

ALKANES – STRUCTURE, PROPERTIES

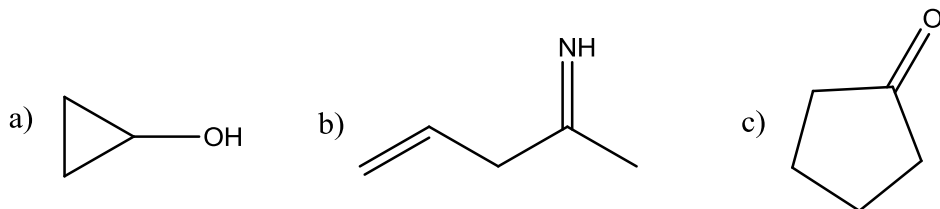
A STUDENT SHOULD BE ABLE TO:

1. Define, recognize, and give examples of constitutional (structural) isomers.
2. Define, recognize, and give examples of geometric (*cis* and *trans*) isomers.
3. Predict relative boiling points of alkanes, in comparison with other alkanes and with compounds containing other functional groups. Intermolecular bonding type (ionic, hydrogen bonds, dipole-dipole, induced dipole-induced dipole) and surface area (among isomers, unbranched compounds have higher surface area and higher boiling points) are important here.
4. Draw conformations of alkanes and cycloalkanes when given the name, and identify conformations when given a structure. For butane and related molecules, the important conformations are eclipsed and staggered (including *gauche* and *anti*). For substituted and unsubstituted cyclohexanes, the most important conformation is the chair. Also recognize cyclohexane's less important boat, twist boat, and half chair conformations.
5. Give the IUPAC names of alkanes, alkyl halides, and alcohols (open chain and cyclic) when given a picture of the conformation. Newman projections and bond-line formulas are important here.
6. Predict the relative stabilities of conformations of alkanes and cycloalkanes, and draw and describe the most stable conformations in these systems. Also, give or identify the types of strain present in different conformations in these systems, and use this information to explain relative stabilities. Important types of strain in conformational analysis are:
 - torsional strain (favors staggered conformations over eclipsed)
 - bond angle strain (which favors conformations with normal bond angles of 109.5° for sp^3 atoms and 120° for sp^2 atoms)
 - steric strain (effects of the bulk of groups, occurring when two groups try to occupy the same space).

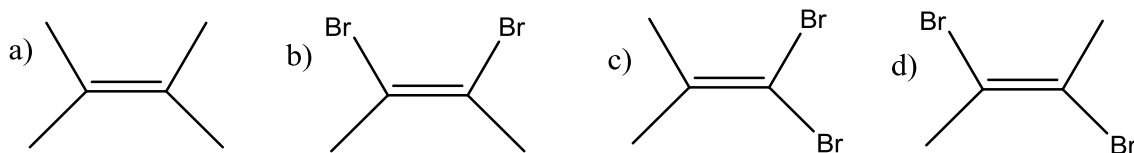
To best prepare for this module, please work Chapter 4 Skill Builder problems in the textbook.
Please use your model kit to prepare for this module.

A STUDENT WHO HAS MASTERED THE OBJECTIVES ON THE PREVIOUS PAGE SHOULD BE ABLE TO SOLVE THE FOLLOWING PROBLEMS AND RELATED ONES:

1.1 Draw the structure of a constitutional isomer of each of the following compounds.



2.1 Which of the following is a *cis* isomer? Which is *trans*?



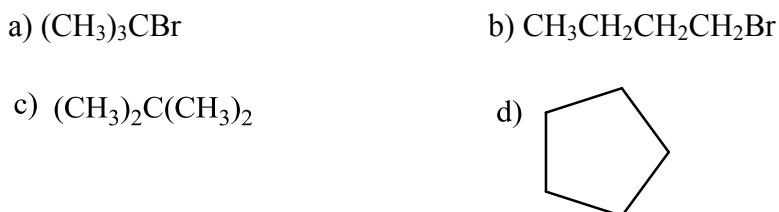
2.2 Which of the following alkenes can be drawn in both *cis* and *trans* configurations?



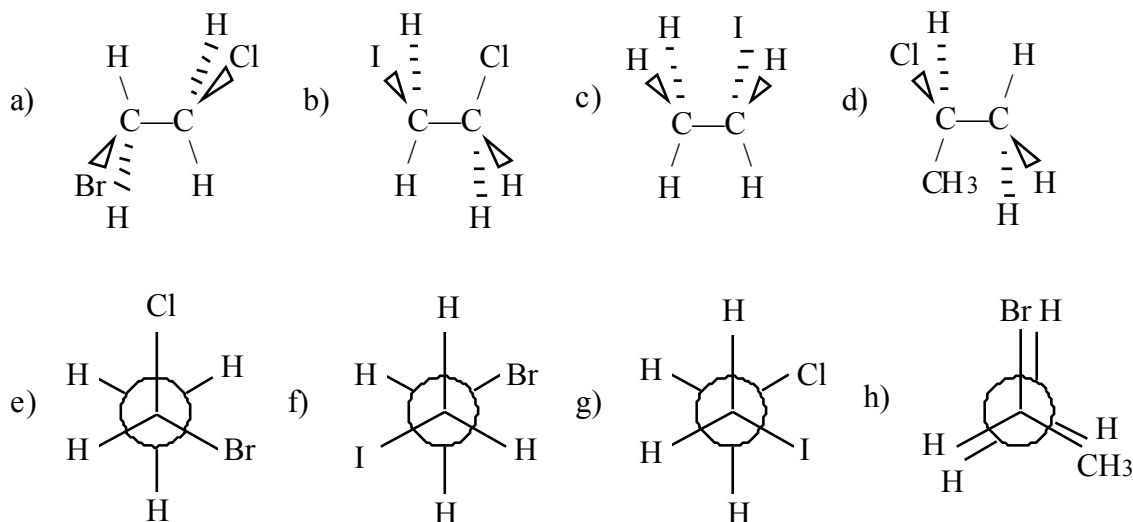
3.1 Which of the following alkanes has the highest boiling point?



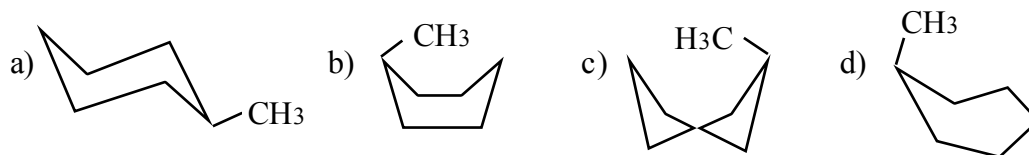
3.2 Which of the following compounds has the highest boiling point?



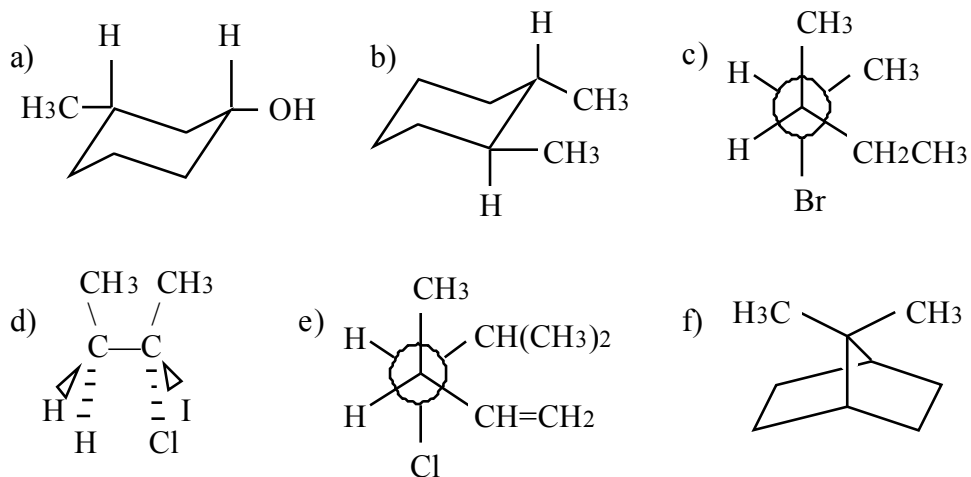
4.1 Use the terms: eclipsed, staggered, gauche, anti to classify each of the following structures. Some structures may need more than one term for a full classification.



4.2 Classify each of the following structures as one of the following: chair, half chair, boat, twist boat.



5.1 Give the IUPAC name of each of the following compounds.



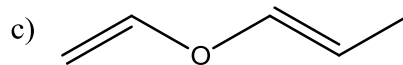
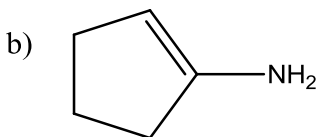
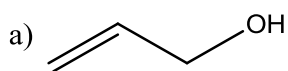
6.1 Which of these describes the most stable conformation of butane? Which describes the least stable?

- Eclipsed, with the methyl groups eclipsing hydrogens
- Eclipsed, with the methyl groups eclipsing each other
- Anti
- Gauche

- 6.2 Draw the most stable conformation of each of the following:
a) 4-methylcyclohexanol b) methylcyclohexane c) 1-fluoropropane d) propane
- 6.3 For 1-iodo-2-methylpropane, draw:
a) the staggered conformation(s) of lowest energy b) the eclipsed conformation(s) of highest energy
- 6.4 a) Which of these describes the most stable conformation of *cis*-3-isopropylcyclohexanol?
I. The isopropyl group is equatorial and the OH is axial
II. The isopropyl group is axial and the OH is equatorial
III. Both substituents are equatorial
IV. Both substituents are axial
- b) Which of the choices A-D above best describes the most stable conformation of *cis*-4-isopropylcyclohexanol?
- 6.5 Underline one or more words in each set of parentheses to make each of the following sentences correct.
- a) The chair form of cyclohexane is (less, more) stable than the boat form because the chair form has (less, more) (torsional, bond angle, steric) strain.
- b) The “flagpole” interaction in the boat form of cyclohexane is an example of (torsional, bond angle, steric) strain.
- c) The staggered form of propane is (less, more) stable than the eclipsed form because the staggered form has (less, more) (torsional, bond angle, steric, torsional and steric) strain.
- d) Unstable conformations have (higher, lower) potential energy than stable ones.

SOLUTIONS TO SAMPLE PROBLEMS:

1.1 There are many other correct isomers. These are just examples.



2.1 *cis* b, *trans* d

2.2 d

3.1 d

3.2 b

4.1 a) staggered, gauche b) staggered, gauche c) eclipsed d) staggered
e) staggered f) staggered, anti g) staggered, gauche h) eclipsed

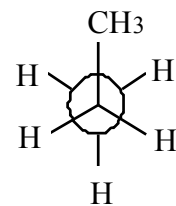
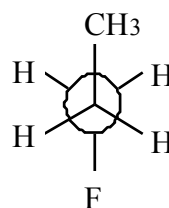
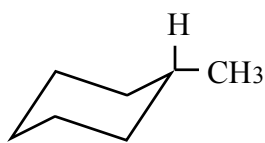
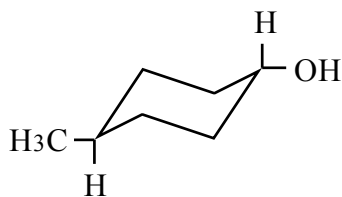
4.2 a) chair b) boat c) twist boat d) half chair

5.1 a) *cis*-3-methylcyclohexanol b) *trans*-1,2-dimethylcyclohexane
c) 2-bromo-3-methylpentane d) 2-chloro-2-iodobutane
e) 4-chloro-3,5-dimethyl-1-hexene f) 7,7-dimethylbicyclo[2.2.1]heptane

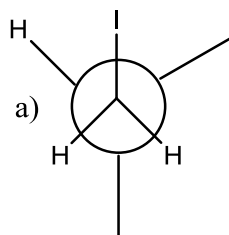
6.1 most stable C, least stable B

6.2 The most stable conformations:

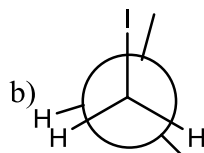
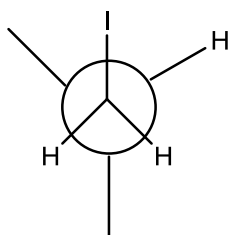
a) 4-methylcyclohexanol b) methylcyclohexane c) 1-fluoropropane d) propane



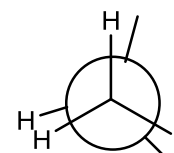
6.3



and



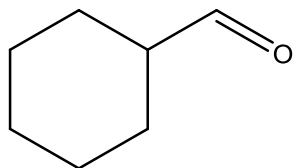
and



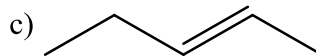
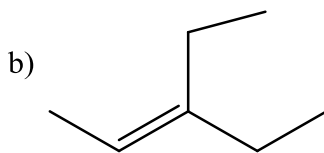
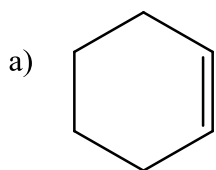
6.4 a) III b) I

6.5 a) more, less, torsional, steric
b) steric
c) more, less, torsional
d) higher

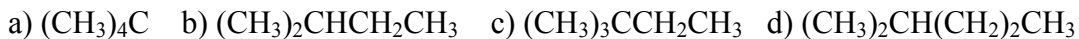
1. Draw an isomer of:



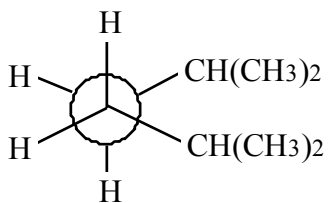
2. Which of the following is a *trans* isomer?



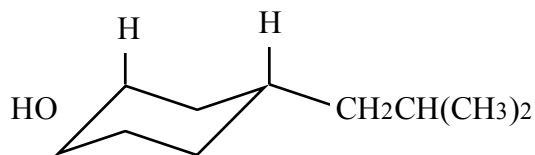
3. Which of the following compounds has the highest boiling point?



4. Give the IUPAC name of:



5. Give the IUPAC name of:



6. Draw the most stable conformation of ethyl chloride.

7. Fill in the blanks. The most stable conformation of *trans*-1-*tert*-butyl-3-fluorocyclohexane has the *tert*-butyl group _____ and the fluorine atom _____ (axial, equatorial).

1. Draw five constitutional (structural) isomers with the molecular formula C_4H_{10}

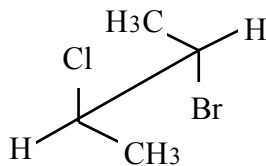
2. Draw the most stable conformation of each of these:

a) *tert*-butylcyclohexane

b) *cis*-1-*tert*-butyl-4-methylcyclohexane

3. Draw both the eclipsed and staggered conformations of 2-chloropropane in the Newman projection looking down the C1-C2 bond. Indicate which is more stable, and state what kind of strain is present in the less stable conformation.

4. Give the IUPAC name of the compound shown. Also, give the name of the conformation in which the compound is drawn.



5. Which of the following has the highest boiling point?

a) $CH_3CH_2CH_2CH_3$ b) $CH_3(CH_2)_3CH_3$ c) $(CH_3)_2CHCH_2CH_3$ d) $(CH_3)_2CHCH_3$