Alcohols, Ethers and Epoxides

- Alcohol, ether and epoxide functional groups contain carbon-oxygen σ bonds

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- Alcohol
- Ether
- Epoxide
**Alcohols—Structure and Bonding**

- **Alcohols** contain a hydroxy group (OH) bonded to an $sp^3$ hybridized carbon.

- They are classified according to the number of alkyl groups attached to carbon bearing the OH.

\[ \text{C} - \text{OH} \]

alcohol

C is $sp^3$ hybridized.

\[ \text{Cortisol} \]

anti-inflammatory steroid

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Enols and Phenols

- Compounds having a hydroxy group on a $sp^2$ hybridized carbon—enols and phenols—undergo different reactions than alcohols.

- $C$ bonded to OH is $sp^2$ hybridized.
• Ethers have two alkyl groups bonded to an oxygen atom.
Epoxides

• Epoxides are ethers having the oxygen atom in a three-membered ring.

• Epoxides are also called oxiranes.

• The C-O-C bond angle for an epoxide must be 60°, a considerable deviation from the tetrahedral bond angle of 109.5°.

• Thus, epoxides have angle strain, making them more reactive than other ethers.
Oxygen Hybridization and Geometry

• The oxygen atom in alcohols, ethers, and epoxides is $sp^3$ hybridized.

• Alcohols and ethers have a bent shape like that in $\text{H}_2\text{O}$.

• The bond angle around the O atom in an alcohol or ether is similar to the tetrahedral bond angle of 109.5°.

• Because the O atom is much more electronegative than carbon or hydrogen, the C-O and O-H bonds are both polar.
Electrostatic Potential Maps

• The oxygen atom in alcohols, ethers, and epoxides is $sp^3$ hybridized.

• Alcohols and ethers have a bent shape like that in $H_2O$.

Figure 9.1
Electrostatic potential maps for a simple alcohol, ether, and epoxide

- Electron-rich regions are shown by the red around the O atoms.
Naming Alcohols

How To  Name an Alcohol Using the IUPAC System

Example  Give the IUPAC name of the following alcohol:

\[
\begin{align*}
\text{Step [1]} & \quad \text{Find the longest carbon chain containing the carbon bonded to the OH group.} \\
\text{6 C's in the longest chain} & \quad \text{Change the -e ending of the parent alkane to the suffix -ol.} \\
6 \text{ C's} & \rightarrow \text{hexane} \rightarrow \text{hexanol}
\end{align*}
\]

\text{Step [2]}  Number the carbon chain to give the OH group the lower number, and apply all other rules of nomenclature.

\begin{enumerate}
\item \textbf{a. Number} the chain.
\item \textbf{b. Name and number} the substituents.
\end{enumerate}

\begin{align*}
\text{Number the chain to put the OH group at C3, not C4.} & \quad \text{methyl at C5} \\
\text{Answer: 5-methylhexan-3-ol} & \quad \text{hexan-3-ol}
\end{align*}
Naming Alcohols Attached to Rings

• When an OH group is bonded to a ring, the ring is numbered beginning with the OH group.
• Because the functional group is at C1, the 1 is usually omitted from the name.
• The ring is then numbered in a clockwise or counterclockwise fashion to give the next substituent the lowest number.

Figure 9.2
Examples: Naming cyclic alcohols

3-methylcyclohexanol

The OH group is at C1; the second substituent (CH₃) gets the lower number.

2,5,5-trimethylcyclohexanol

The OH group is at C1; the second substituent (CH₃) gets the lower number.
Common Names of Alcohols

• Common names are often used for simple alcohols. To assign a common name:
  • Name all the carbon atoms of the molecule as a single alkyl group.
  • Add the word alcohol, separating the words with a space.
Naming Ethers

• Simple ethers are usually assigned common names. To do so:
  • Name both alkyl groups bonded to the oxygen, arrange these names alphabetically, and add the word ether.
  • For symmetrical ethers, name the alkyl group and add the prefix “di-”.

\[
\text{sec-butyl methyl ether}
\]

Alphabetize the b of butyl before the m of methyl.

\[
\text{diethyl ether}
\]
Naming Complex Ethers

• More complex ethers are named using the IUPAC system.
• One alkyl group is named as a hydrocarbon chain, and the other is named as part of a substituent bonded to that chain:
  • Name the simpler alkyl group as an alkoxy substituent by changing the -yl ending of the alkyl group to -oxy.
  • Name the remaining alkyl group as an alkane, with the alkoxy group as a substituent bonded to this chain.

• Cyclic ethers have an O atom in the ring. A common example is tetrahydrofuran (THF).
Naming Epoxides

- Epoxides can be named in three different ways—epoxyalkanes, oxiranes, or alkene oxides.
- To name an epoxide as an epoxyalkane, first name the alkane chain or ring to which the O atom is attached, and use the prefix “epoxy” to name the epoxide as a substituent.
- Use two numbers to designate the location of the atoms to which the O is bonded.

1,2-epoxycyclohexane 1,2-epoxy-2-methylpropane cis-2,3-epoxypentane
hexane + 01 → 2 x

dimethyl

chlorine

3 - chloro - 4,4 - dimethyl

2 - hexanol
3-chloro-4,4-dimethyl hexane-2-ol

CH₃-CH₂-CH₂-CH₂-C-CH₂-C₄H₆O₂H

ethane

heptane

4-ethyl-1-heptanol

4-ethyl hexan-1-ol
alkyl
alkyl
er
ether
smaller
alkoxy
alkane
more
complex

CH₃CH₂O-CH₂C₆H₄-CH₃
1 2 3

ethoxy
butane

3- methyl
3- chloro
3- chloro-1- ethoxy-3- methyl
butane
heptane

2,4-dimethyl

2,4-dimethyl-3-methoxy heptane

3-methoxy 5-2,4-dimethyl heptane
\[
\begin{align*}
\text{C}_8 & \quad \text{C}_7 & \quad \text{C}_6 & \quad \text{C}_5 & \quad \text{C}_4 & \quad \text{C}_3 & \quad \text{C}_2 & \quad \text{C}_1 \\
4 & \quad 5 & \quad 6 & \quad 7 & \quad 8 & \quad 9 & \quad 10 & \quad 11 & \quad 12 & \quad 13
\end{align*}
\]

- \text{4,5-epoxy} \\
- \text{ethane} \\
- \text{chlorine}

3-chloro-4,5-epoxy-6-ethyl octane