

1.1: INTRODUCTION

OBJECTIVE

After completing this section, you should be able to determine whether or not a molecule contains a conjugated system, given its Kekulé, condensed, or shorthand formula.

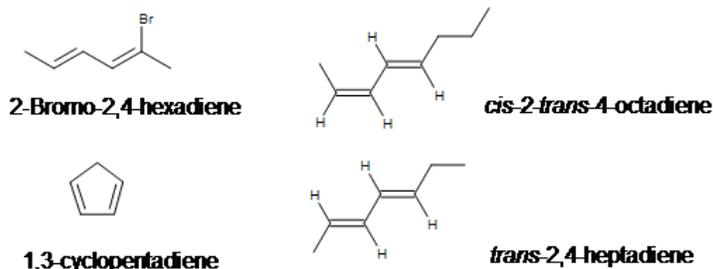
DIENES

A diene is a hydrocarbon chain that has two double bonds that may or may not be adjacent to each other. This section focuses on the delocalization of π systems by comparing two neighboring double bonds. The arrangements of these double bonds have varying effects on the compound's reactivity and stability.

NAMING DIENES

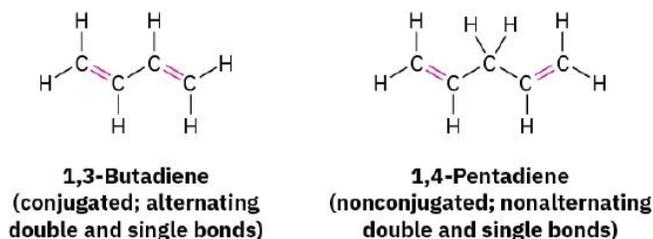
First identify the longest chain containing both carbons with double bonds in the compound. Then, give the lowest possible number for the location of the carbons with double bonds and any other functional groups present (remember when naming alkenes that some groups take priority, such as alcohols). Do not forget [stereochemistry](#) or any other orientation of the double bond such as (E/Z, cis or trans).

Examples:



CLASSIFICATION OF DIENES

Most of the unsaturated compounds we looked at in the previous chapters on alkenes had only one double bond, but many compounds have numerous sites of unsaturation. If the different unsaturations are well separated in a molecule, they react independently, but if they're close together, they may interact. In particular, compounds that have alternating single and double bonds—so-called conjugated compounds—have some distinctive characteristics. The conjugated diene 1,3-butadiene, for instance, has some properties quite different from those of the nonconjugated 1,4-pentadiene.



CONJUGATED VS. NON-CONJUGATED DIENES

Dienes are compounds that contain two double bonds. These dienes can be conjugated, non-conjugated (isolated), or cumulated dienes. Conjugated dienes have properties and reactivity distinctly different from non-conjugated or cumulated dienes. Determining if double bonds are conjugated represents a critical skill in organic chemistry.

Conjugated dienes have the two double bonds separated by a single bond.

Nonconjugated (Isolated) dienes are two double bonds separated by more than one single bond. The two double bonds are separated by at least one sp^3 hybridized atom, and can not resonate.



3,5-Octadiene
(Conjugated)



2,5-Octadiene
(Non-Conjugated)



1,3-Cyclohexadiene
(Conjugated)



1,4-Cyclohexadiene
(Non-Conjugated)



1,3-Butadiene
(Conjugated)



1,4-Pentadiene
(Non-Conjugated)

CUMULATED DIENES

Another Classification for dienes are **Cumulated dienes** (allenes). Two double bonds are connected to the same atom, a sp hybridized atom

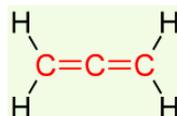


Figure
1.1.1

: 1,2-Propadiene. (credit: Jü, Wikimedia Commons, CC BY 1.0)

CONJUGATED DIENES IN NATURE

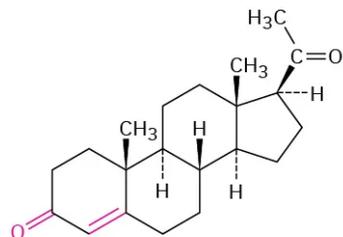
Conjugated compounds of many different sorts are common in nature. Many of the pigments responsible for the brilliant colors of fruits, flowers, and even animals have numerous alternating single and double bonds. β -Carotene, for instance, the orange pigment responsible for the color of carrots and an important source of vitamin A, is a conjugated *polyene* with 11 double bonds. Conjugated *enones* (alkene + ketone) are common structural features of many biologically important molecules, such as progesterone, the hormone that prepares the uterus for the implantation of a fertilized ovum. Cyclic conjugated molecules such as benzene are a major field of study in themselves. In this chapter, we'll look at some of the distinctive properties of conjugated molecules and at the reasons for those properties.



Figure 1.1.2: Saffron, derived from stigmas of the saffron crocus, is the world's most expensive spice. Its color is caused by the presence of alternating single and double bonds. (credit: "Welcome to My World! ~ Huron River Watershed" by j van cise photos/Flickr, CC BY 2.0)



β -Carotene
(orange pigment and vitamin A precursor)



Progesterone, a conjugated enone



Benzene,
a cyclic conjugated molecule

KEY TERMS

Make certain that you can define, and use in context, the key terms below.

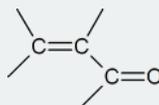
- Conjugated dienes / double bonds
- Nonconjugated (Isolated) dienes
- Cumulated dienes
- enone
- polyene

STUDY NOTES

Conjugated double bonds are double bonds separated by one carbon-carbon single bond. Thus, the double bonds in butadiene, $\text{CH}_2=\text{CH}-\text{CH}=\text{CH}_2$, are conjugated, and this compound is an example of a *conjugated diene*.

Just as the term *diene* indicates the presence of two carbon-carbon double bonds in a compound, the term *polyene* is used to describe compounds containing many carbon-carbon double bonds.

An *enone* is a compound containing a carbon-carbon double bond (ene) and a carbonyl group (one). A conjugated enone contains the structural unit:



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