Chapter #8 Lecture Slides

Alkenes

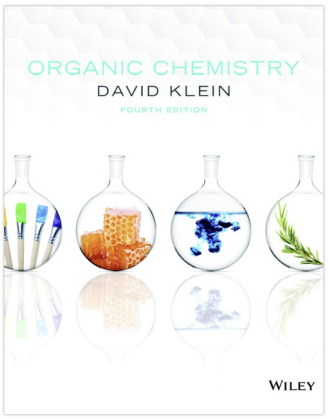
Part #2 – Nomenclature of Olefins

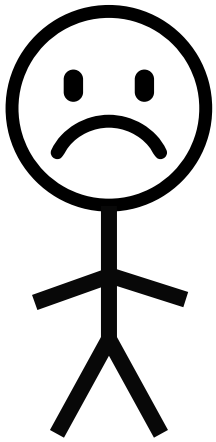
08-018

1

Nomenclature of Alkenes

1. **Our textbook—despite being published in 2021—does not reflect the updated IUPAC guidance from 2013 regarding the systematic nomenclature of olefins.**





a disappointed IUPAC apparatchik

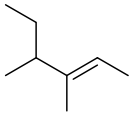
- Failure to adopt international standards is why Americans still use inches, yards, miles, ounces, and pounds, among other antediluvian units

08-019

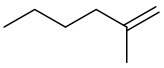
2

Nomenclature of Alkenes

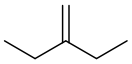
2. **Alkenes are named based on the longest continuous chain of carbon atoms in the molecule, regardless of whether the chain contains the double bond or not. If the chain includes the C=C bond, replace the –ane suffix from the parent alkane hydrocarbon with –ene.**



this is a hexene



this is a hexene



this is a pentane
not a butene

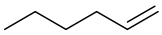
- Note: Klein's 4th edition (your textbook, published in 2021) perpetuates the outdated rule of selecting the parent chain as the longest chain of carbon atoms *that includes the π bond*. This used to be the IUPAC preference before 2013.

08-020

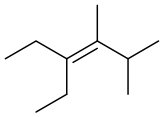
3

Nomenclature of Alkenes

3. **When the parent chain includes both carbons in the double bond, number the chain starting from the end that gives the start of the double bond the lower locant number. Insert the locant number directly in front of the –ene suffix.**

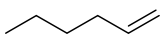


hex-1-ene
not hex-5-ene

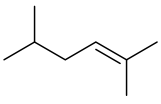


4-ethyl-2,3-dimethylhex-3-ene
not 3-ethyl-4,5-dimethylhex-3-ene

- In case of a tie, apply the nomenclature rules we already know as the tiebreakers:
  1. number the chain to give the lower locant to the first substituent (and so on…)
  2. number the chain to give the lower locant to the first substituent that comes earliest in the alphabet
- It is not uncommon to encounter the locant for the double bond in front of the name of the parent chain:



1-hexene



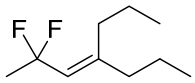
2,5-dimethyl-2-hexene

08-021

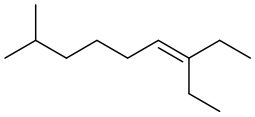
4

Nomenclature of Alkenes

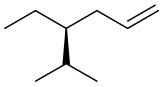
4. **Notice how we simply incorporate these new rules for alkenes into all the rules of nomenclature we learned for alkanes and alkyl halides.**



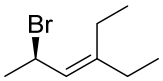
2,2-difluoro-4-propylhept-3-ene



3-ethyl-8-methylnon-3-ene
not 7-ethyl-2-methylnon-6-ene



(4*S*)-4-ethyl-5-methylhex-1-ene
not (4*S*)-4-isopropylhex-1-ene



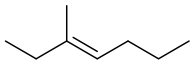
(2*R*)-2-bromo-4-ethylhex-3-ene
not (5*R*)-5-bromo-3-ethylhex-3-ene

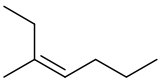
08-022

5

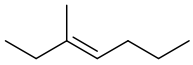
Nomenclature of Alkenes

5. **Recall that C=C double bonds in which each olefinic carbon atom is substituted with two different groups can exist as a pair of diastereomers.**

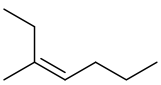




6. **We differentiate these stereoisomers with *E*/*Z* descriptors added as prefixes.**



(3*E*)-3-methylhept-3-ene



(3*Z*)-3-methylhept-3-ene

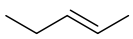
- **If the higher priority groups (using the Cahn–Ingold–Prelog system) on each carbon atom are on "opposite sides" of the double bond, the descriptor *E* is used. If the higher priority groups are on the "same side", the descriptor *Z* is used.**

08-023

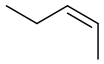
6

Nomenclature of Alkenes

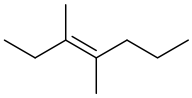
7. **In cases where each carbon atom of the C=C bond is only monosubstituted, it is acceptable to use the descriptors *cis-* and *trans-***



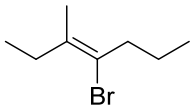
(2*E*)-pent-2-ene
trans-pent-2-ene
trans-2-pentene



(2*Z*)-pent-2-ene
cis-pent-2-ene
cis-2-pentene



(3*E*)-3,4-dimethylhept-3-ene
not *trans*-3,4-dimethylhept-3-ene
certainly not *cis*-3,4-dimethylhept-3-ene



(3*Z*)-4-bromo-3-methylhept-3-ene

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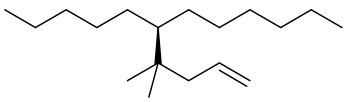
7

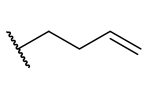
Nomenclature of Alkenes

8. **When the parent chain of an alkene does not include the double bond, it will be included in the name of a substituent of the parent chain.**

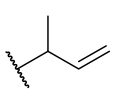


(6*S*)-6-(2-methylpent-4-en-2-yl)dodecane

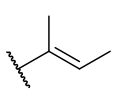
9. **Alkene-containing substituents are named as alkenes, except after you identify the longest chain of the substituent, you number it from the end that gives its point of attachment to the parent chain the lower locant number. The substituent name is made by dropping the final –e, then appending the locant of the point of attachment followed by –yl.**



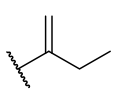
a but-3-en-1-yl group



a but-3-en-2-yl group



a but-2-en-2-yl group



a but-1-en-2-yl group

08-025

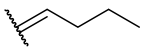
8

Nomenclature of Alkenes

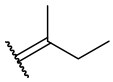
10. Groups attached via a double bond to the parent chain are named as ylidenes.

a methylidene group

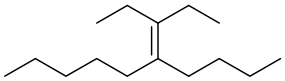
sometimes seen as its common name: a methylene group



a butan-1-ylidene group



a butan-2-ylidene group



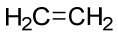
5-(pentan-3-ylidene)decane

08-026

9

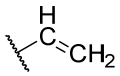
Nomenclature of Alkenes

11. IUPAC allows common names for some alkenes and alkene-containing substituent groups

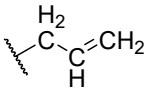


ethylene
but ethene preferred

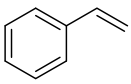
propylene
but propene preferred



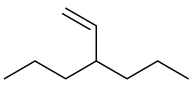
vinyl group
but ethenyl preferred



allyl group
but prop-2-en-1-yl preferred



styrene
also vinylbenzene
but ethenylbenzene preferred



4-ethenylheptane preferred
also 4-vinylheptane
not 3-propylhex-1-ene

08-027

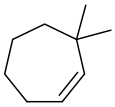
10

Nomenclature of Cycloalkenes

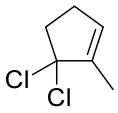
1. **Cycloalkenes are compounds with a C=C bond between two carbons in a ring.**

2. **Cycloalkenes are named by numbering the ring such that the C=C bond is between C1 and C2.**

cyclohexene
not cyclohex-1-ene



3,3-dimethylcycloheptene
not 1,1-dimethylcyclohept-2-ene
not 7,7-dimethylcycloheptene



5,5-dichloro-1-methylcyclopentene
not 5,5-dichloromethylcyclopentene
not 1,1-dichloro-2-methylcyclopent-2-ene
not 3,3-dichloro-2-methylcyclopentene

- **The locant "1" for the position of the C=C bond in a cycloalkene is omitted when alone as it is implied.**

08-028

11

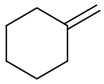
Nomenclature of Cycloalkenes

1. **When contained in small rings—fewer than 8 atoms—it is assumed all double bonds are *cis*- with respect to the ring sides if no *E*- or *Z*- descriptor is given.**

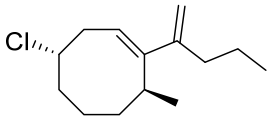
1-methylcyclobutene
(1*Z*)-1-methylcyclobutene

1-bromocyclobutene
(1*E*)-1-methylcyclobutene

2. **Incorporate these rules for cycloalkenes with the other rules for nomenclature we have learned.**



methylidenecyclohexane



(1*E*,4*S*,8*S*)-4-chloro-8-methyl-1-(pent-1-en-2-yl)cyclooctene

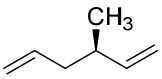
08-029

12

Nomenclature of Polyenes and Cyclopolyenes

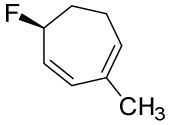
1. **Compounds with multiple C=C double bonds are called polyenes.**
2. **When multiple C=C bonds appear in the longest chain, replace the –ne suffix from the parent hydrocarbon with –diene (for 2), –triene (for 3), etc.**

cycloocta-1,3,6-triene
also 1,3,6-cyclooctatriene
not cycloocta-1,4,6-triene



(3*R*)-3-methylhexa-1,5-diene

3. **Give preference to lower locants for double bonds before substituents.**



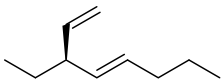
(5*S*)-5-fluoro-2-methylcyclohepta-1,3-diene
not (5*S*)-5-fluoro-1-methylcyclohepta-1,6-diene
not (7*S*)-7-fluoro-3-methylcyclohepta-1,3-diene

08-030

13

Nomenclature of Polyenes and Cyclopolyenes

4. **If there is a tie for longest chain in a polyene, choose the chain with the most double bonds.**



(3*S*,4*E*)-3-ethylocta-1,4-diene
not (3*S*,4*E*)-3-ethenyloct-4-ene

08-031

14

Chapter #9 Lecture Slides

Alkynes

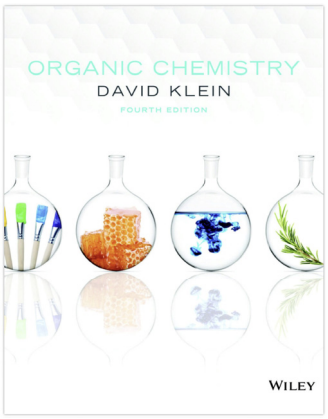
Part #2 – Nomenclature of Alkynes

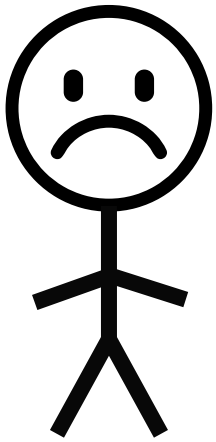
09-009

15

Nomenclature of Alkynes

1. **Our textbook—despite being published in 2021—does not reflect the updated IUPAC guidance from 2013 regarding the systematic nomenclature of alkynes.**





a disappointed IUPAC apparatchik

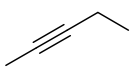
- Failure to adopt international standards is why Americans still use inches, yards, miles, ounces, and pounds, among other antediluvian units

09-010

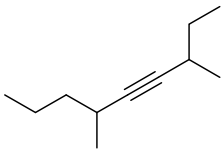
16

Nomenclature of Alkynes

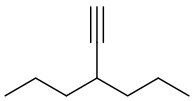
2. **Alkynes are named based on the longest continuous chain of carbon atoms in the molecule, regardless of whether the chain contains the triple bond or not. If the chain includes the C≡C bond, replace the –ane suffix from the parent alkane hydrocarbon with –yne.**



this is a pentyne

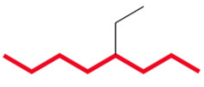


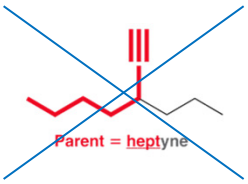
this is a nonyne



this is a heptane
not a hexyne

- Note: Klein's 4th edition (your textbook, published in 2021) perpetuates the outdated rule of selecting the parent chain as the longest chain of carbon atoms *that includes the C≡C bond*. This used to be the IUPAC preference before 2013.





09-011

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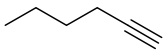
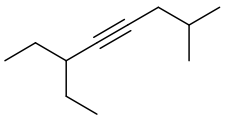
Nomenclature of Alkynes

3. **When the parent chain includes both carbons in the triple bond, number the chain starting from the end that gives the start of the triple bond the lower locant number. Insert the locant number directly in front of the –yne suffix.**

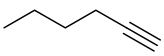


hex-1-yne
not hex-5-yne



6-ethyl-2-methyloct-4-yne
not 3-ethyl-7-methyloct-4-yne

- In case of a tie, apply the nomenclature rules we already know as the tiebreakers:
  1. number the chain to give the lower locant set for the substituents (based on first difference)
  2. number the chain to give the lower locant to the first substituent that comes earliest in the alphabet
- It is not uncommon to encounter the locant for the triple bond in front of the name of the parent chain:



1-hexyne
but hex-1-yne preferred

09-012

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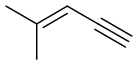
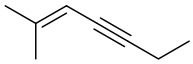
Nomenclature of Alkynes

4. If the parent chain includes both C=C and C≡C bonds, number the chain to give the first instance of a multiple bond the lower locant. These compounds are named as an enynes. (In the name, the ene part always precedes the yne part.)

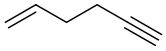


4-methylpent-3-en-1-yne
not 2-methylpent-2-en-4-yne



2-methylhept-2-en-4-yne
not 6-methylhept-5-en-3-yne

5. In the event of a tie for lower locant between a C=C and C≡C bond, give seniority to the C=C bond and number the chain to assign it the lower locant.



hex-1-en-5-yne
not hex-5-en-1-yne

09-013

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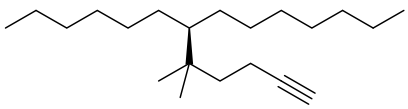
Nomenclature of Alkynes

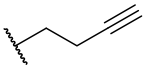
6. When the parent chain of an alkene does not include the triple bond, it will be included in the name of a substituent of the parent chain.



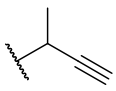
(7*S*)-7-(2-methylhex-5-yn-2-yl)tetradecane

7. Alkyne-containing substituents are named as alkynes, except after you identify the longest chain of the substituent, you number it from the end that gives its free valence (i.e., the point of attachment to the parent chain) the lower locant number. The substituent name is made with elision of the final –e, then appending the locant of the point of attachment followed by –yl.

an ethynyl group



a but-3-yn-1-yl group



a but-3-yn-2-yl group

09-014

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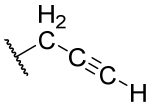
Nomenclature of Alkynes

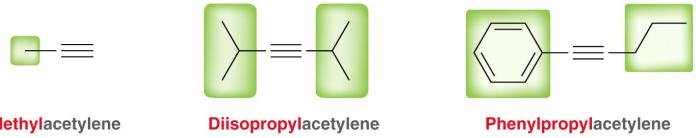
8. You may encounter common names for alkynes and alkynyl groups.

acetylene
preferred over ethyne



propargyl group
prop-2-ynyl preferred

- **IUPAC actually prefers the common name acetylene over the systematic name ethyne.**



Methylacetylene — **propyne**

Diisopropylacetylene — **2,5-dimethylhex-3-yne**

Phenylpropylacetylene — **(pent-1-yn-1-yl)benzene**

- **Alkynes can be named as substituted acetylenes, but IUPAC discourages this convention.**

09-015

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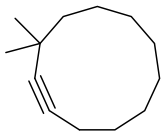
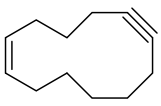
Nomenclature of Cycloalkynes

1. Cycloalkynes are compounds with a C≡C bond between two carbons in a ring.

2. Cycloalkynes are named by numbering the ring such that the C≡C bond is between C1 and C2.



3,3-dimethylcycloundecyne
not 1,1-dimethylcycloundec-2-yne
not 11,11-dimethylcycloundecyne



cyclododec-1-en-6-yne
not cyclododec-6-en-1-yne
not cyclododec-1-en-8-yne

- **The locant "1" for the position of the C≡C bond in a cycloalkene is omitted when alone (because it is implied)**
- **When both C=C and C≡C bonds are in the ring, give seniority to the C=C bond**

09-016

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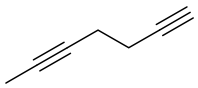
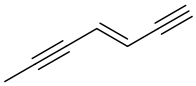
Nomenclature of Alkynes and Cycloalkynes

1. **Chains and rings containing multiple C≡C bonds are named as diynes, triynes, tetraynes, etc.**



hepta-1,5-diyne
not hept-1,5-yne



(3*E*)-hept-3-en-1,5-diyne

- **When the multiplier directly follows the parent chain, the "a" is not included in the elision of the ending "–ane" because it sounds better (e.g., hexa-1,5-diyne sounds better than "hex-1,5-diyne")**

09-017

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Review

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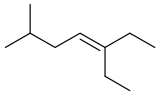
Nomenclature of Alkenes Using the Updated 2013 IUPAC Preferences

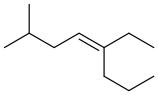
(1) Identify the parent chain—the longest chain of carbon atoms regardless of whether it includes the C=C bond

(2) Number the chain to give the first carbon of the C=C bond the lower locant number



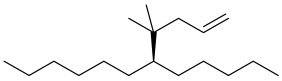
3-ethyl-6-methylhept-3-ene
not 5-ethyl-2-methylhept-4-ene

(3) When different diastereomers are possible, assign *E*- or *Z*- as a stereodescriptor prefix



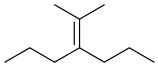
(4*Z*)-5-ethyl-2-methyloct-4-ene

(4) For substituents that contain C=C bonds, name the group as an alkene, giving preference to the carbon bonded to the parent, and use it as an enyl group



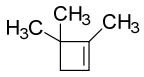
(6*S*)-6-(2-methylpent-4-en-2-yl)dodecane

(5) Substituents joined to the parent chain by a C=C bond are named as ylidene groups



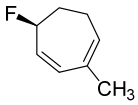
4-(propan-2-ylidiene)heptane
not 2-methyl-3-propylhex-2-ene

(6) For cycloalkenes, the C=C bond is numbered between C1 and C2. The C=C locant is usually omitted



1,4,4-trimethylcyclobutene
not 2,3,3-trimethylcyclobutene
not 1,1,2-trimethylcyclobut-2-ene

(7) Polyenes are named by applying a multiplier prefix to the ene suffix



(5*S*)-5-fluoro-2-methylcyclohepta-1,3-diene
not (5*S*)-5-fluoro-1-methylcyclohepta-1,6-diene
not (7*S*)-7-fluoro-3-methylcyclohepta-1,3-diene

08-R02

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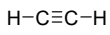
Nomenclature of Alkynes Using the Updated 2013 IUPAC Preferences

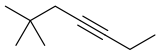
(1) The IUPAC-preferred name of C_2H_2 is acetylene



acetylene
preferred over ethyne

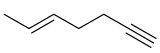
(2) Identify the parent chain—the longest chain of carbon atoms regardless of whether it includes the C≡C bond

(3) Number the chain to give the first carbon atom of the C≡C bond the lower locant number



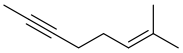
6,6-dimethylhept-3-yne
not 2,2-dimethylhept-4-yne

(4) For chains containing both C=C and C≡C bonds, number to give the lowest locant set possible regardless of type



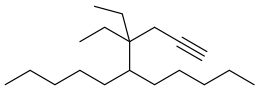
(5*E*)-hept-5-en-1-yne
not (2*E*)-hept-2-en-6-yne

(5) If C=C and C≡C bonds would be tied for smallest locant, give seniority to the C=C bond



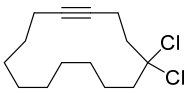
2-methyloct-2-en-6-yne
not 7-methyloct-6-en-2-yne

(6) For substituents that contain C≡C bonds, name the group as an alkyne, giving seniority to the carbon bonded to the parent, and use it as an ynyl group



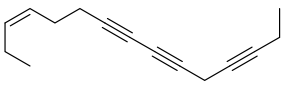
6-(3-ethylhex-5-yn-3-yl)undecane
not 5-pentyl-4,4-diethyldec-1-yne

(7) For cycloalkynes, the C≡C bond is numbered between C1 and C2. The locant of 1 is omitted if it stands alone



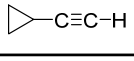
5,5-dichlorocyclotetradecyne
over 5,5-dichlorocyclotetradec-1-yne
not 12,12-dichlorocyclotetradecyne
not 1,1-dichlorocyclotetradec-4-yne

(8) Apply multipliers to chains with multiple C≡C bonds



(12*Z*)-pentadec-12-en-3,6,8-triyne
not (12*Z*)-pentadeca-12-en-3,6,8-triyne
not (3*Z*)-pentadec-3-en-7,9,12-triyne

(9) Alkynes should not be named as substituted acetylenes



ethynylcyclopropane
not cyclopropylacetylene

09-R02

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Problems

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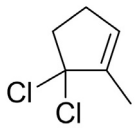
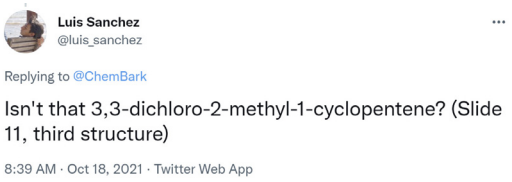
Practice Problem – Nomenclature

Q: A gentleman on Twitter flagged a possible error in the name of the structure on the left. Is he correct?



5,5-dichloro-1-methylcyclopentene



A: No, the name given in green is correct. While the locant of the C=C bond is minimized at 1 for both names, the locant set of the substituents is minimized with 1,5,5 rather than 2,3,3 – as 1 is lower than 2.

08-P01-1

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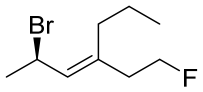
Practice Problem – Olefin Nomenclature

Q: Provide a name acceptable to IUPAC for the following compound.



A:

(2*R*,3*E*)-2-bromo-4-(2-fluoroethan-1-yl)hept-3-ene

08-P03-1

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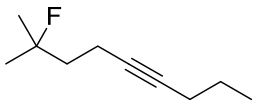
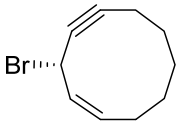
Practice Problem – Nomenclature of Alkynes

Q1: Provide the IUPAC-preferred name for the following two compounds





A1: 8-fluoro-8-methylnon-4-yne (3*S*)-3-bromocyclodec-1-en-4-yne

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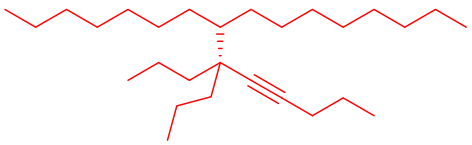
Q2: Draw the structure of the alkyne with the IUPAC name (8*R*)-8-(4-propylnon-5-yn-4-yl)hexadecane

A2:



30