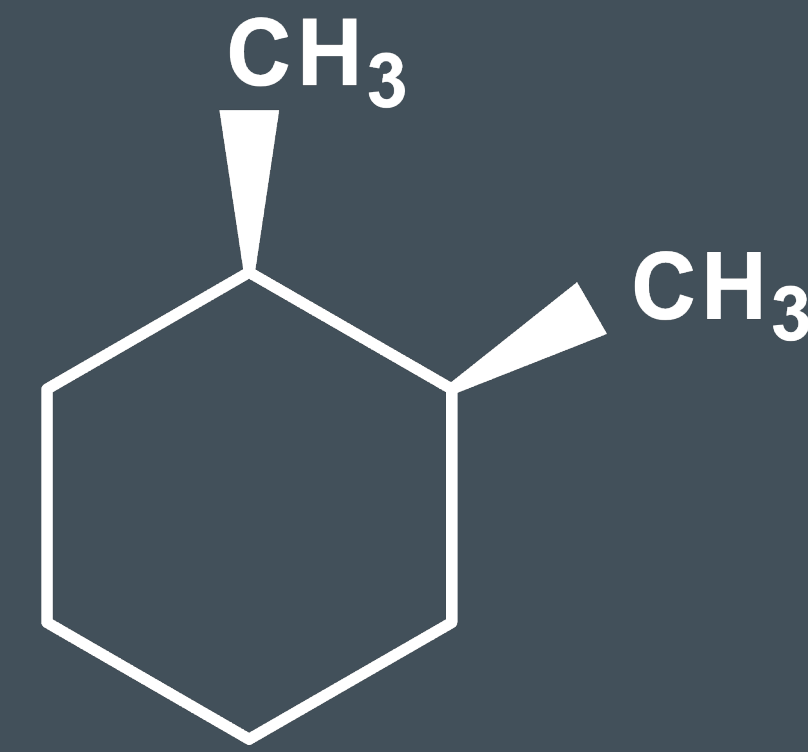


trans

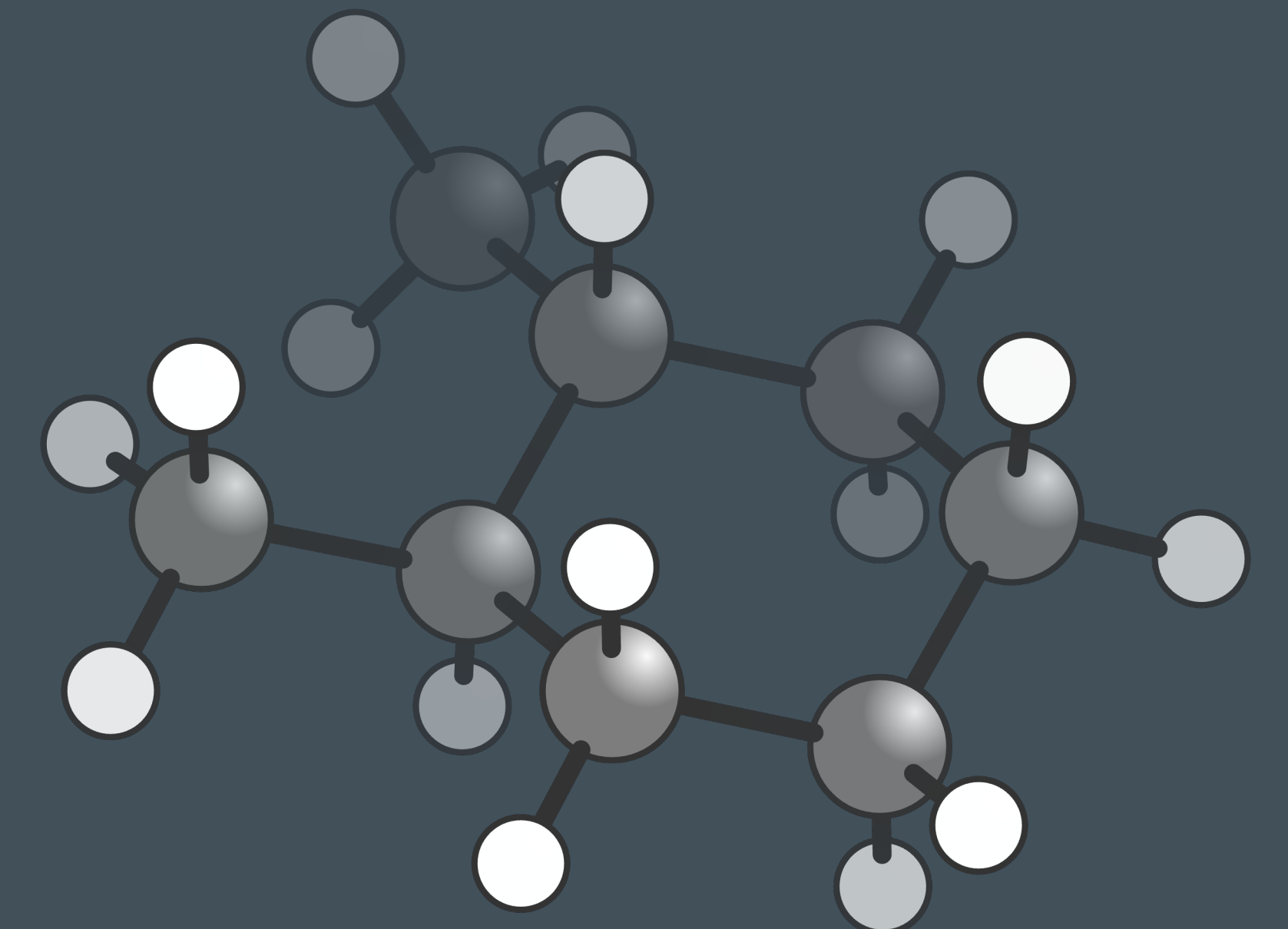
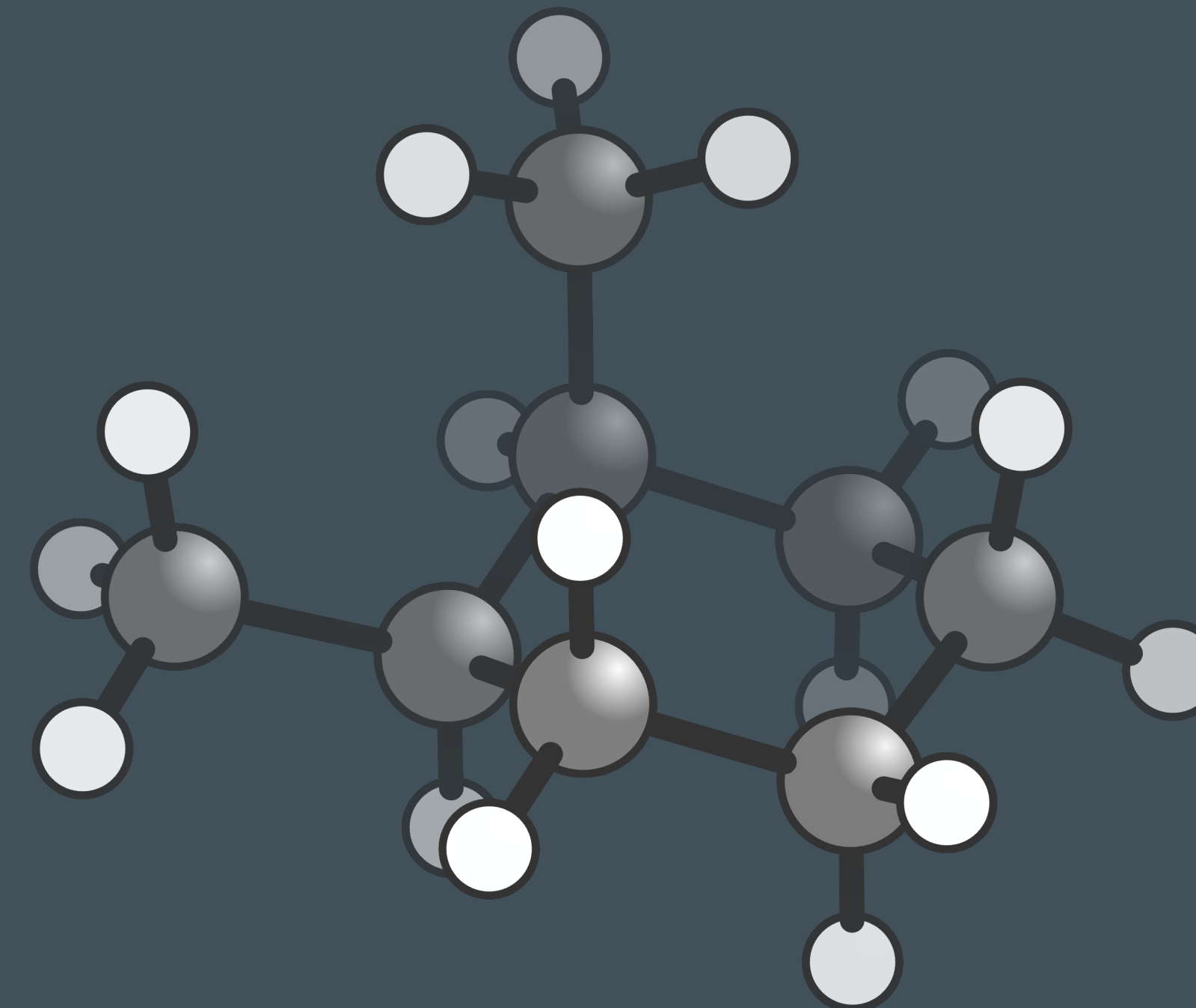
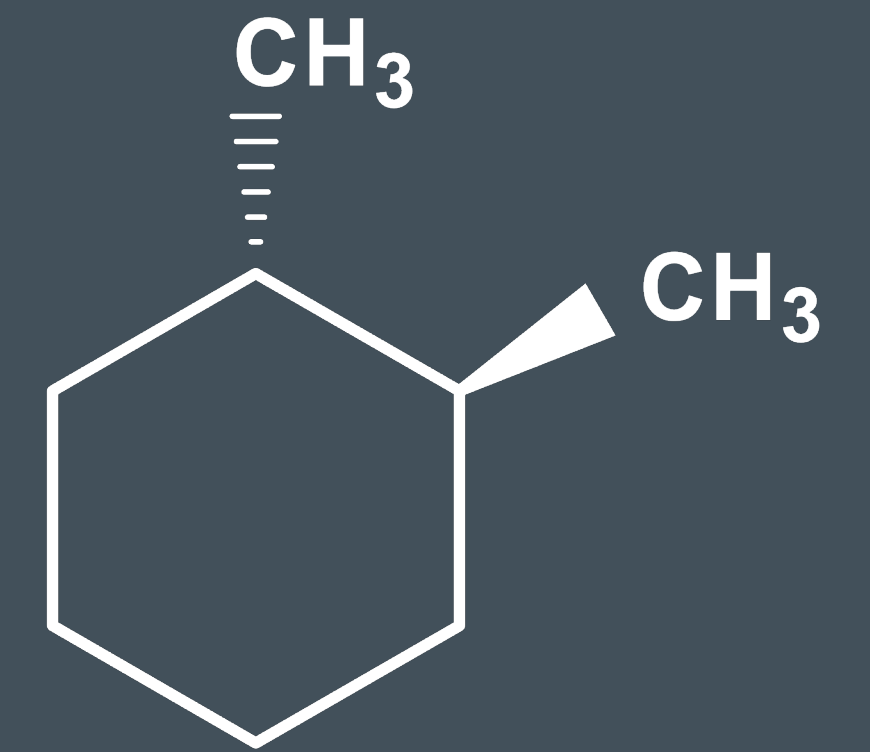


Cyclic alkanes

cis



trans



Same composition, Same bonding pairs, **Different shape** (not related by symmetry)

Chirality

A chiral molecule is a structure that is not identical to its mirror image



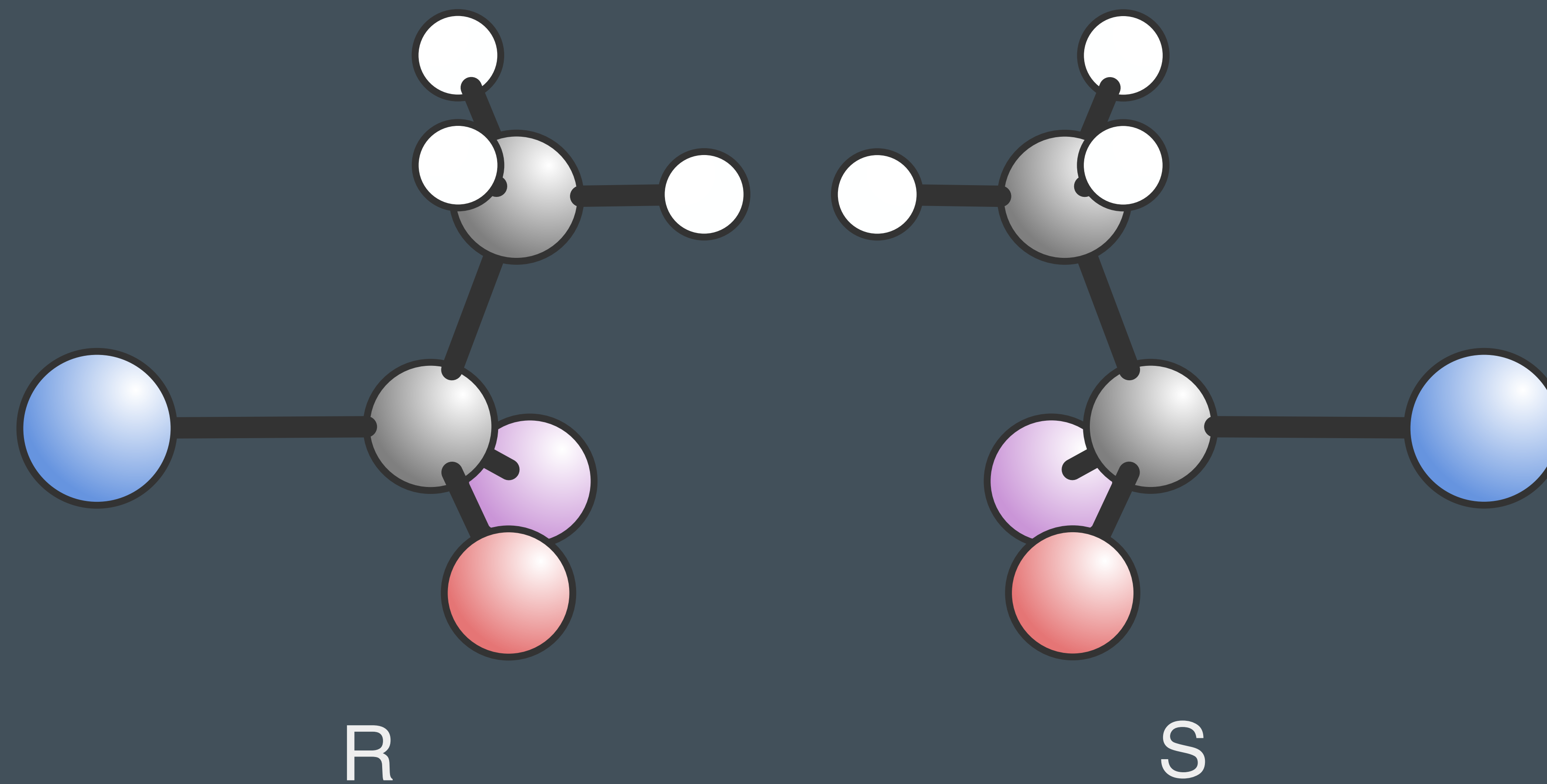
Left-handed



Right-handed

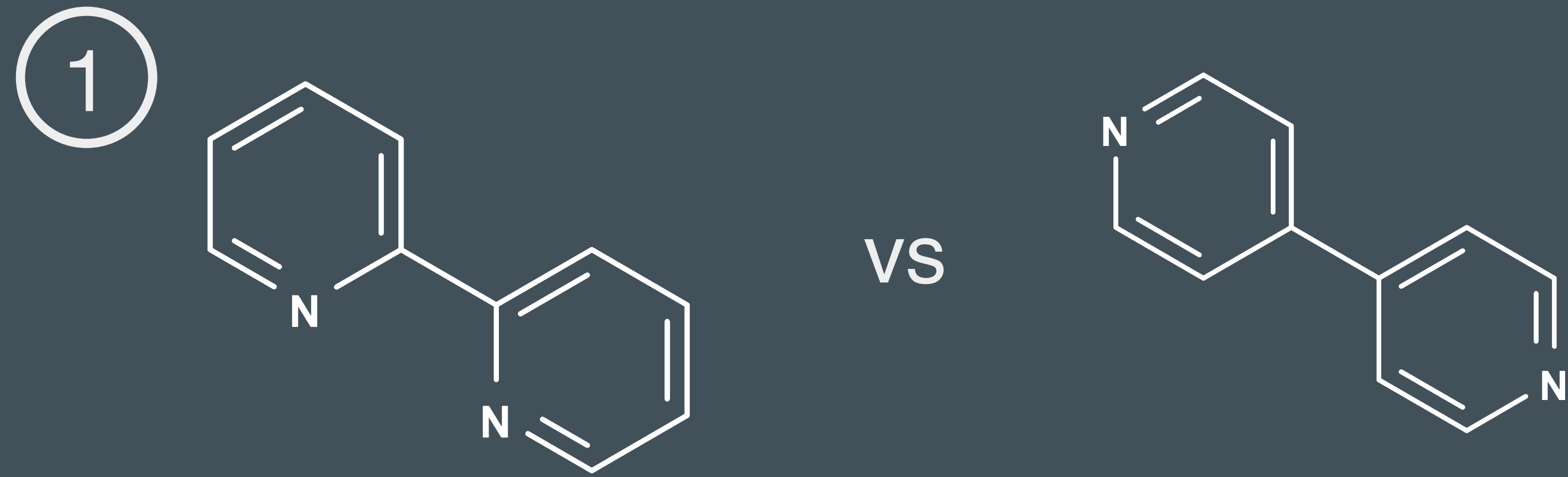
Sometimes we'll also refer to this as "handedness"

Optical Isomers: Same atoms, same connectivity, same arrangement *different handedness (chirality)*



The R molecule is the *enantiomer* of the S molecule

What is the relationship?

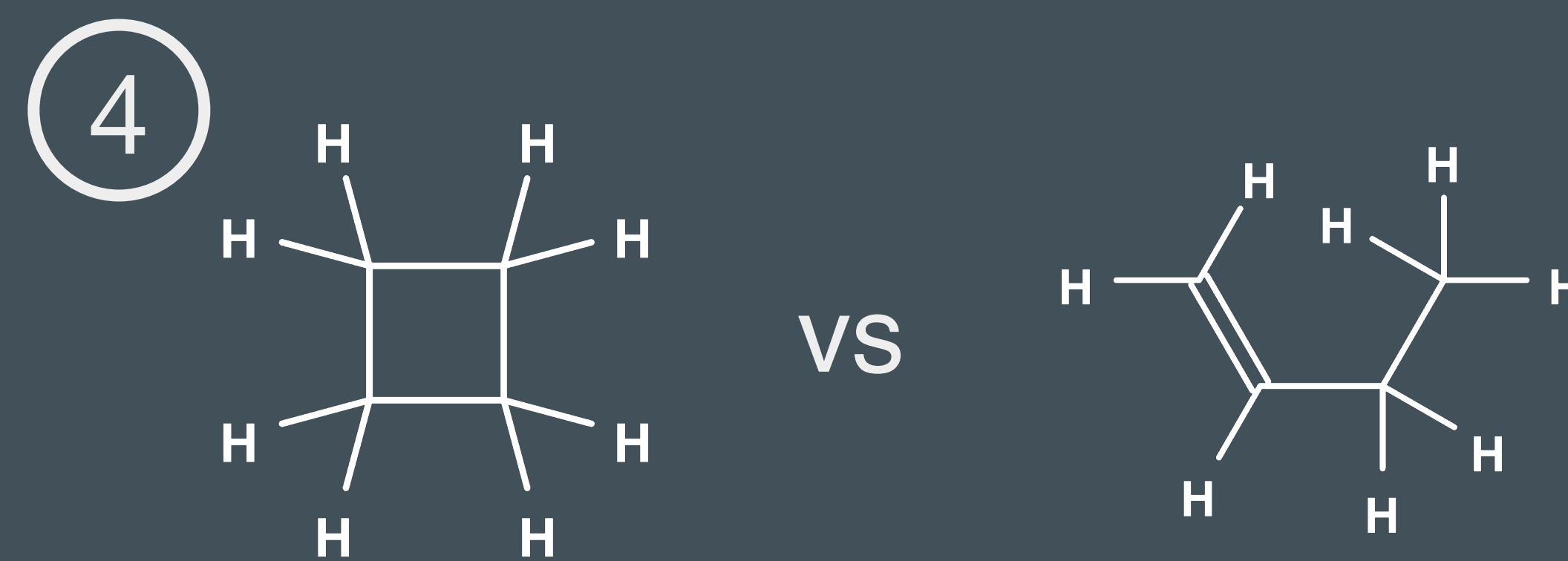
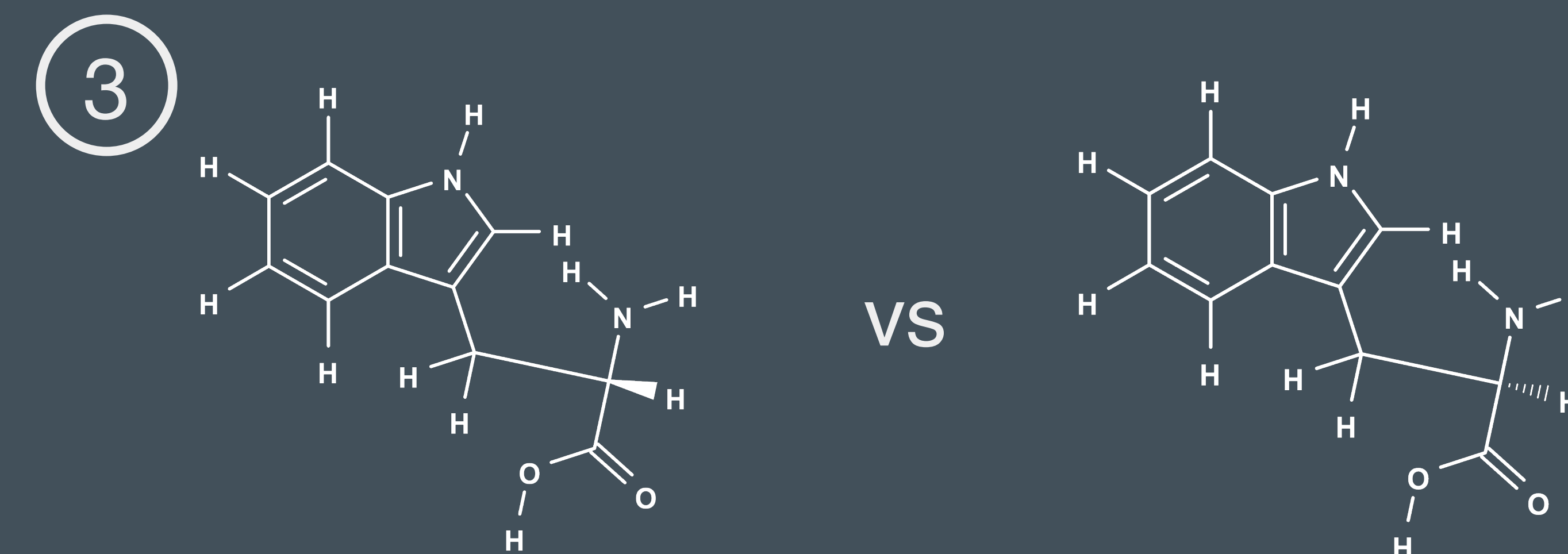
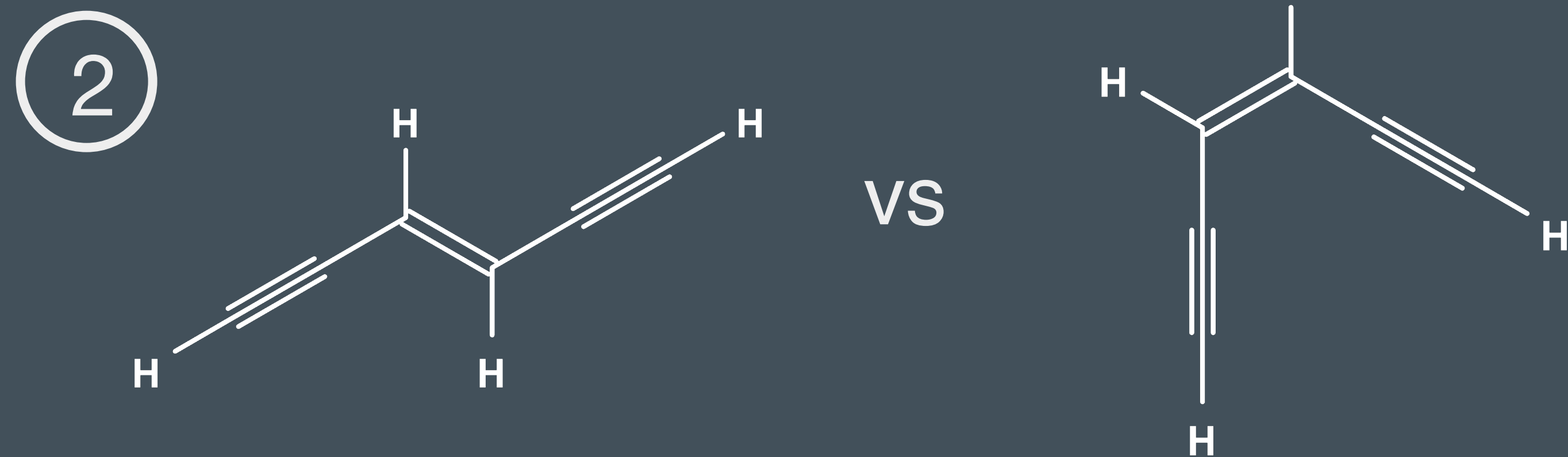


A. Different compounds

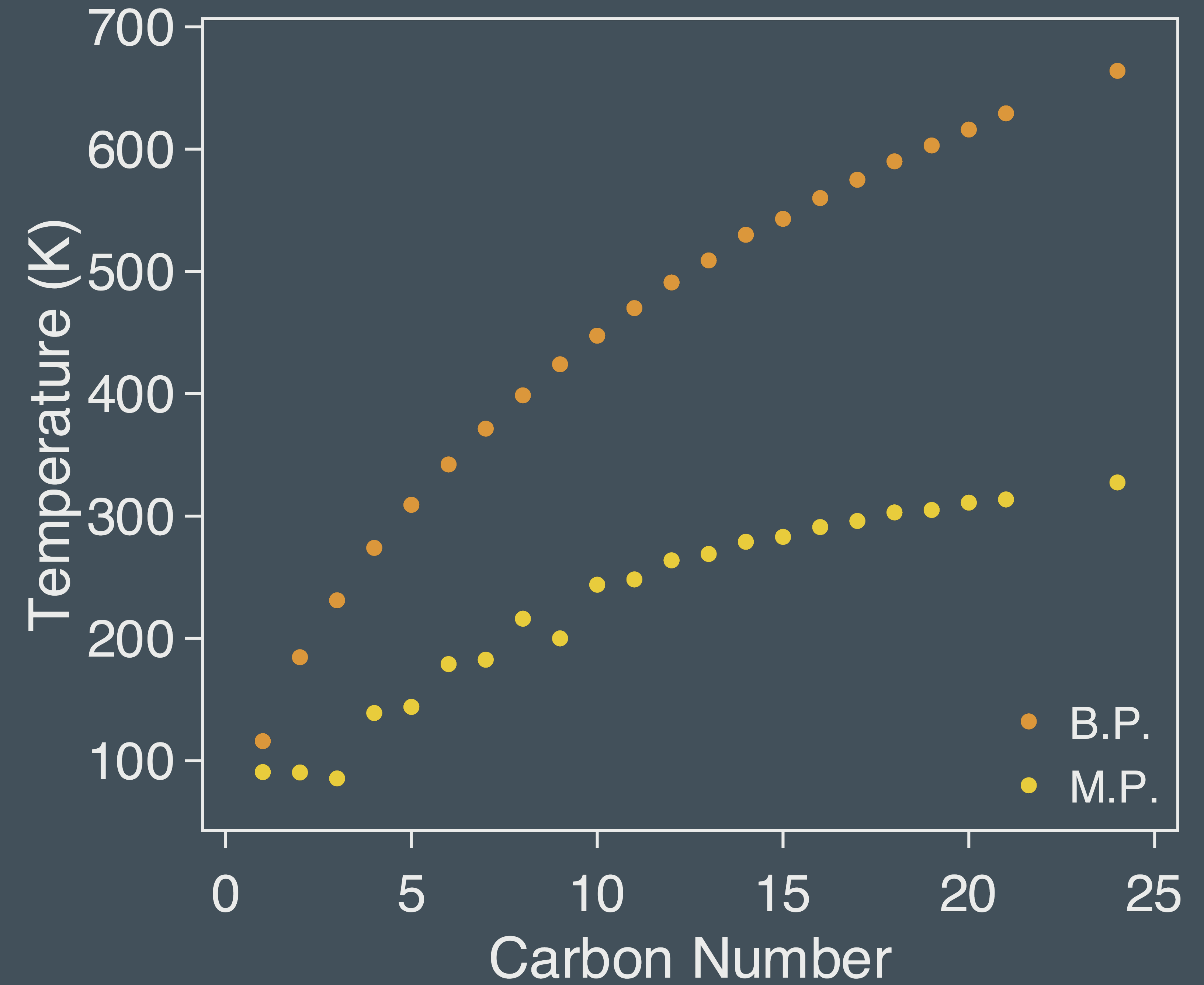
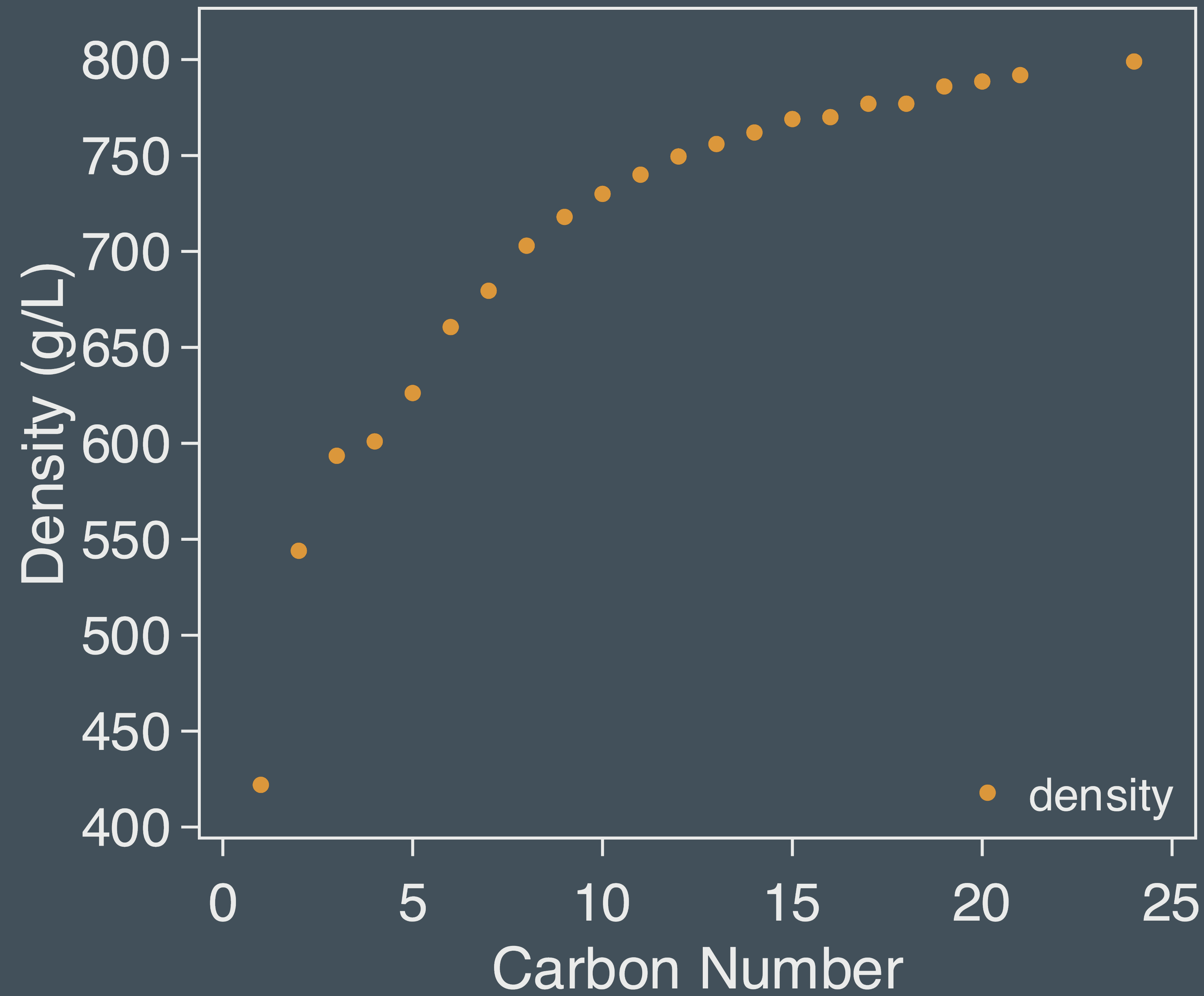
B. Structural Isomer

C. Geometric Isomer

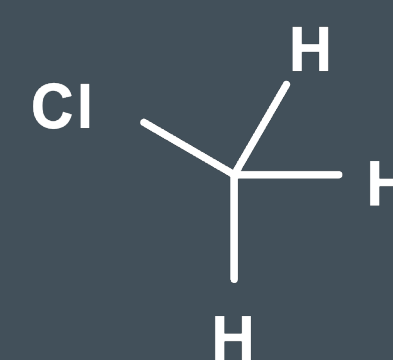
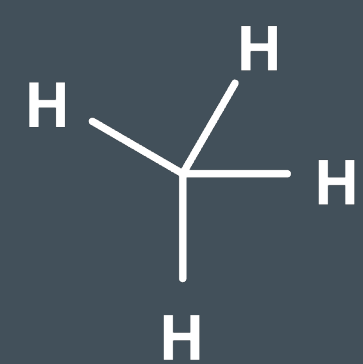
D. Enantiomer (Optical Isomer)



Some Properties of Alkanes

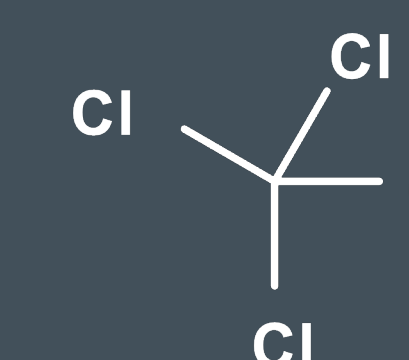
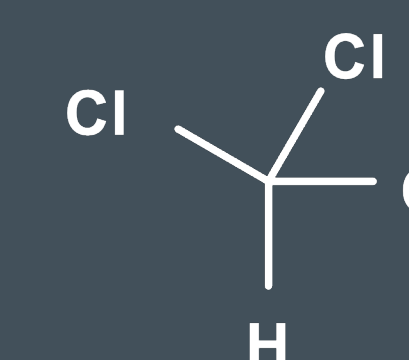
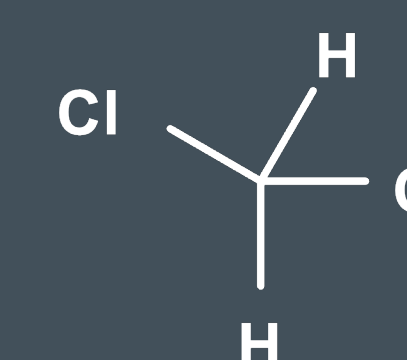
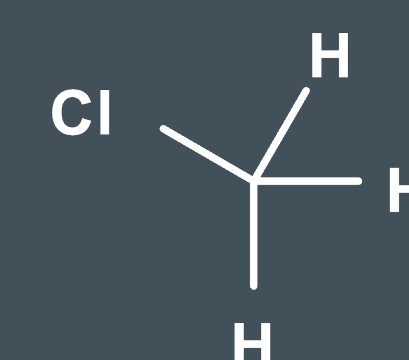
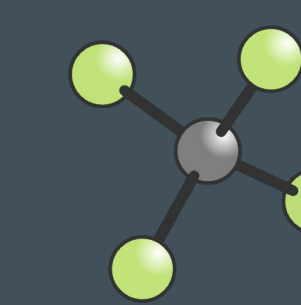
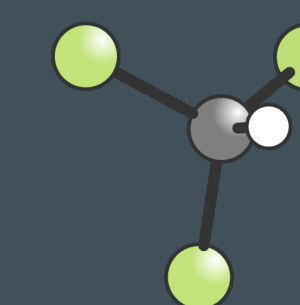
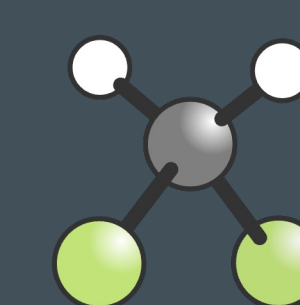
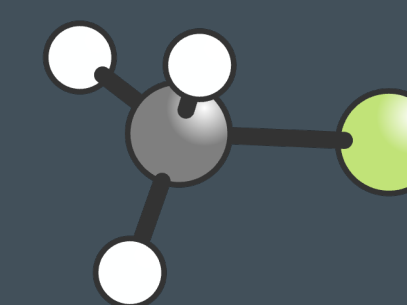


Reactions of Alkanes: Substitution

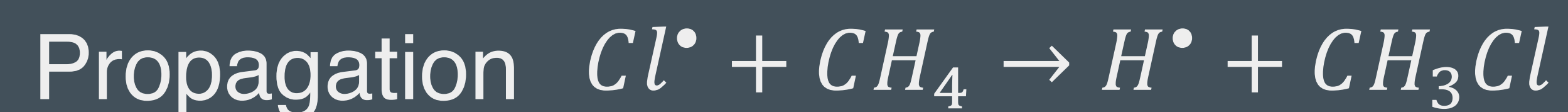
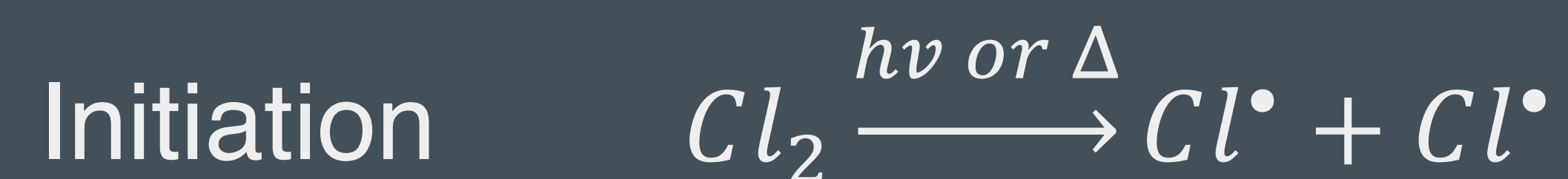


Yield distribution of:

CH_3Cl , CH_2Cl_2 , CHCl_3 , and CCl_4

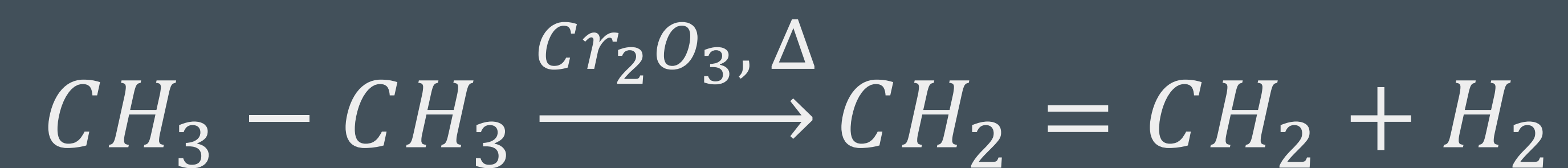


A radical reaction mechanism:



Reactions of Alkenes:

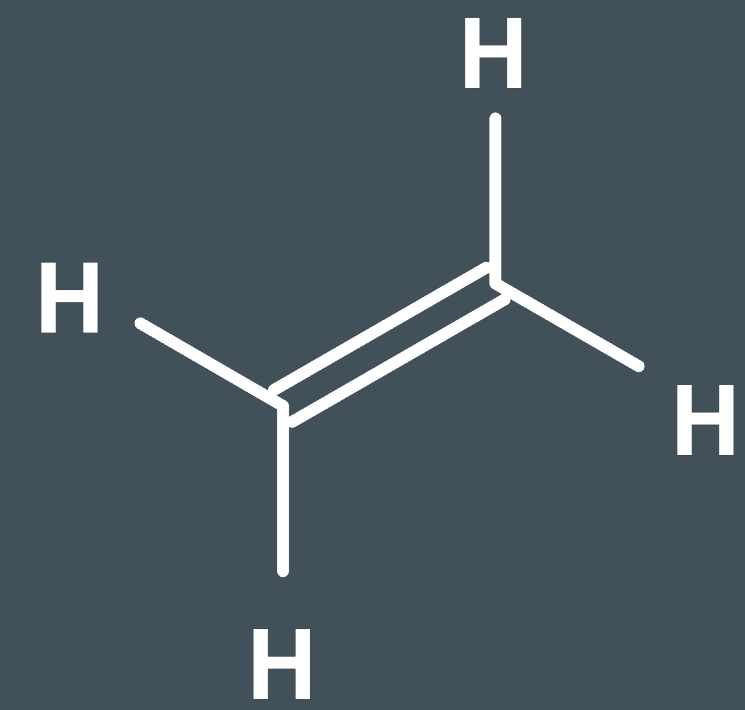
Oxidation of Alkanes to Alkenes (Elimination)



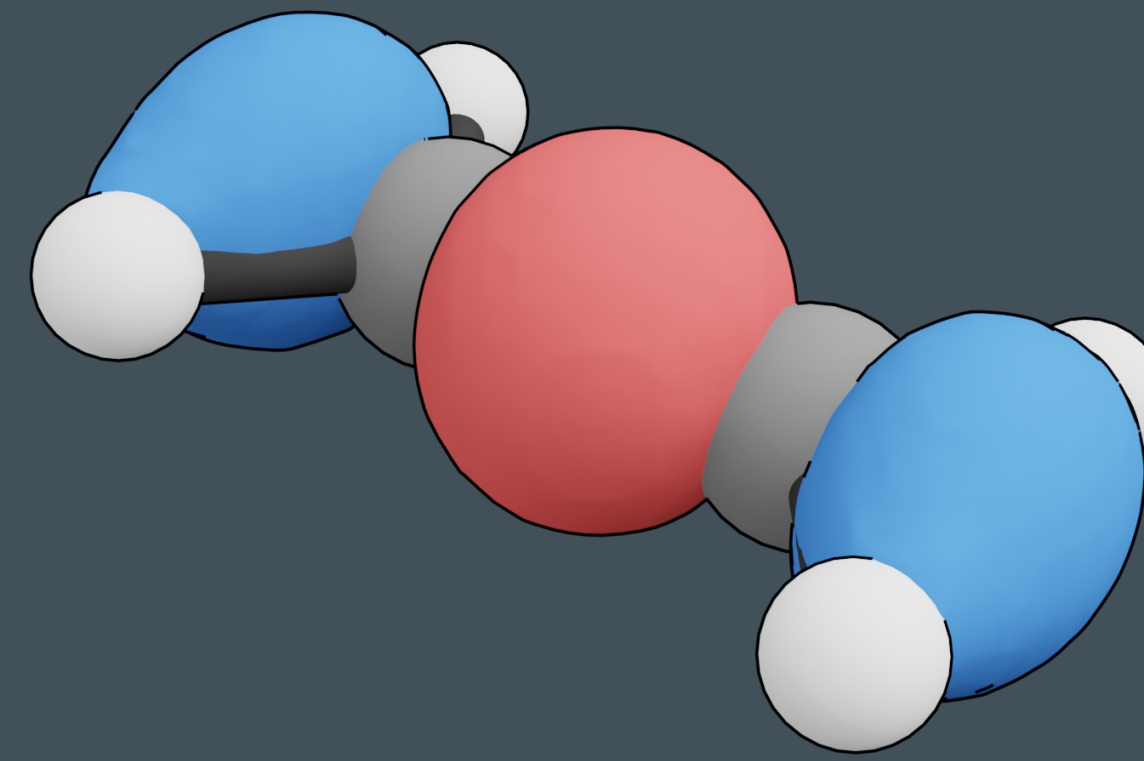
DEF: Elimination | a reaction in which atoms are “removed” from the reactant

Conversion of petroleum to a high value reagent
(goes on to make arenes, polyethylene, PVC...)

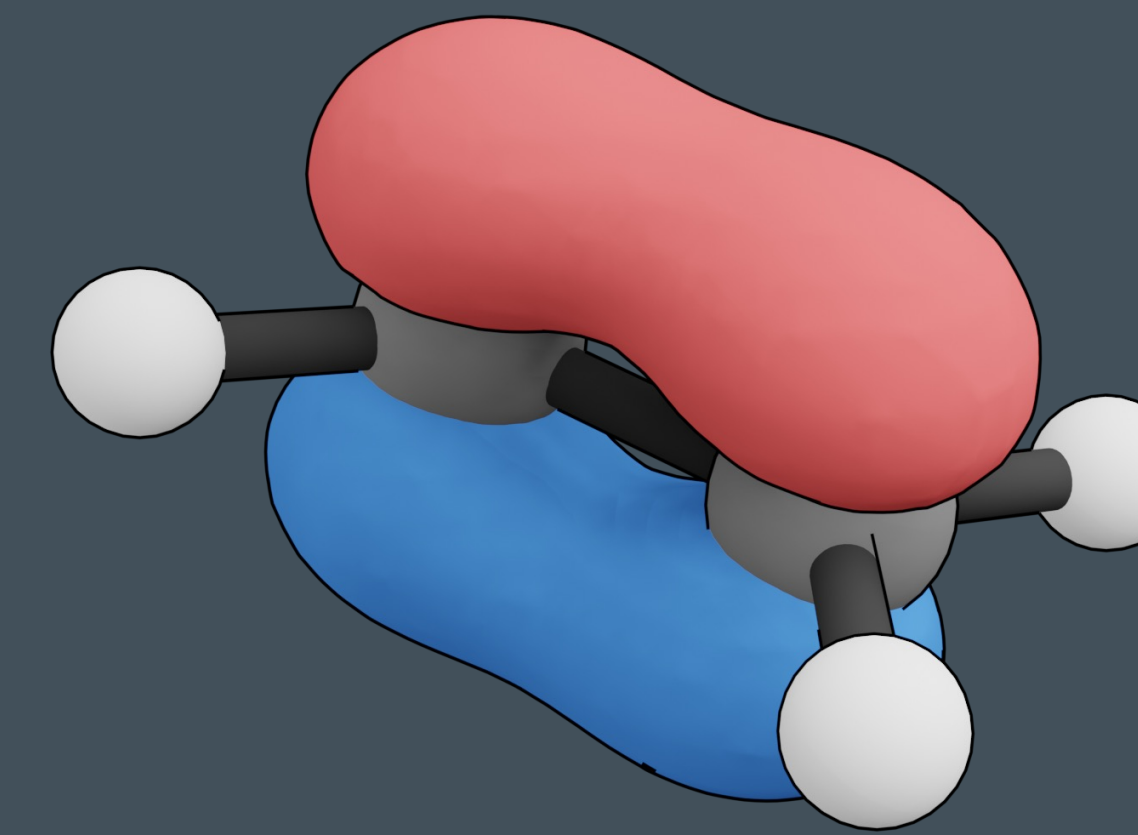
Nature of alkenes and alkynes



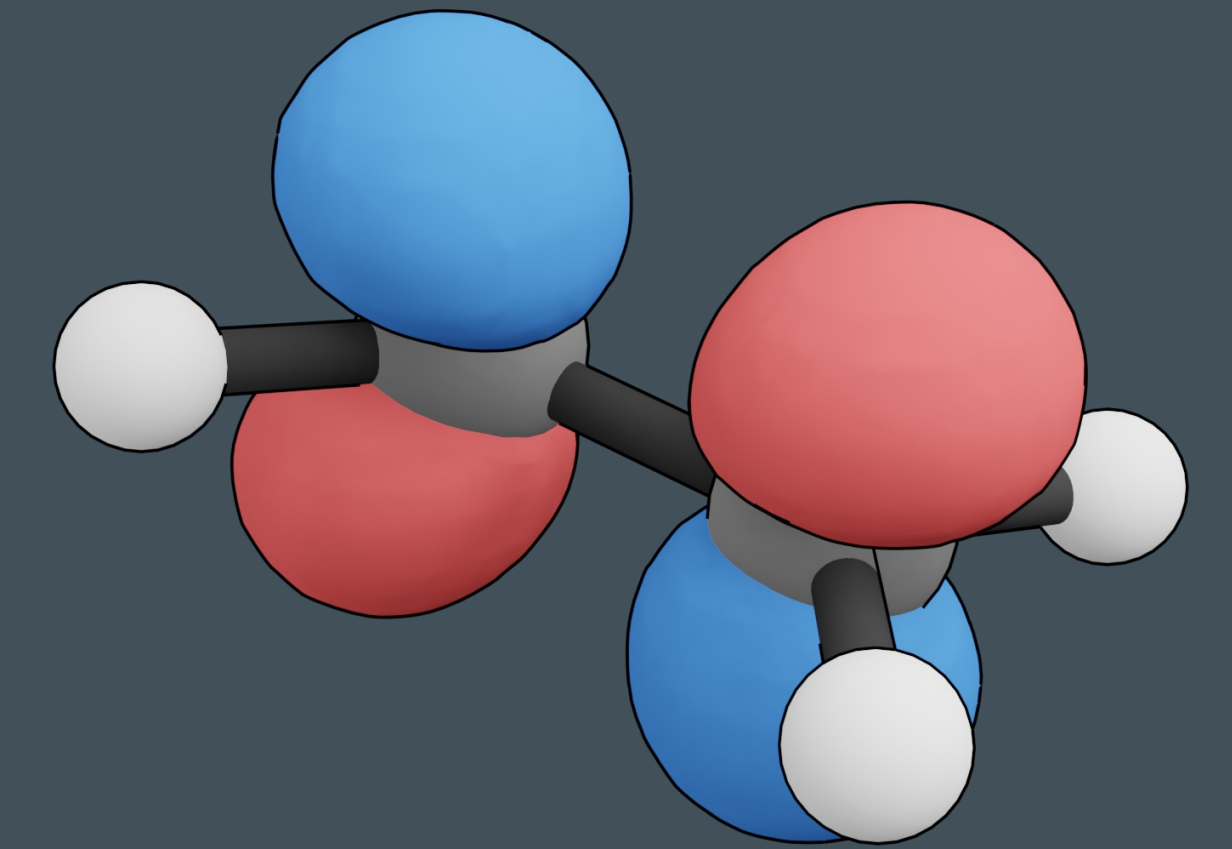
σ -bond



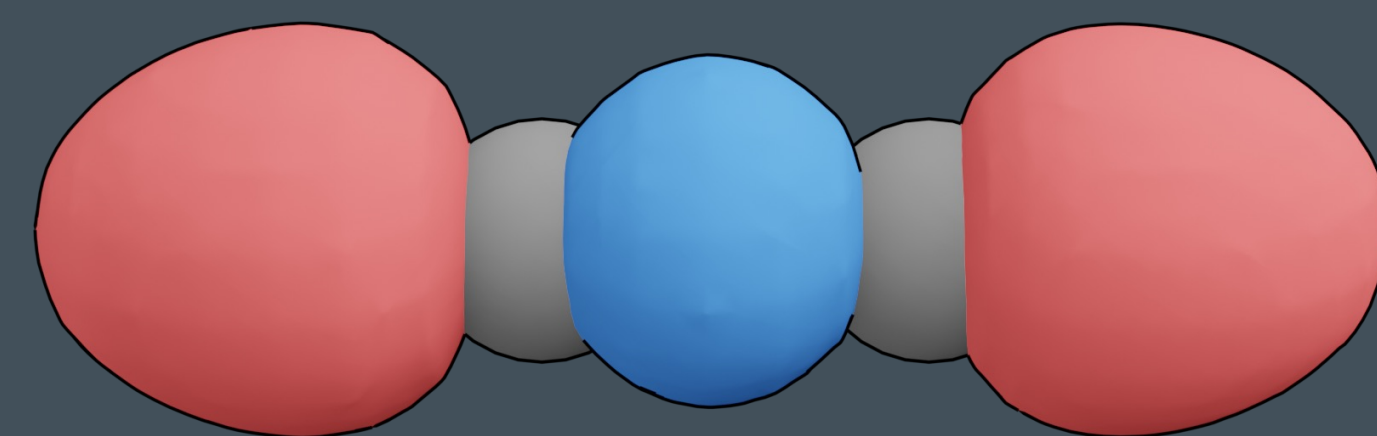
π -bond



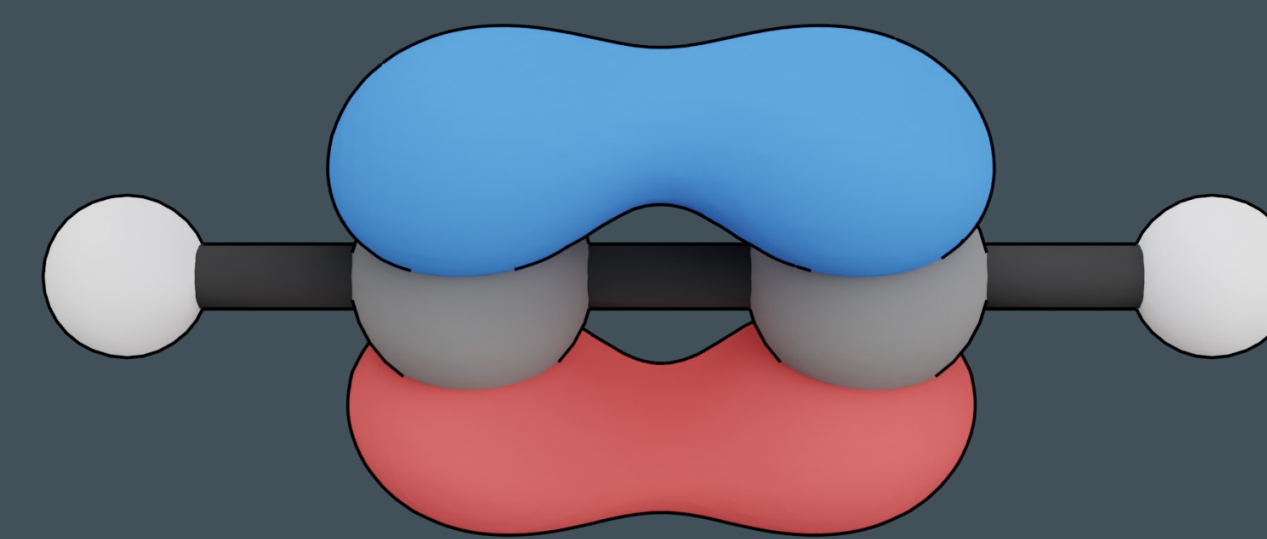
π^* -bond



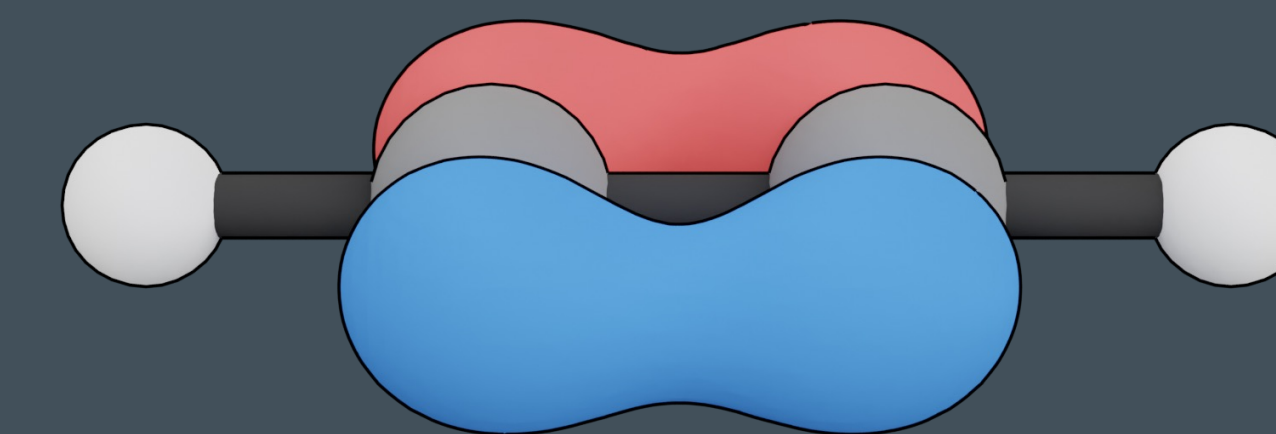
σ -bond



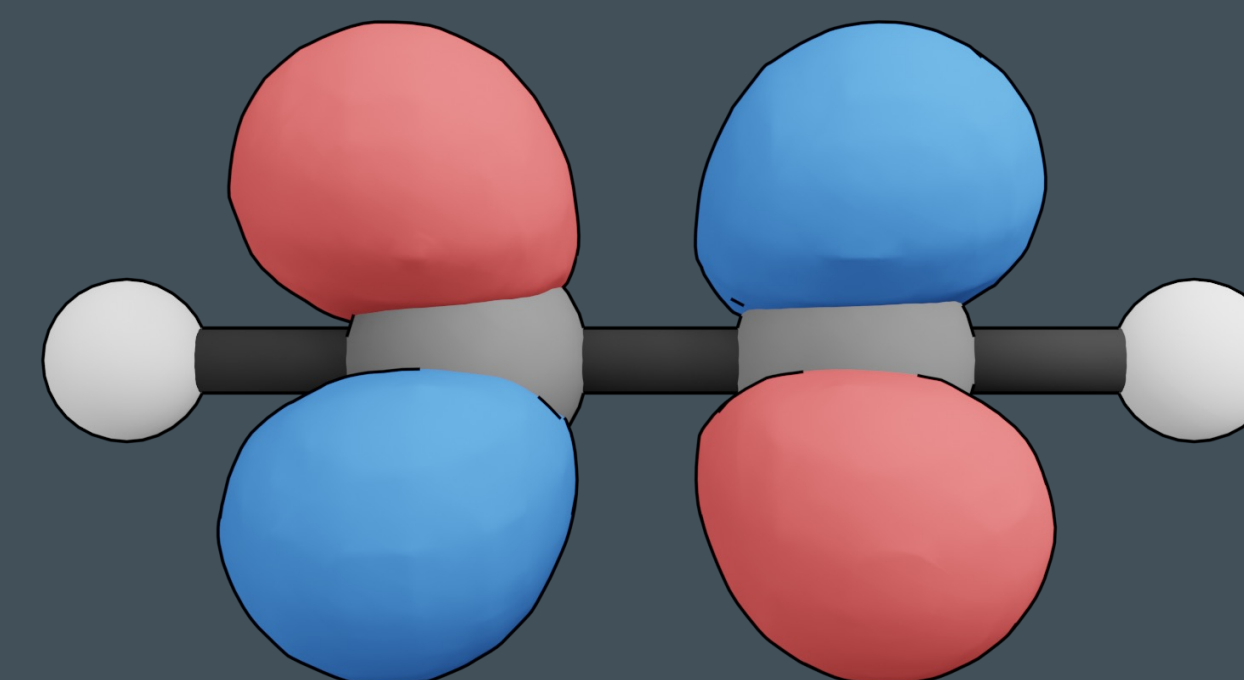
π -bond



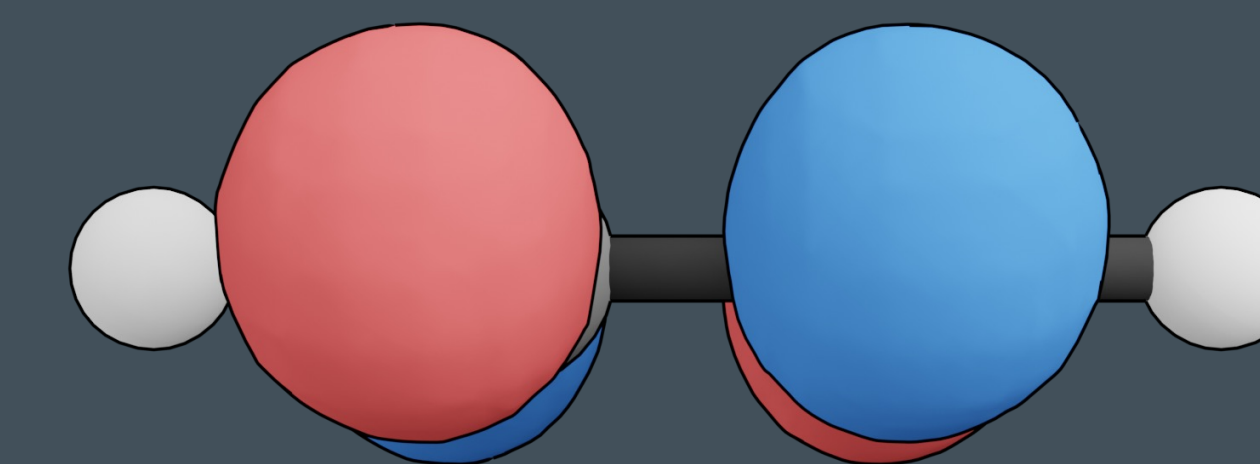
π -bond



π^* -bond

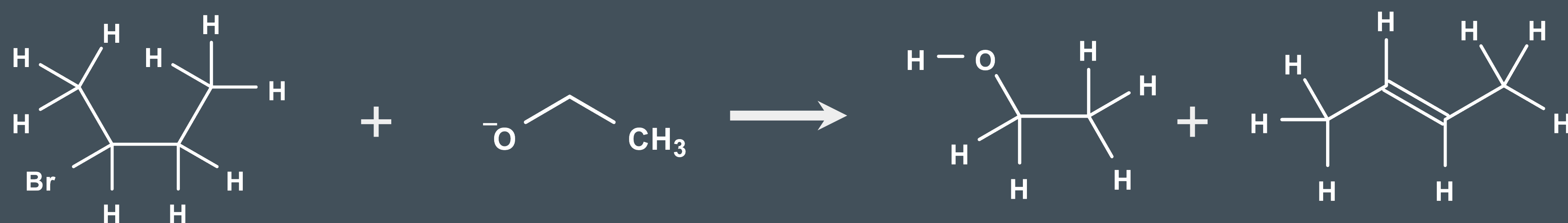


π^* -bond



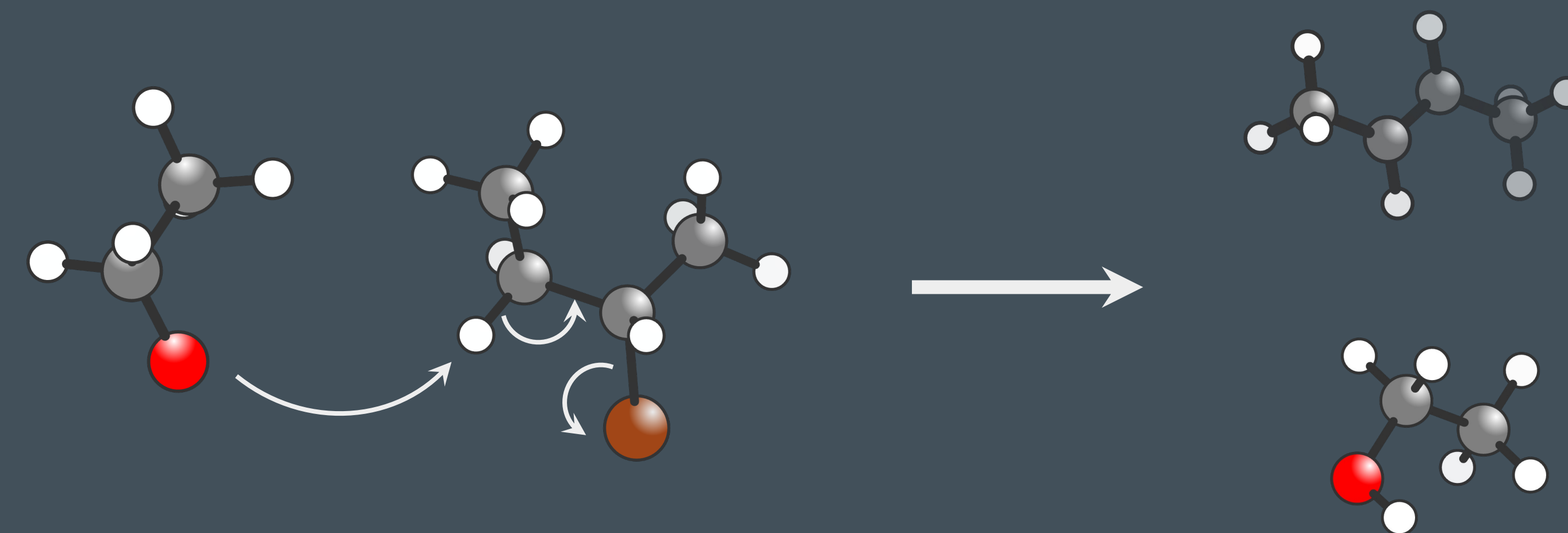
Reactions of Alkenes:

① Dehydrohalogenation



(an alternative route to alkenes)

“Arrow pushing” rxn mechanism



② Electrophilic Addition



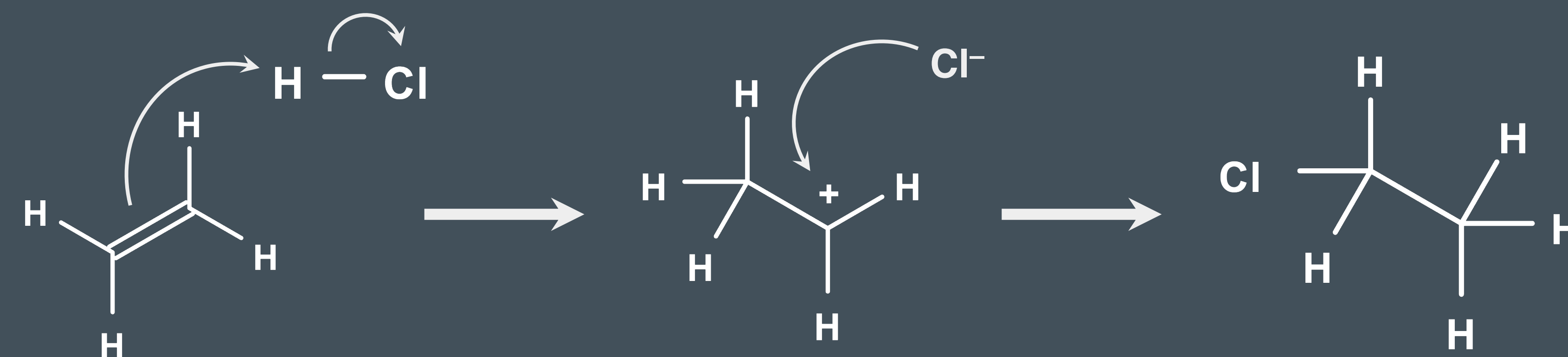
DEF: Addition | a reaction in which atoms are “added” to the reactant

DEF: Electrophile | a reagent attracted to regions of other molecules with high electron density

③ Hydrohalogenation

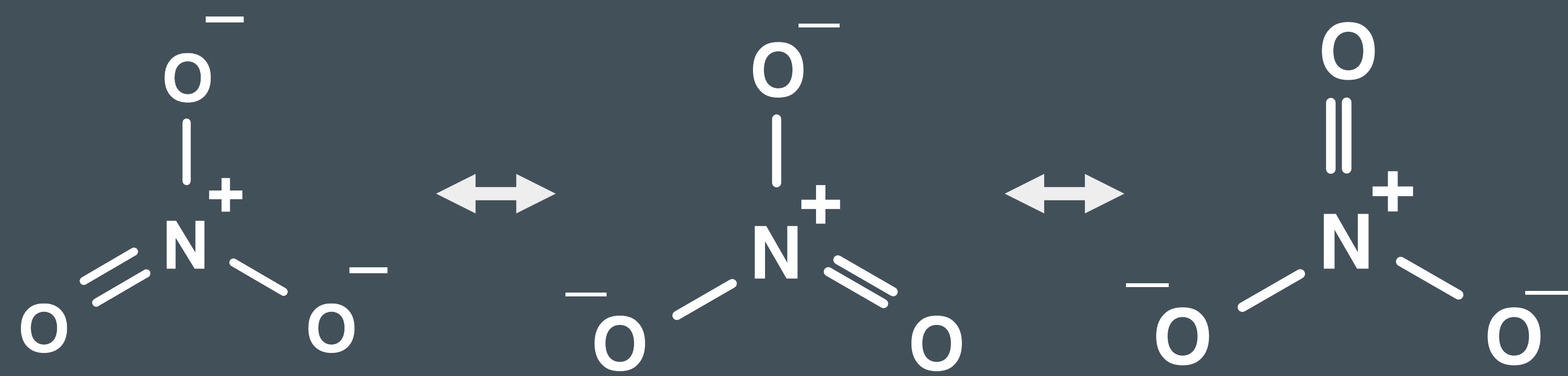


(a specific electrophilic addition)

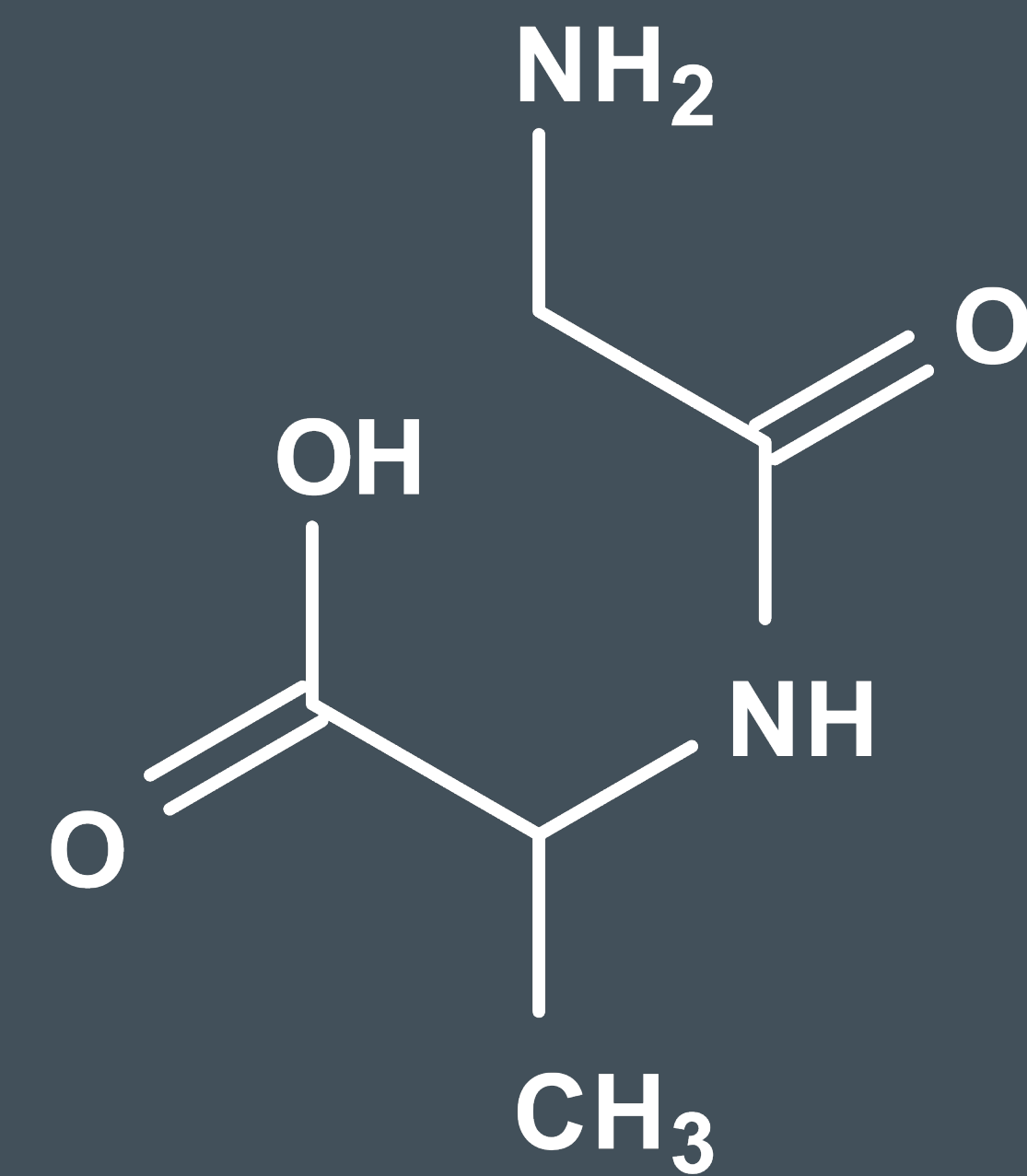


Resonance Structures

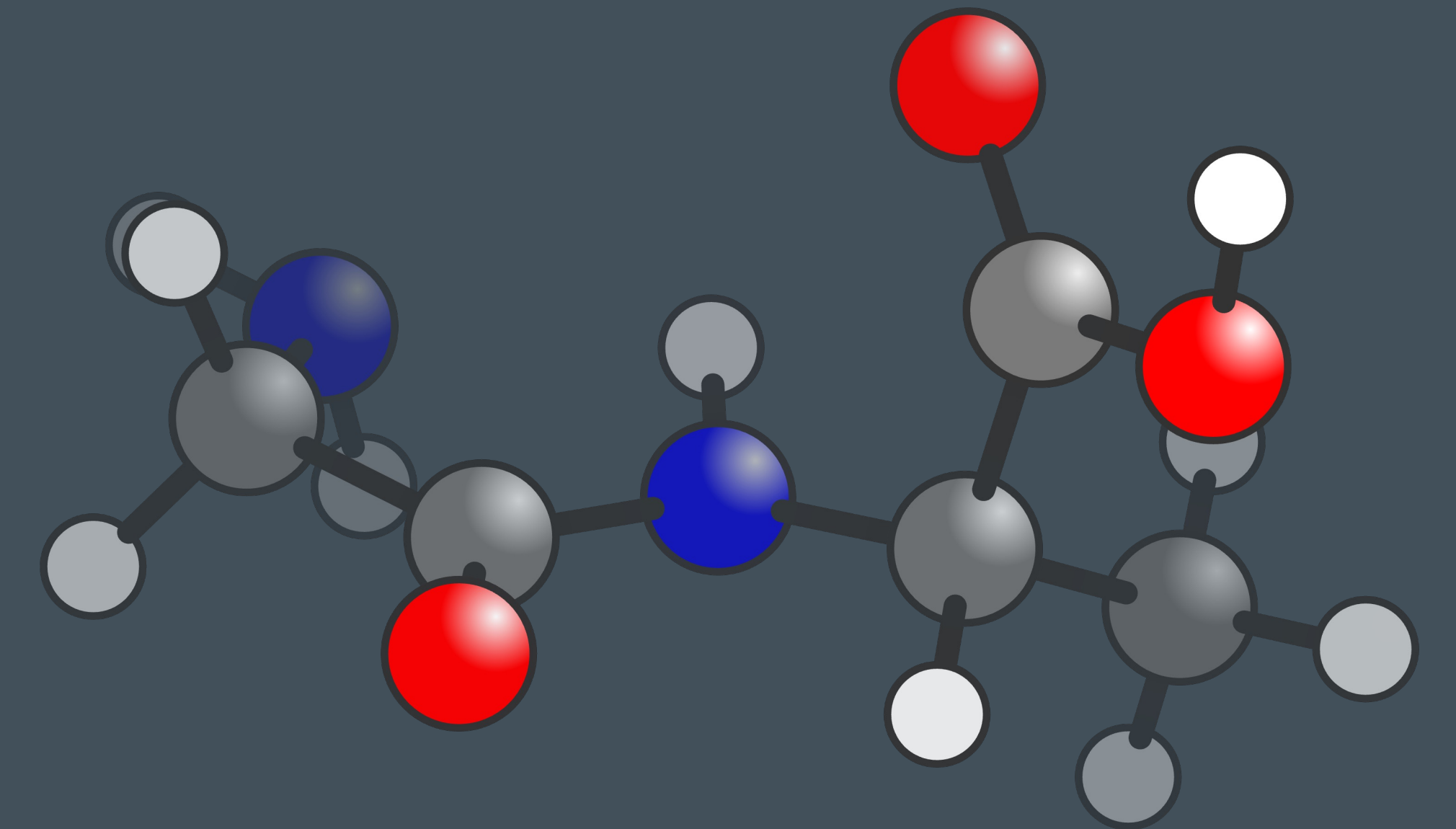
Equienergetic resonance structures



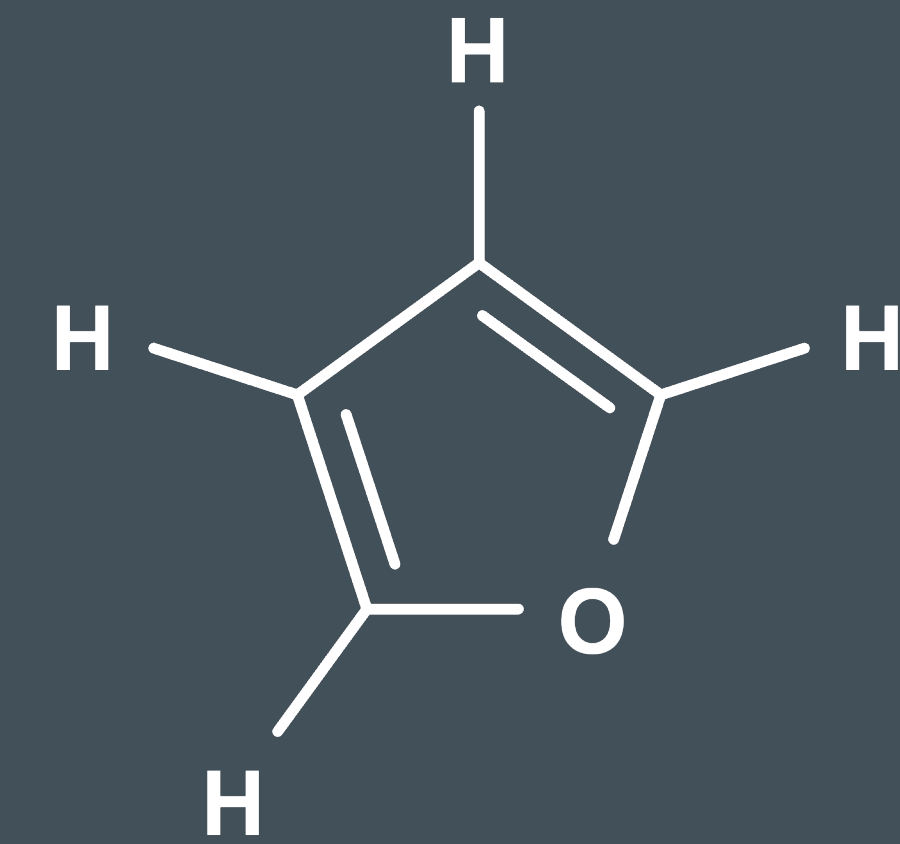
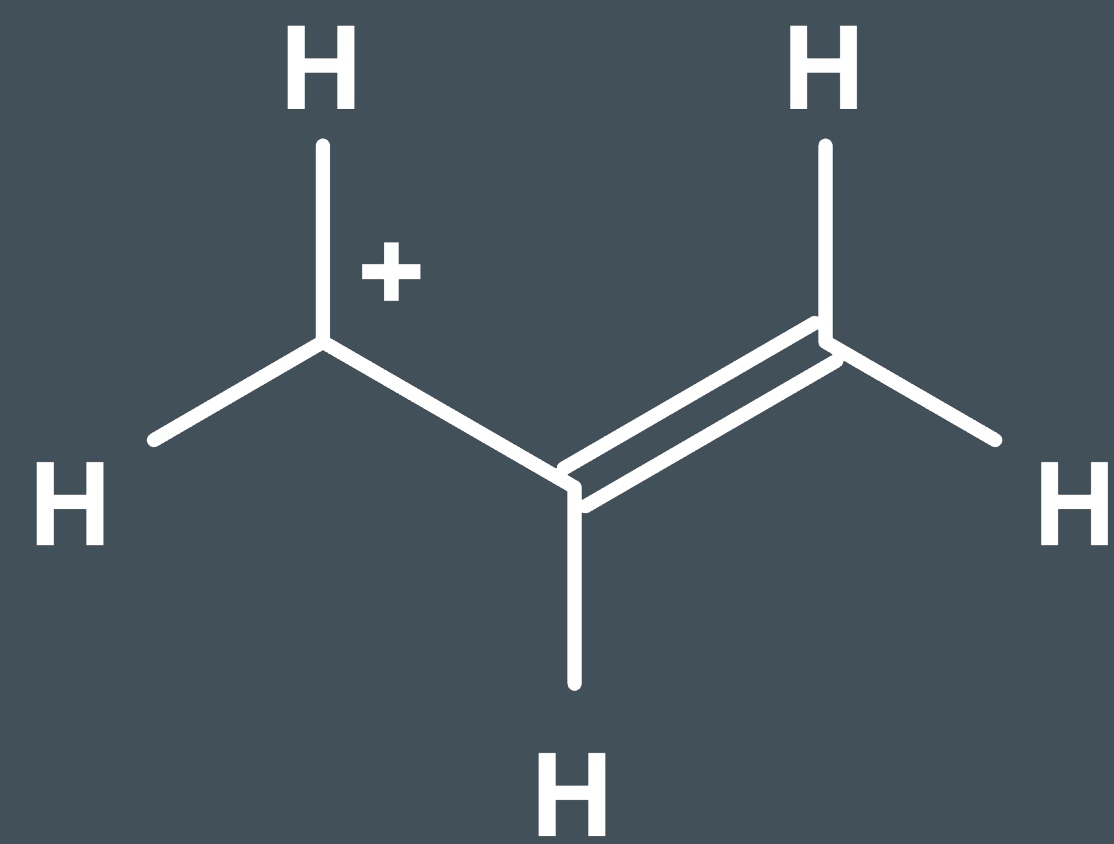
Non-equienergetic resonance structures



Glycine-Alanine

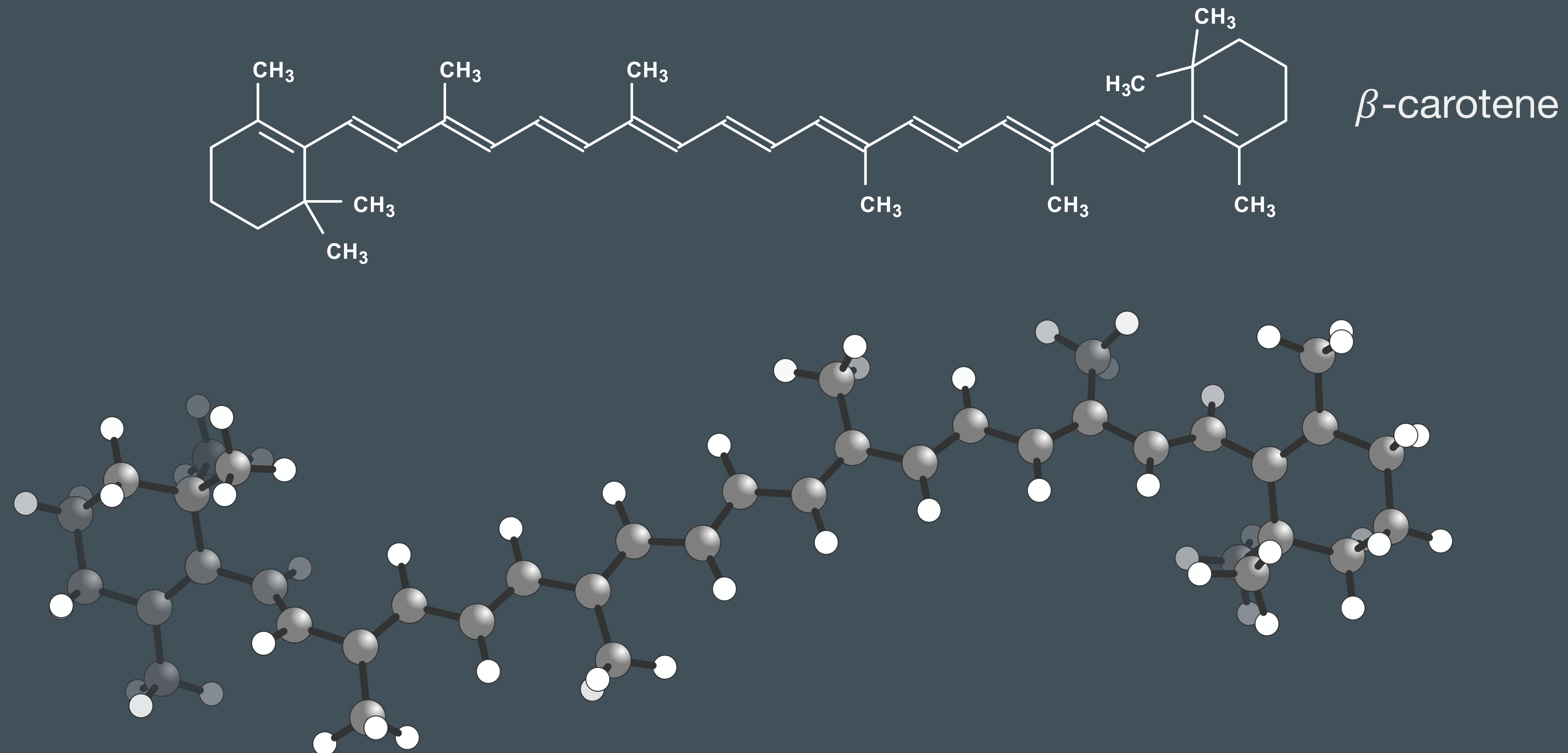


Draw the equivalent resonance structures



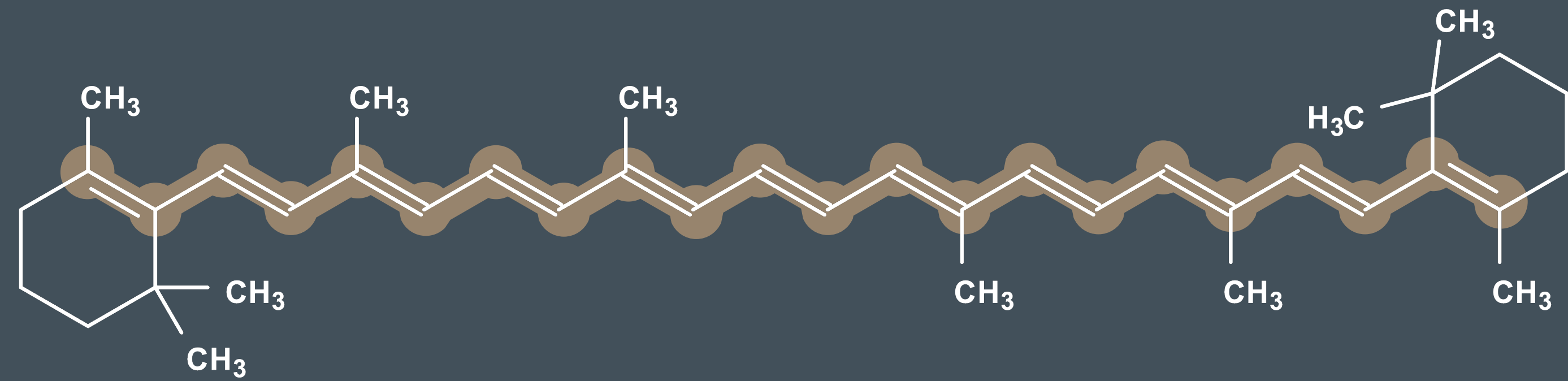
Conjugation

DEF **Conjugation**: An alternation of single and double bonds that yield a planar structure.

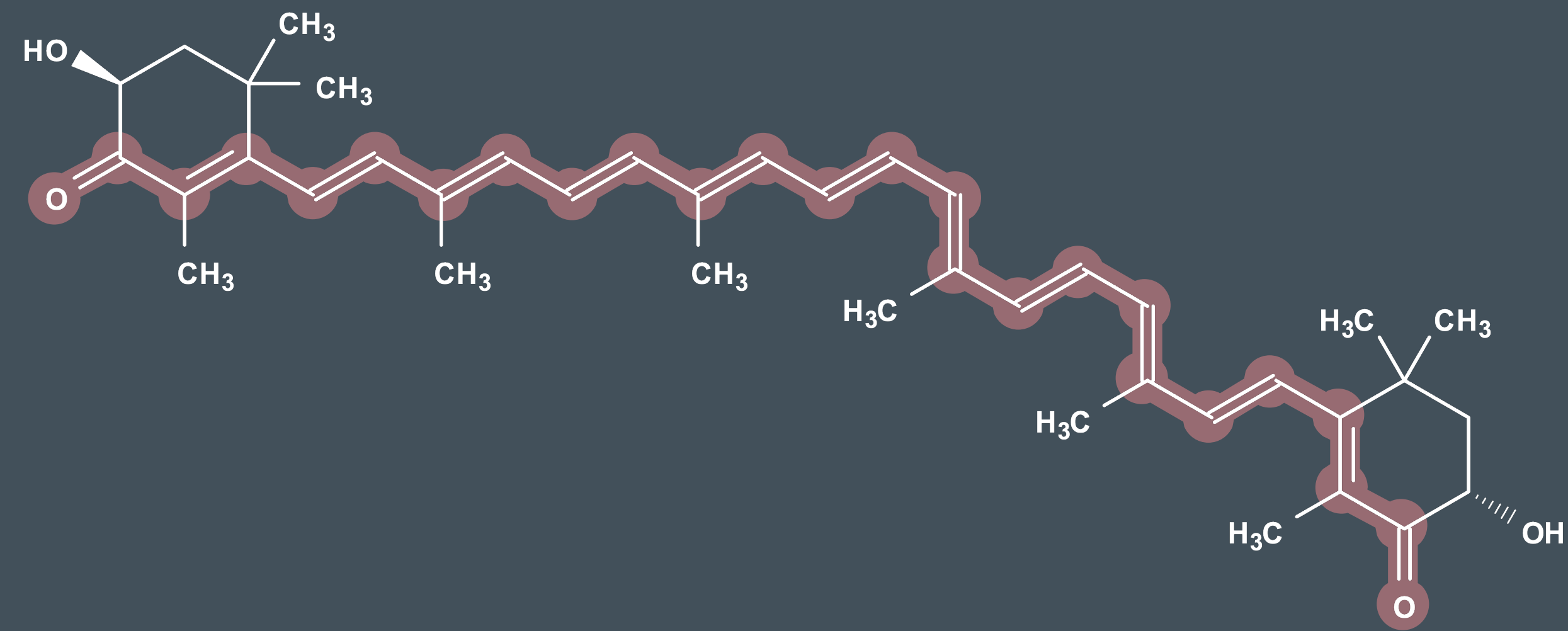


Conjugation results in the delocalization of electrons across many atoms. Extensive conjugation over yields richly colored compounds used as dyes and color sensors.

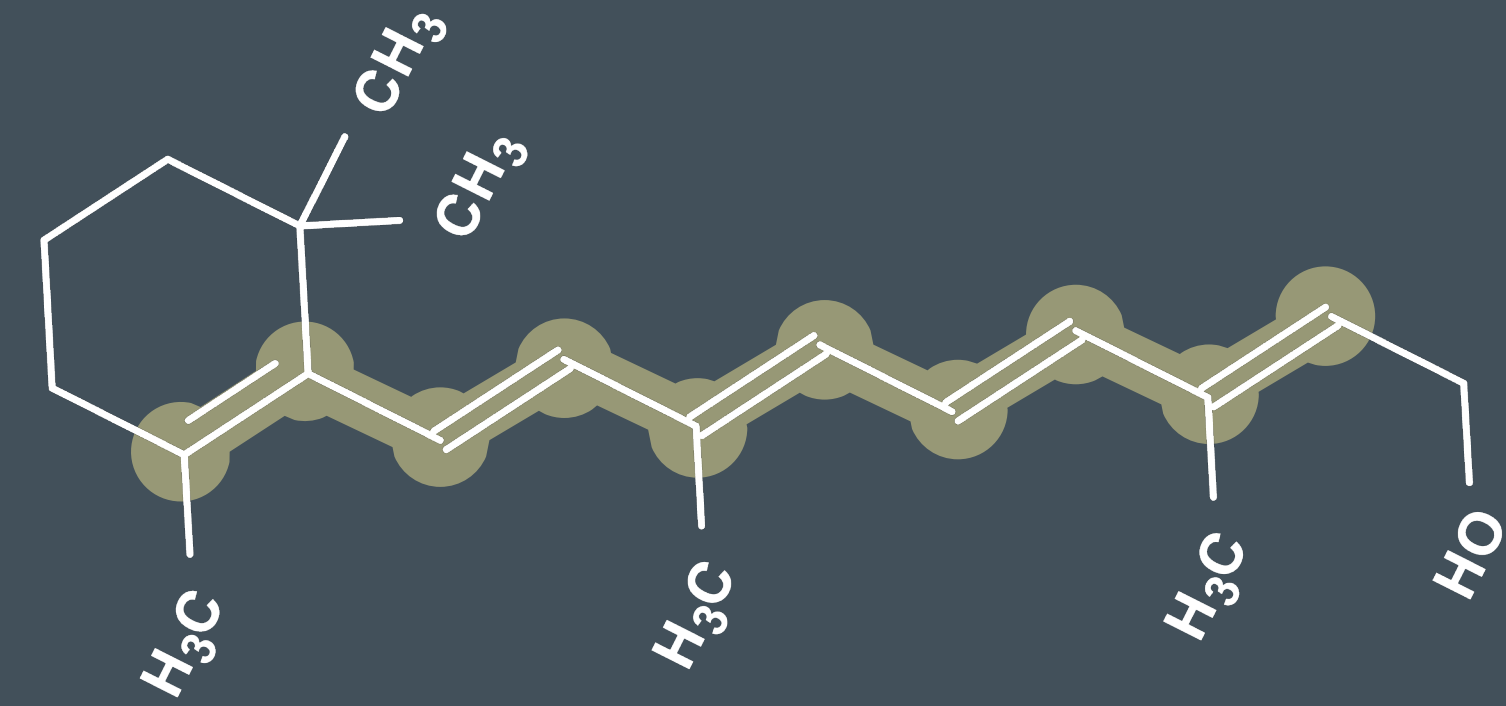
Conjugation



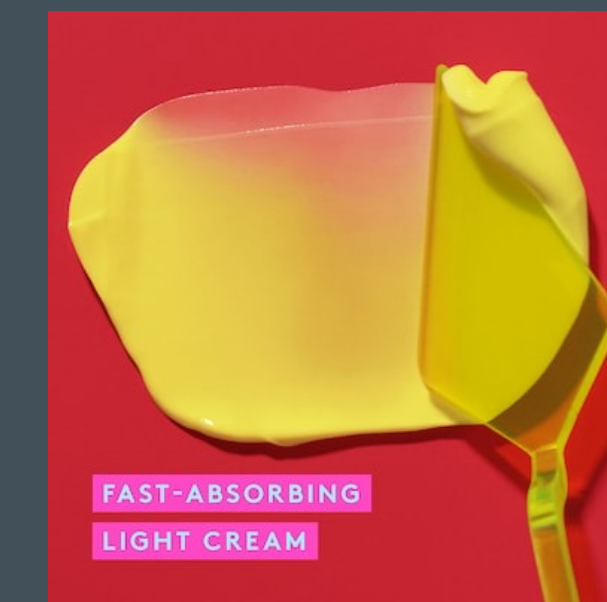
β -carotene



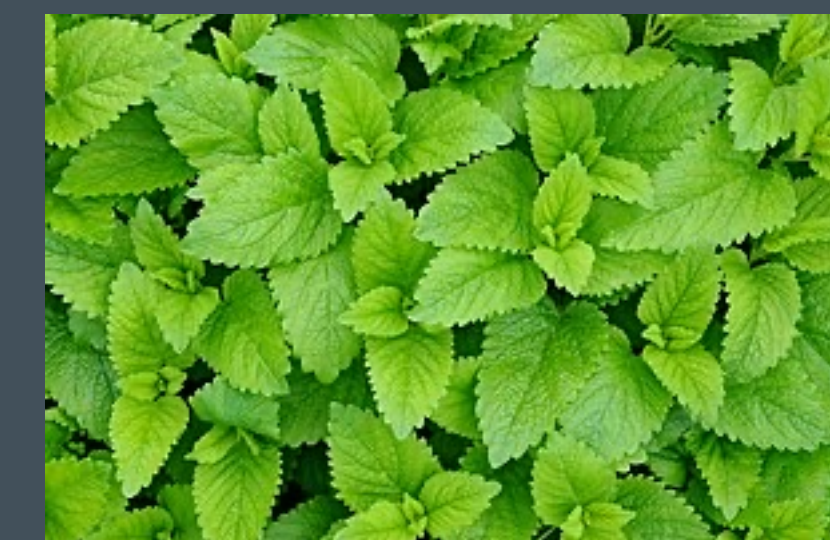
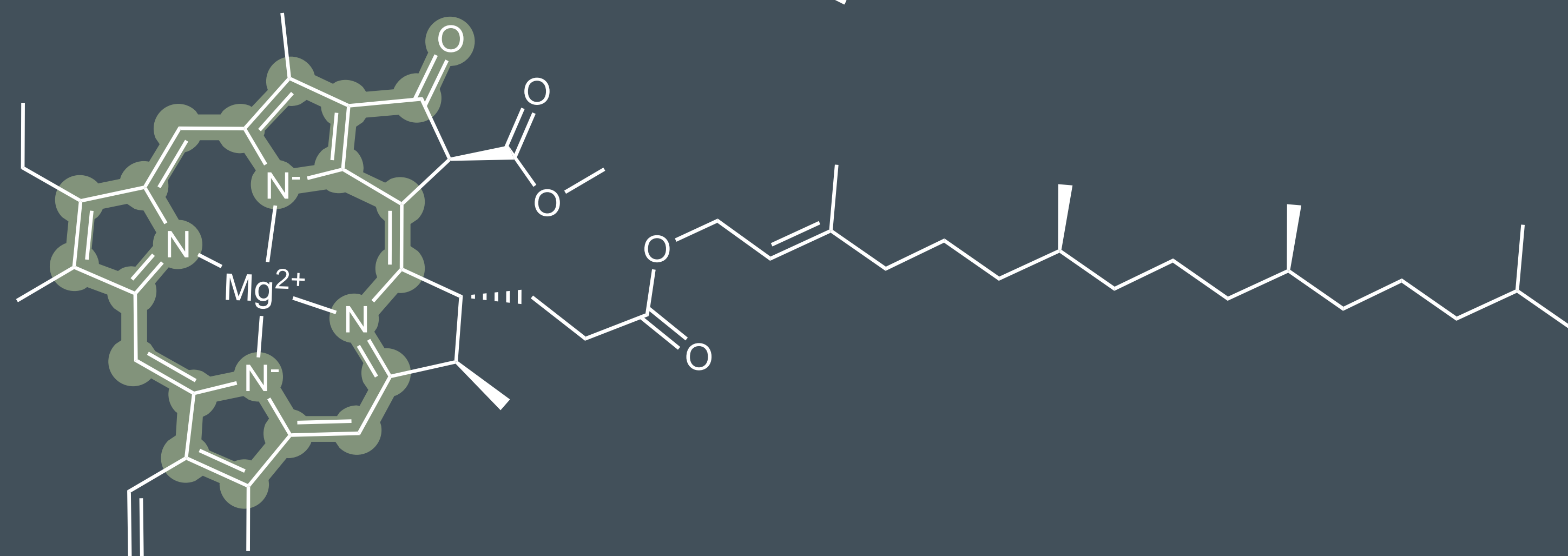
Astaxanthin



Retinol



Chlorophyll a



The downfall of the Kekulé structures of benzene (aka resonance)

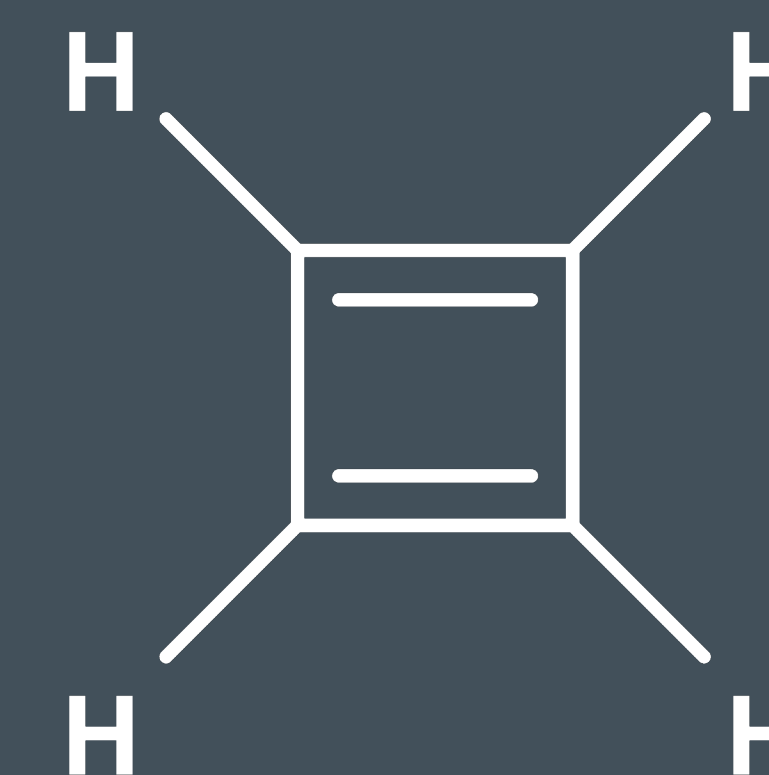


Resonance stabilize certain
cyclic aromatics...

benzene

Particularly stable

...but not others

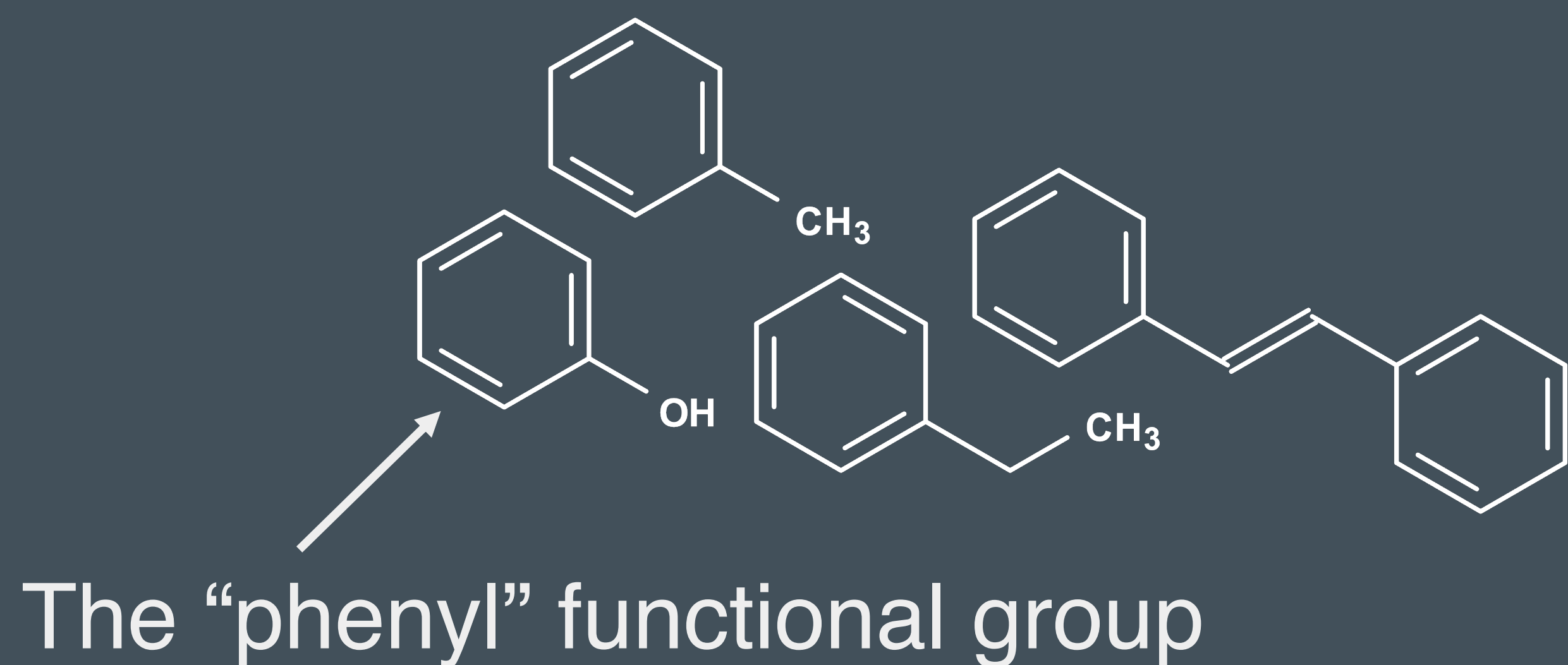


cyclobutadiene

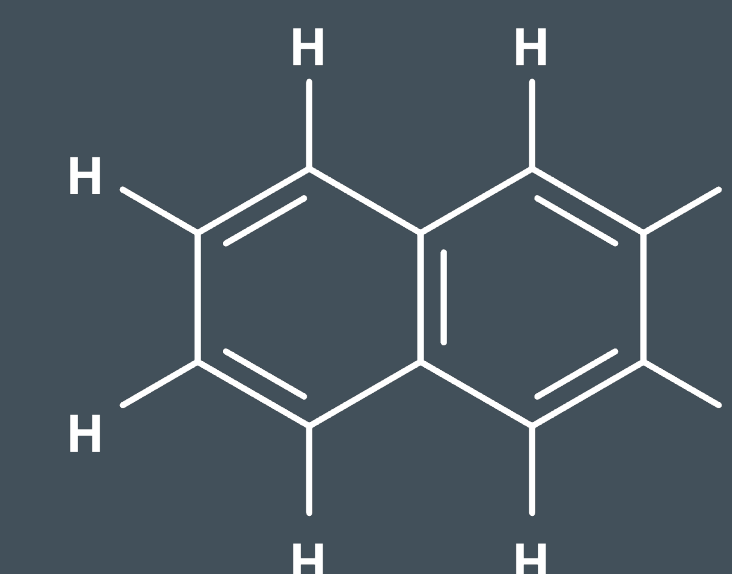
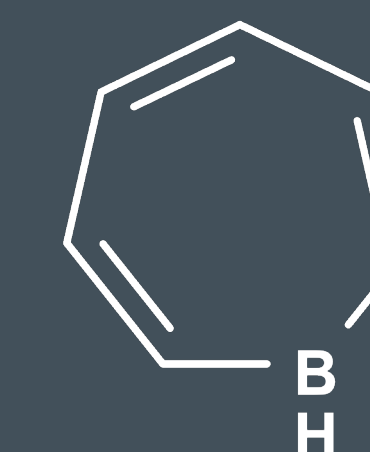
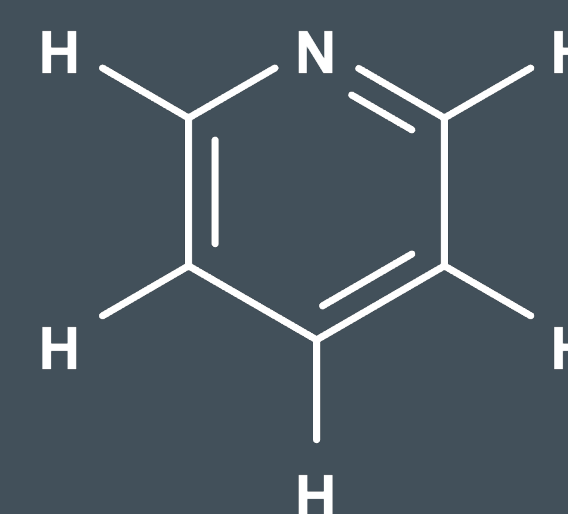
Particularly unstable

Aromaticity

Aromatic ($4n+2$ electrons)

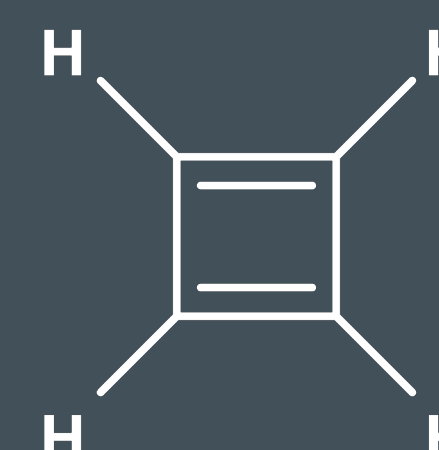
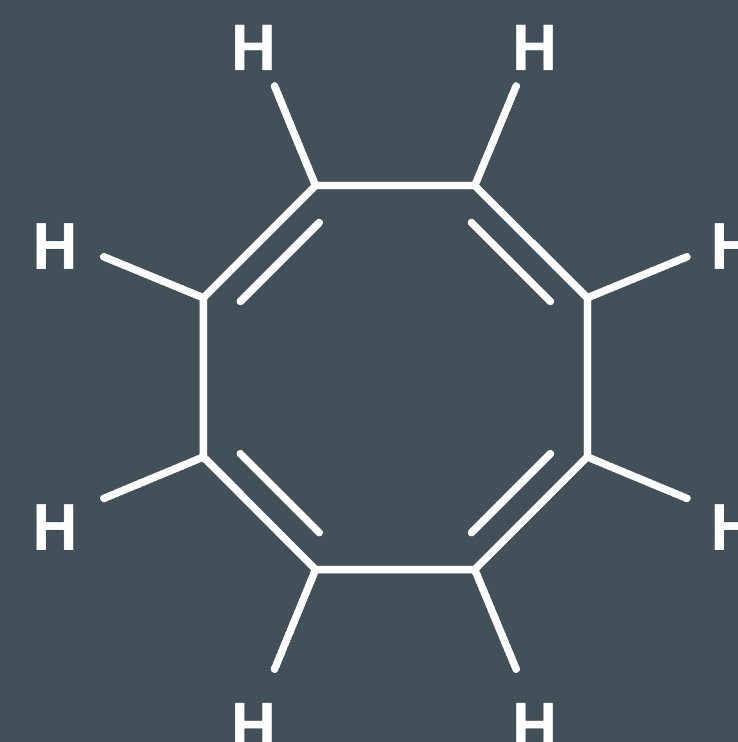
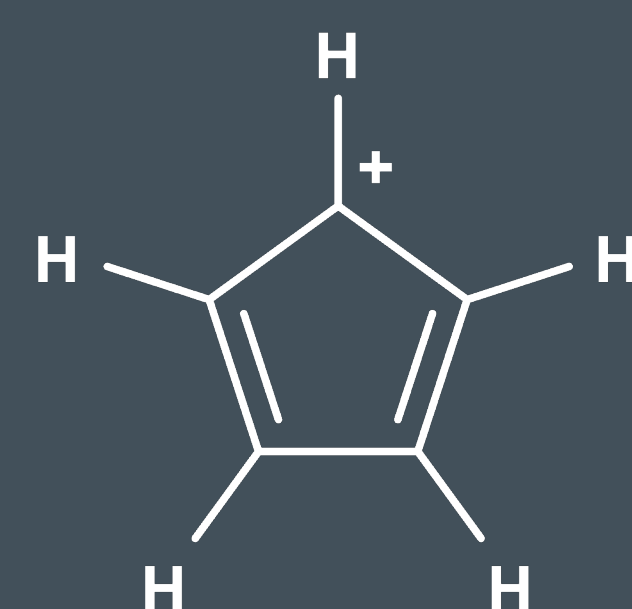


benzene



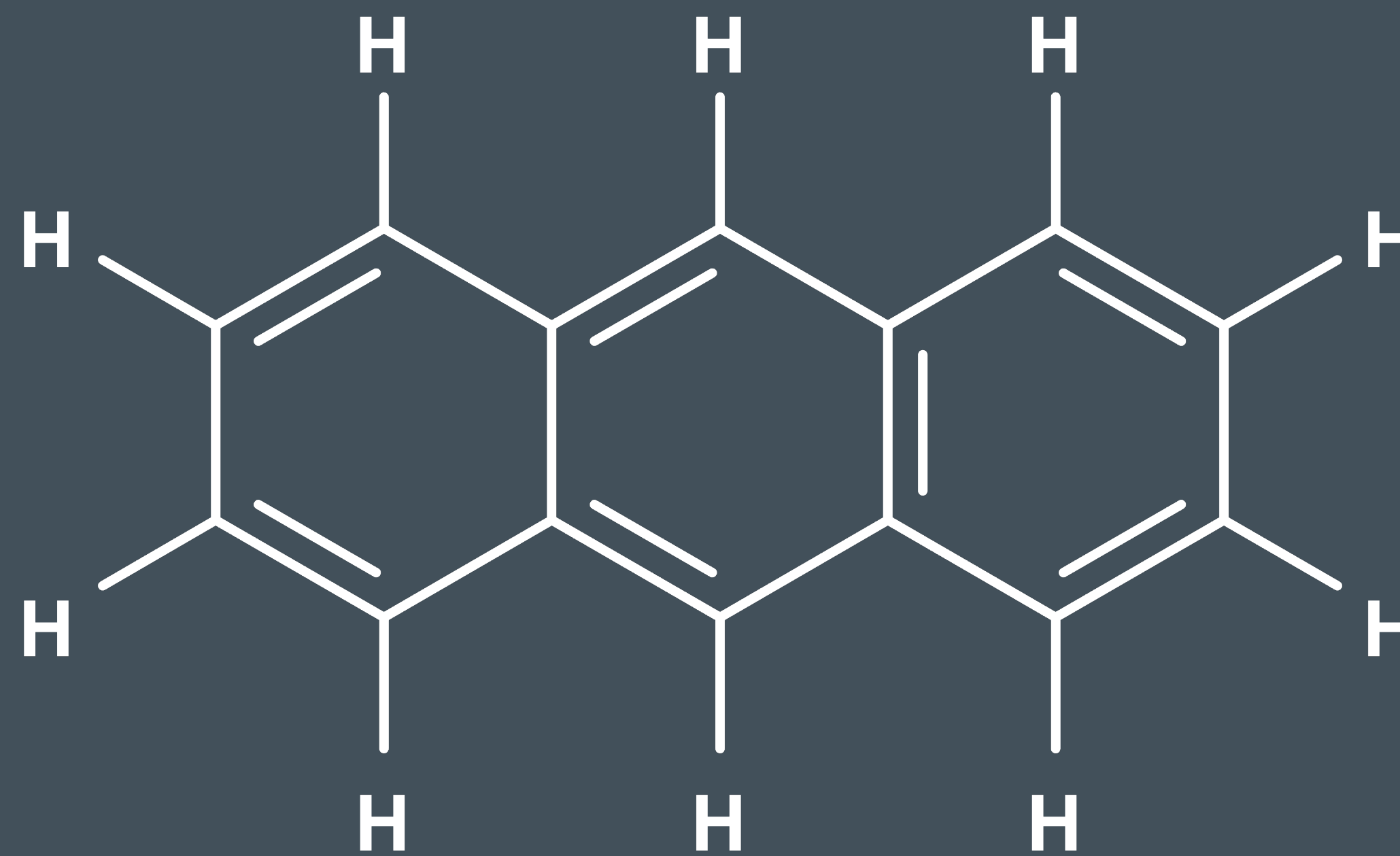
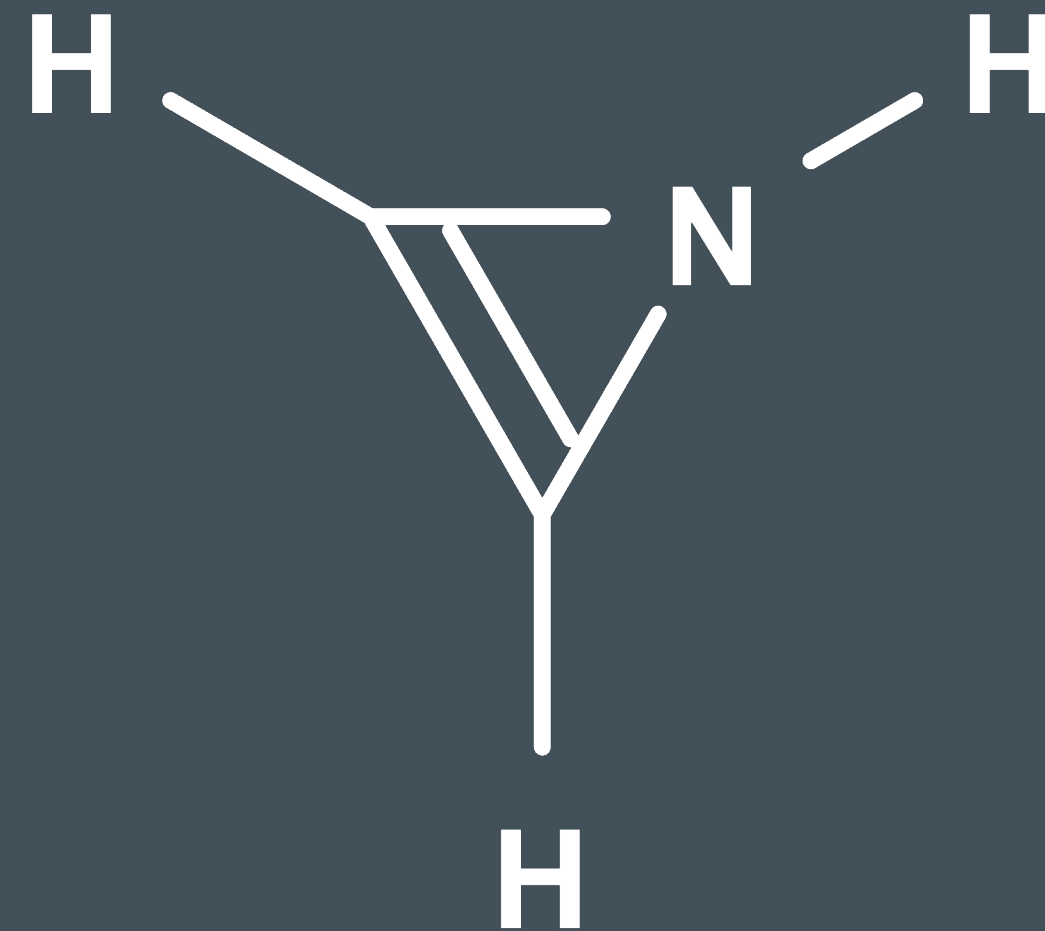
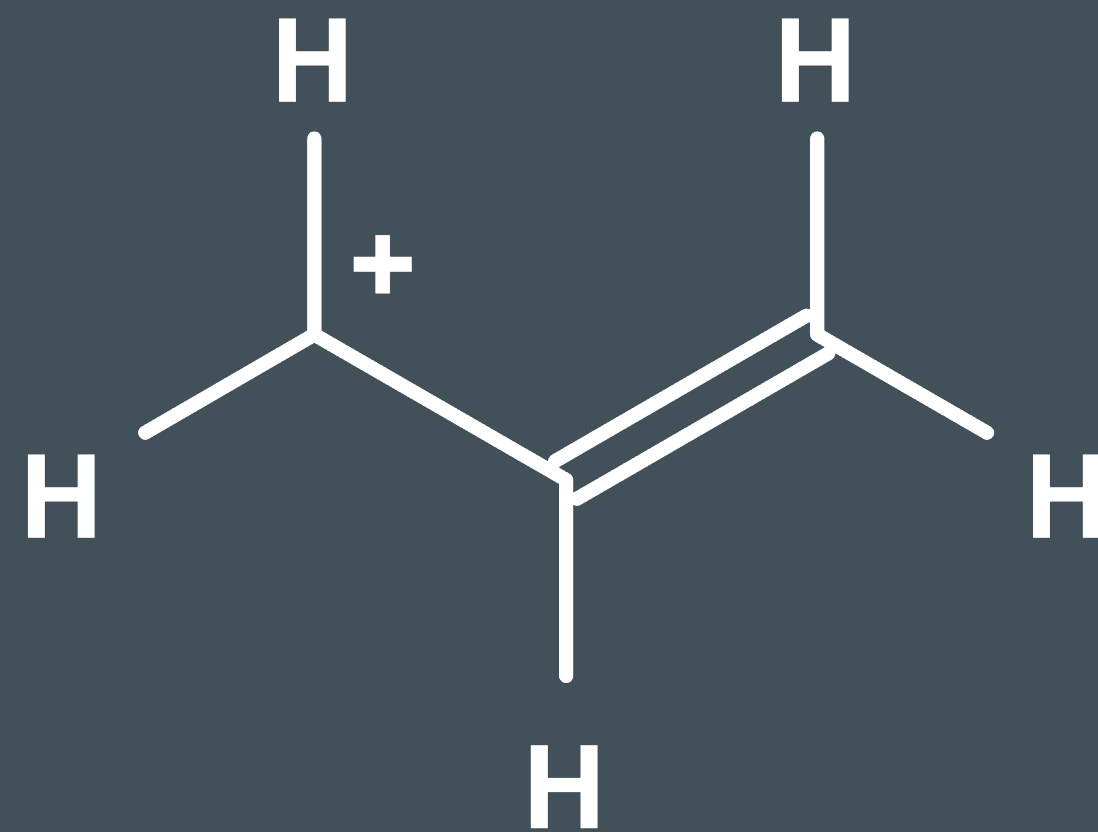
Aromatic compounds are **stable**

Antiaromatic ($4n$ electrons)



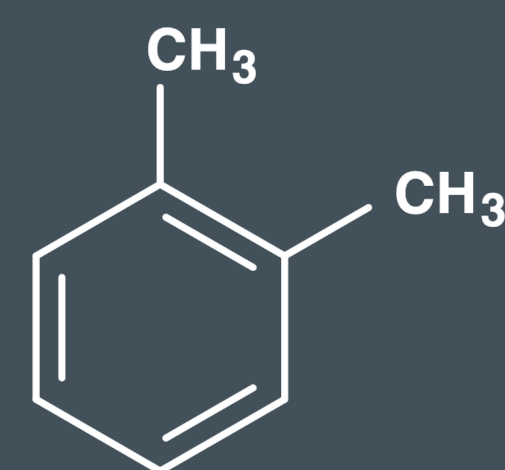
Antiaromatic compounds are **NOT stable**

Aromatic or Antiaromatic?



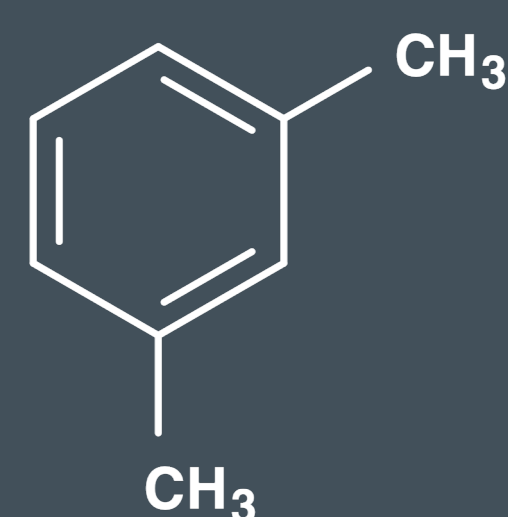
Positional substitution on benzene

Ortho (next to)



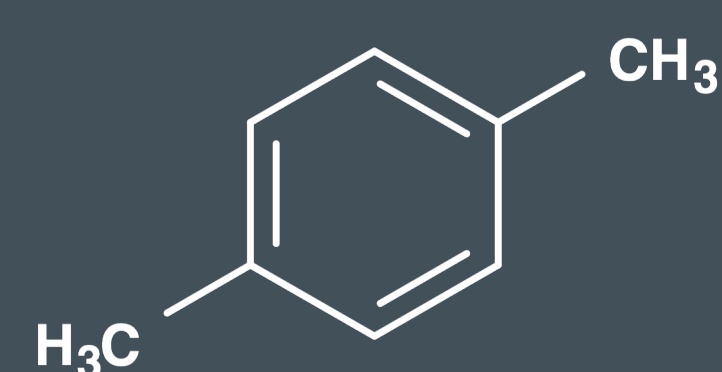
ortho-xylene

Meta (skip one)



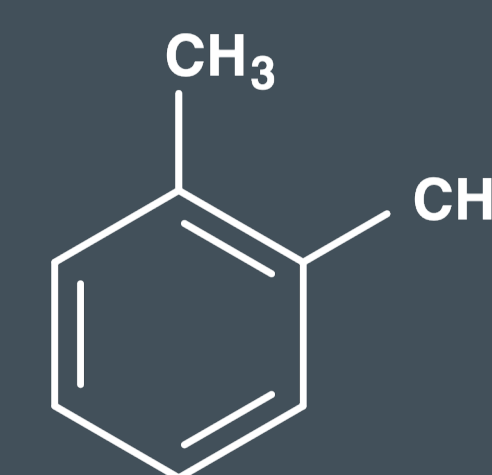
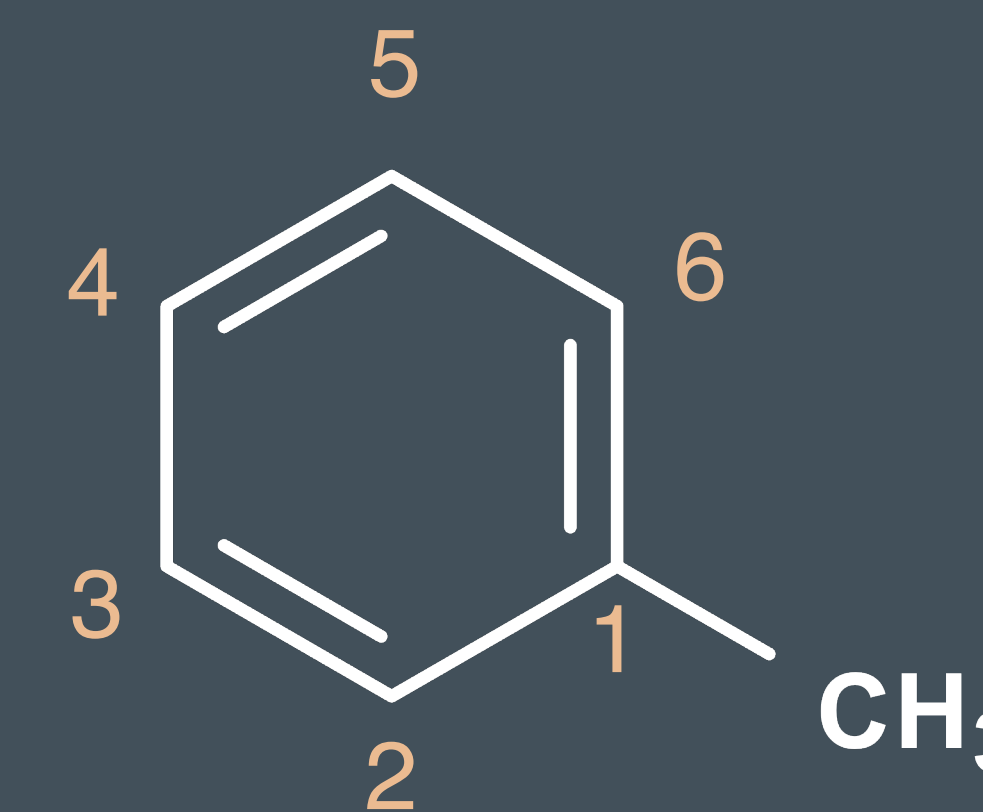
meta-xylene

Para (opposite)

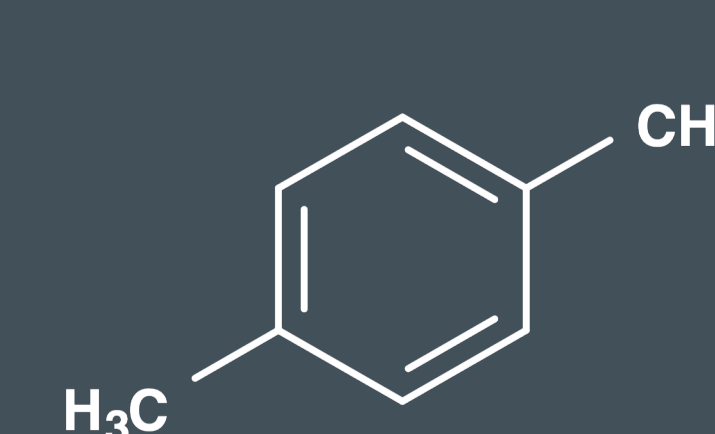


para-xylene

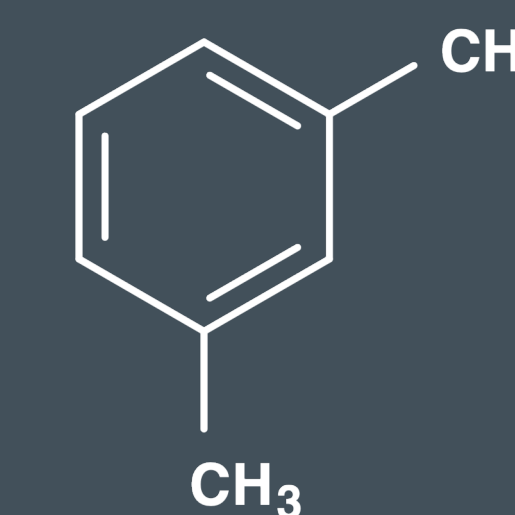
Numbering



1,2-dimethyl-benzene



1,4-dimethyl-benzene

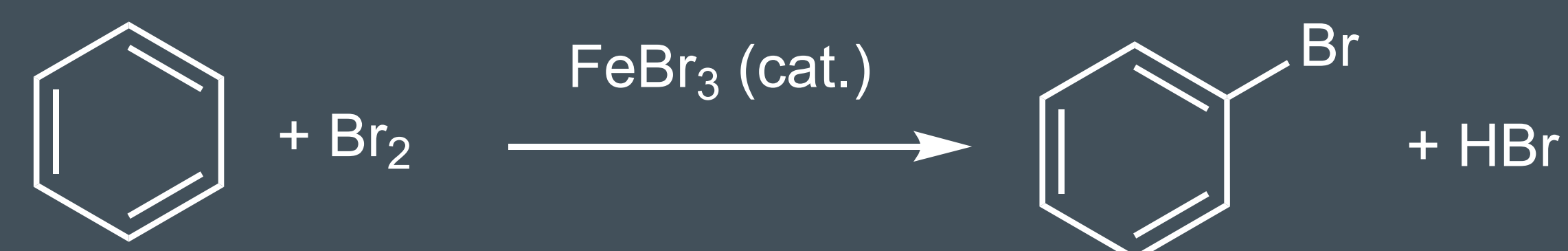


1,3-dimethyl-benzene

Frost Circles

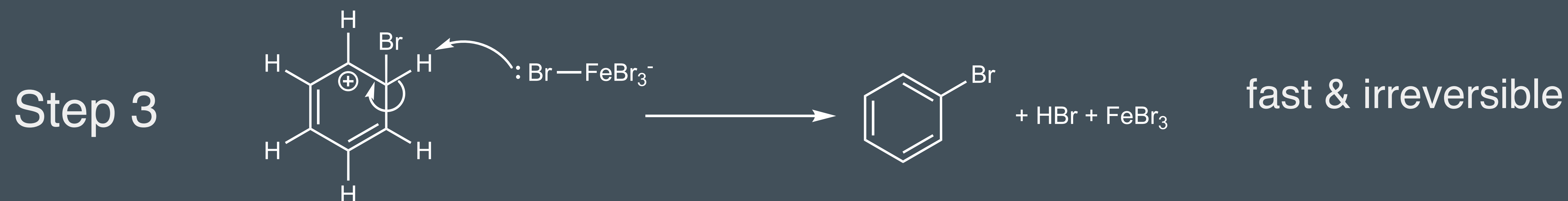
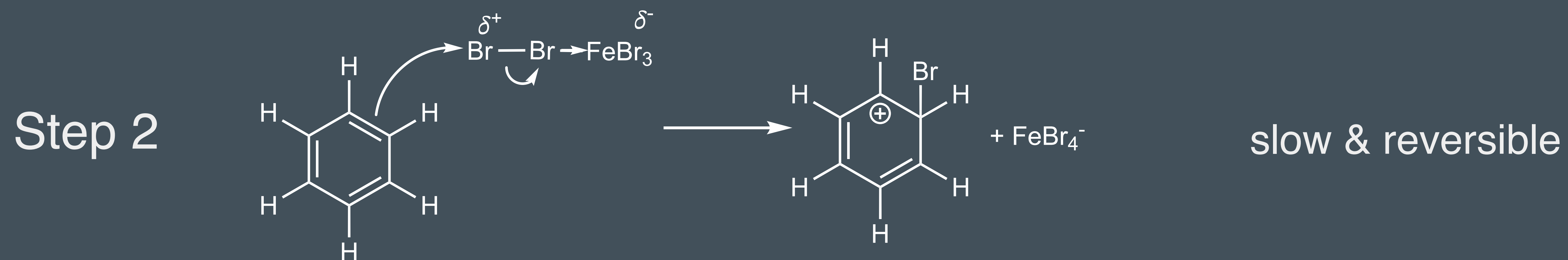
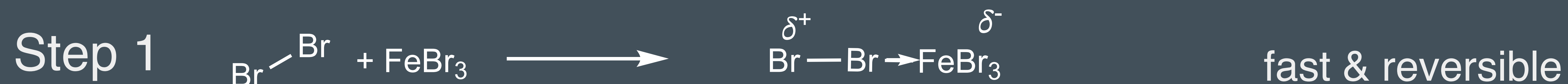
Reactions of aromatics

Electrophilic Substitution is more for aromatics than in alkenes



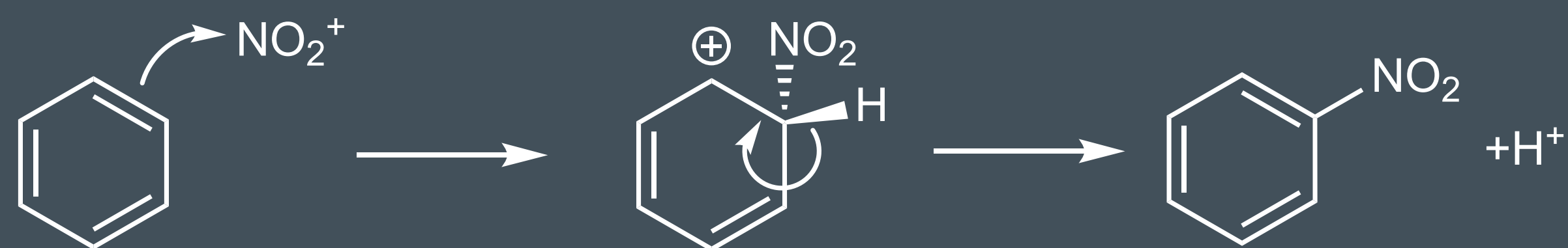
Aromaticity stabilizes the double bonds
A catalyst is required to accelerate the reaction

Mechanism

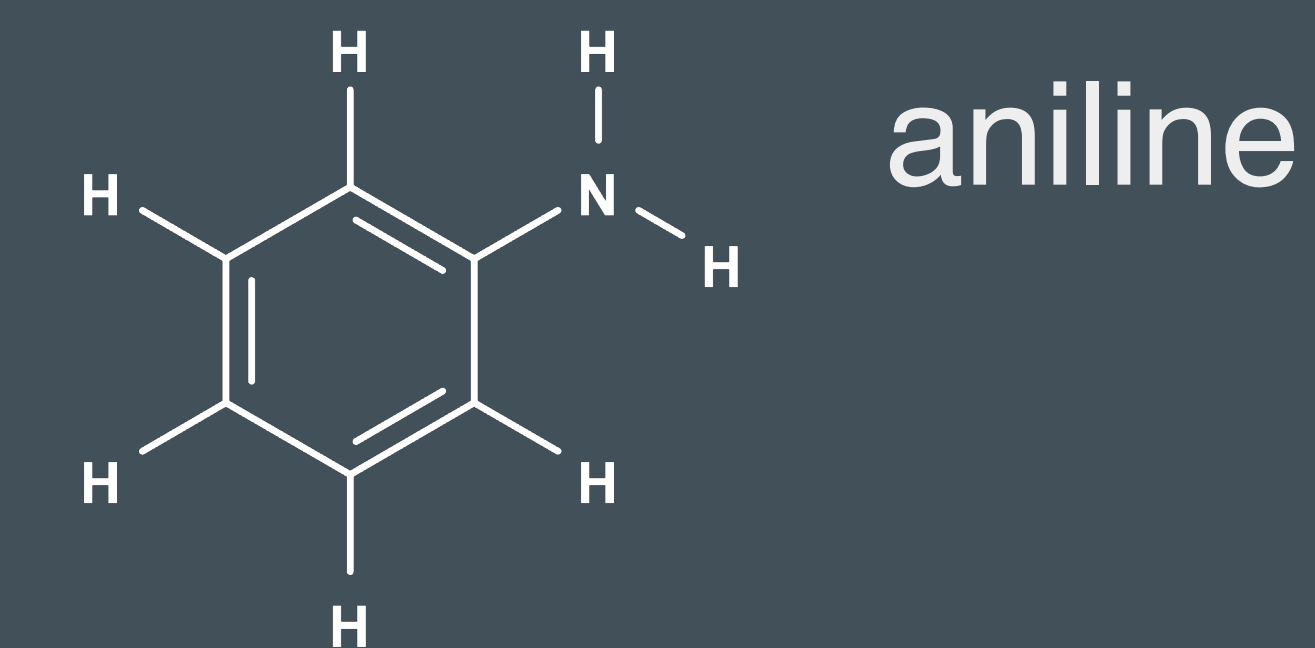
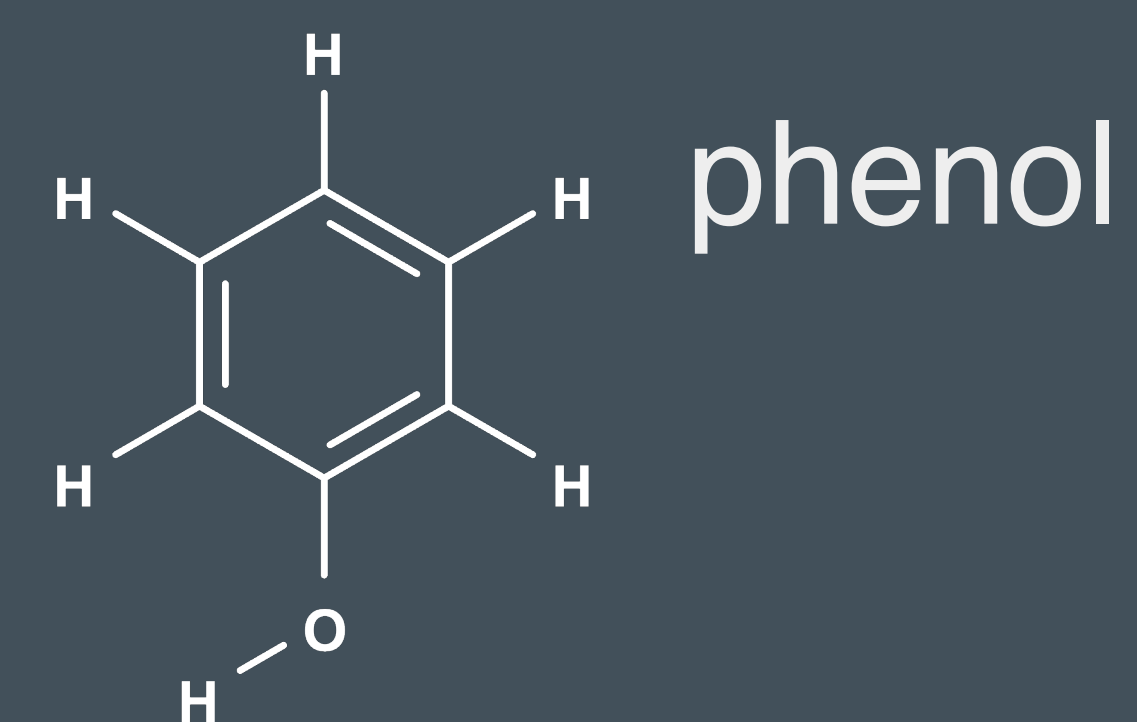


Controlling the rate of reaction by structural modification

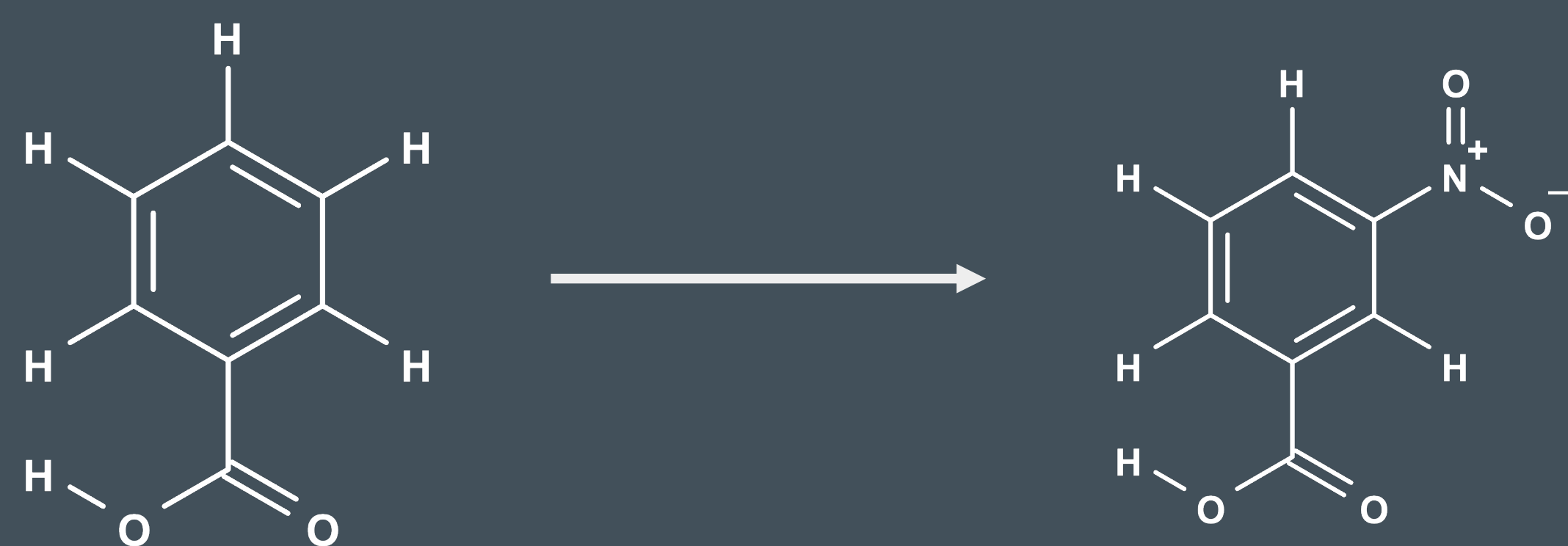
Electrophilic substitution of Nitrate



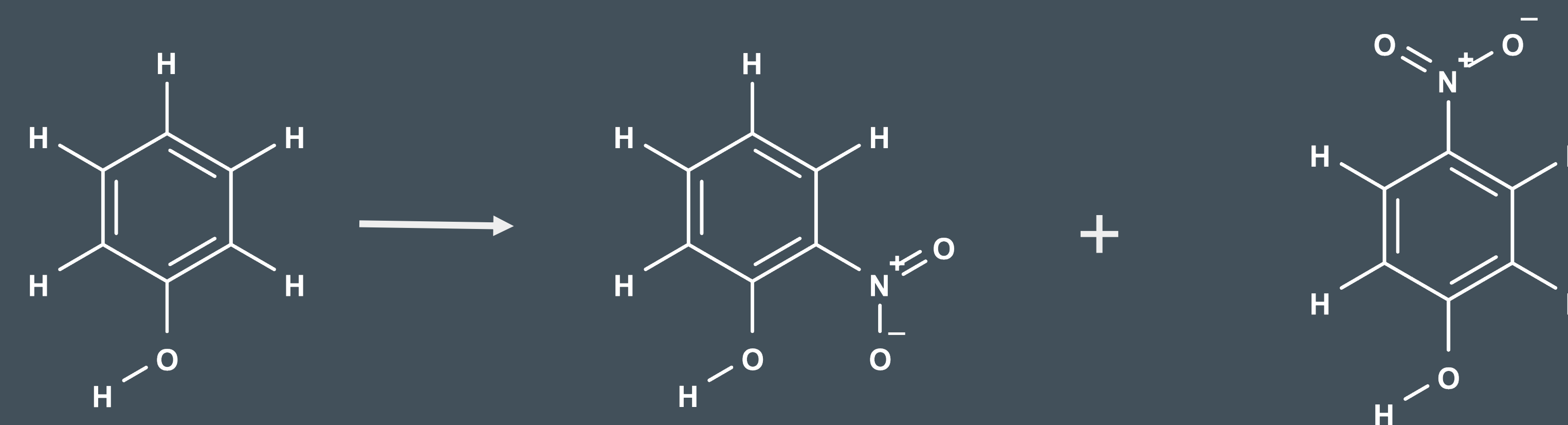
π -donor substituents speed up the reaction



π -acceptor substituents slow down the reaction

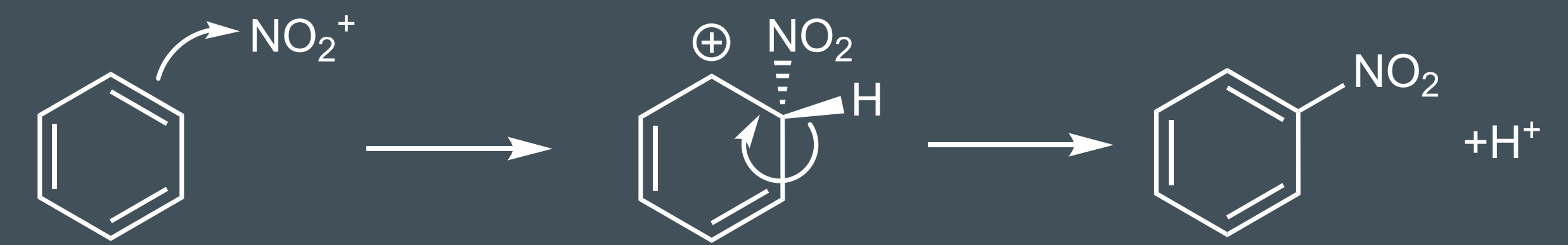
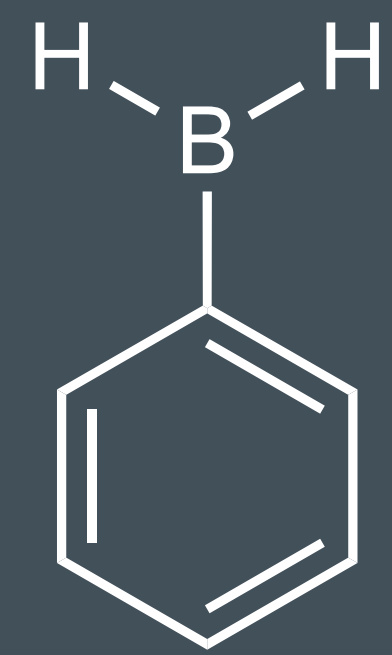


Selectively substitute at *meta* position



Selectively substitute at *ortho* or *para* position

Where will nitrate substitute?



Will this reaction be faster or slower than for benzene?