Objective 6: Draw conformational isomers of chains (staggered, eclipsed) and rings (chair – axial/equatorial, boat, cis/trans) using skeletal structures, Newman projections, wedge-dash, sawhorse. Identify most stable conformer.

Quiz Practice problems

Key ideas:

Molecules are NOT static structures. Molecules are not solitary, individual structures, like the Lewis or skeletal structures we draw but exist with other molecules in a state of matter (gas, liquid, solid). Outside forces cause molecules to move (translational motion), spin like a top (rotational motion), bonds between atoms in the molecule to stretch or bend (vibrational motion).

We looked at structural (constitutional) isomers earlier – same chemical formula, different connectivity (bonding).

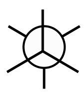
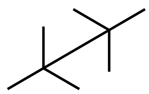
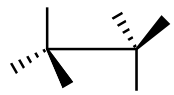
We will look at stereoisomers - same chemical formula, same bonding, different orientation in space.

We will look at a specific type of stereoisomer - conformational isomers.

Conformational isomers (shortcut name = conformers) of an organic compound occur when there is a rotation around a carbon-carbon bond axis.

We will look at three ways to represent (draw) conformational isomers:

Newman projection sawhorse wedge-and-dash

Imagine pointing a pencil straight at your nose. In a Newman projection, the pencil is a carbon-carbon bond and you are looking straight at the C-C bond.

Rotate the pencil 45°. This is a sawhorse representation.

Rotate the pencil another 45° so you are looking at the pencil from the side. This is a wedge-and-dash representation. You are looking at a side view of the C-C bond.

The atoms bonded to each carbon "feel" each other's presence due to the electrons around the atoms. Since electrons have a negative charge, the atom repel each other. The distance between the atoms determine how much the atoms repel each other. The farther apart the atoms, the less repulsion so the atoms in a molecule arranges itself so the repulsion between atoms is lowest to form the most stable (lowest energy) conformer.

We will look at conformational isomers of cyclohexane rings – chair and boat conformers.

Skills:

Give a Lewis or skeletal structure, draw a Newman projection, sawhorse, and wedge-and-dash representations of various conformational isomers of chains and rings.

Determine the most stable conformer of a chain compound.

Determine the least stable conformer of a chain compound.

Identify the axial and equatorial atoms in a chain and boat confomers.

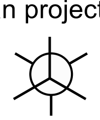
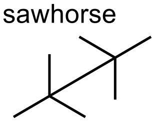
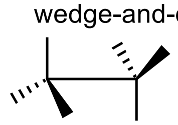
Identify the atoms or groups that are cis or trans to each other in a ring conformer.

Determine the most stable conformer of a ring compound.

Determine the least stable conformer of a ring compound.

1. The Newman projection, sawhorse representation, and wedge-and-dash representation of an alkane are shown. Match the atom in the Newman projection to the sawhorse and wedge-and-dash representations.

Newman projection sawhorse wedge-and-dash

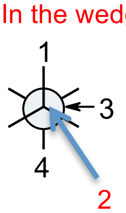




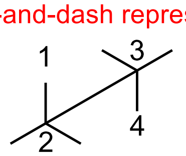
Answers: Atoms 1, 2, 3, and 4 are labeled in each structure.

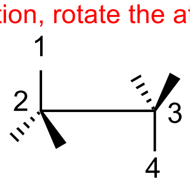
In the Newman projection, look along the atom 2-atom 3 bond.

In the sawhorse representation, rotate the atom 2-atom 3 bond 45°.

In the wedge-and-dash representation, rotate the atom 2-atom 3 bond another 45°.







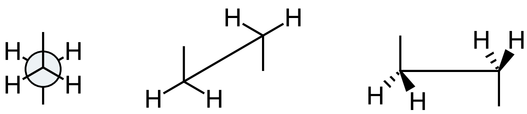
2. n-butane has the formula $CH_3CH_2CH_2CH_3$. Draw the Newman projections along C-2 and C-3 bond, sawhorse representations, and wedge-and-dash representations of:

a. the most stable staggered conformational isomer (conformer).

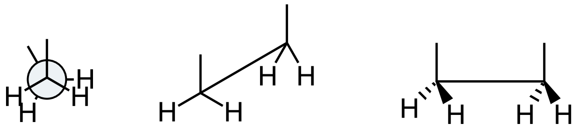
b. the least stable eclipsed conformer.

Answers:

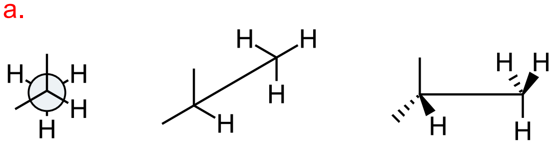
a.



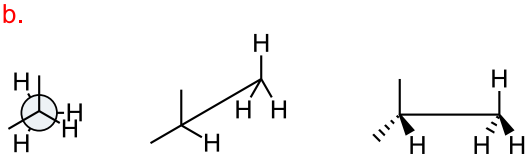
b. In the Newman projection, the methyl groups and H’s are directly behind each other.



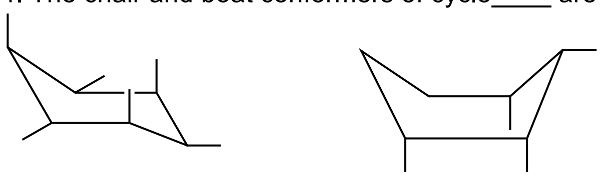
3. Iso-butane has the formula $(CH_3)_2CHCH_3$. Draw the Newman projections along C-2 and C-3 bond, sawhorse representations, and wedge-and-dash representations of:
a. the most stable staggered conformer.
b. the least stable eclipsed conformer.
Answers:
a.



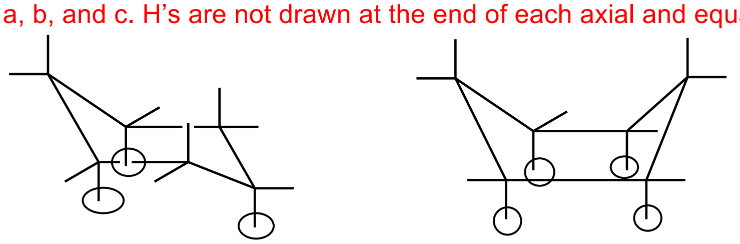
b.



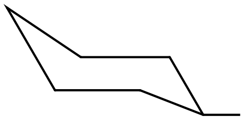
4. The chair and boat conformers of cyclo____ are shown.

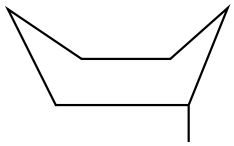


a. Some of the axial and equatorial H’s are shown. Draw in the rest of the axial and equatorial H’s.
Note: the axial and equatorial H’s that are shown in the chair confomer are <u>above</u> the plane of the ring.
Note: the axial and equatorial H’s that are shown in the boat conformer are <u>below</u> the plane of the ring.
b. In the chair conformer, circle the H’s that cause the most ring strain.
c. In the boat conformer, circle the H’s that cause the most ring strain.
Answers:
Hexane
a, b, and c. H’s are not drawn at the end of each axial and equatorial line.

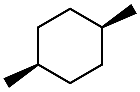


5. Draw the skeletal structure of methylcyclohexane.
a. Draw most stable chair conformer. Circle the axial or equatorial groups that cause the most ring strain.
b. Draw least stable boat conformer. Circle the axial or equatorial groups that cause the most ring strain.
Answers:
a. Methyl group is in an equatorial position.
b. Methyl group is in an axial position.

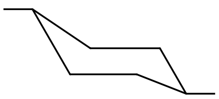


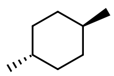


6. Draw the skeletal structure of 1,4-dimethylcyclohexane.
a. Draw most stable chair conformer. Circle the two axial or equatorial groups that cause the most ring strain. Are the methyl groups cis or trans to each other? Draw the wedge-and-dash representation to support your answer.
E.g., the wedge-and-dash representation of cis-1,4- dimethylcyclohexane is shown below. Remember: a wedge is above the plane of the ring and dash is below the plane of the ring. Relate the wedge and dash to the Note in Question 4a.

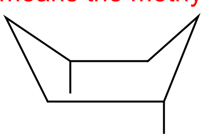


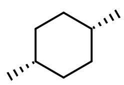
b. Draw least stable boat conformer. Circle the two axial or equatorial groups that cause the most ring strain. Are the methyl groups cis or trans to each other? Draw the wedge-and-dash representation to support your answer.
Answers:
a. Methyl groups are in equatorial positions.
One methyl group is above the ring. The other methyl group is below the ring. This means the methyl groups are trans to each other.



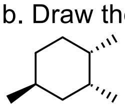


b. Methyl groups are in axial positions.
Each methyl group is below the ring. (You can draw this compound with the two methyl groups above the ring.) This means the methyl groups are cis to each other.

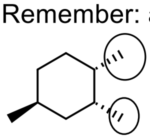


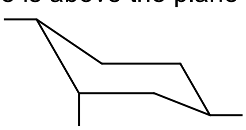


7. a. What is the name of the compound shown below?
b. Draw the chair conformer. Circle the methyl groups that are cis.

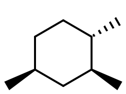


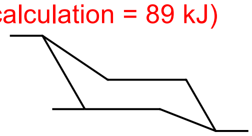
c. Is this conformer the most stable? If not, draw the most stable conformer.
Answers:
a. 1,2,4-trimethylcyclohexane
b. cis means the same side. In this compound, two methyl groups below the ring are cis to each other.
Remember: a wedge is above the plane of the ring and dash is below the plane of the ring.



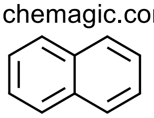


c. This conformer is not the most stable. The methyl group in C-2 is in the axial position. (Marvin Sketch conformer calculation = 93 kJ)
The most stable conformer has the three methyl groups in equatorial positions. (Chemagic.org energy = 44 kJ. Marvin Sketch conformer calculation = 89 kJ)

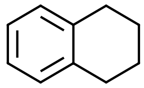




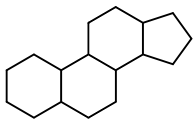
8. a. Naphthalene (shown below) is used in mothballs and smells. Which ring is planar? Which ring is chair? Go to chemagic.com to confirm your answer.



b. Part of naphthalene is hydrogenated (H_2 reacts at the C=C bond (we'll look at this reaction later in Chem 12A). Which ring is planar? Which ring is chair? Go to chemagic.com to confirm your answer.



c. The general structure of a steroid is shown below. Which ring is planar? Which ring is chair? Go to chemagic.com to confirm your answer.



Answers:
a. Each ring is planar. Each C has a trigonal planar shape with sp^2 hybridization.

b. Aromatic ring is planar. Each C has a trigonal planar shape with sp^2 hybridization.
Cyclohexane ring is chair. Four C's with sigma bonds only has a tetrahedral shape with sp^3 hybridization.
c. None of the rings are planar. All four rings are chair. Each C has a tetrahedral shape with sp^3 hybridization.