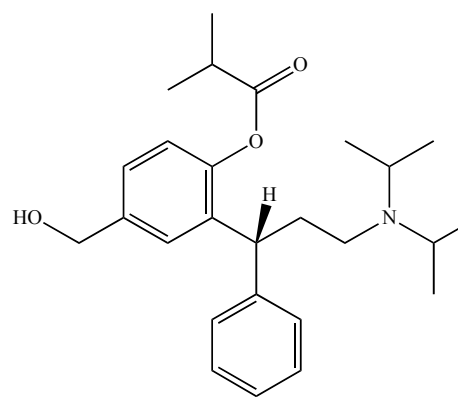


Toviaz is a muscarinic receptor antagonist that inhibits urinary bladder smooth muscle receptors. This drug is currently prescribed for the treatment of overactive bladder symptoms. Toviaz is a salt, formed by the reaction of molecule A (a base) with an acid.



Molecule A

- (2) Write the chemical formula (i.e., C_4H_6O) of molecule A.
- (2) List the atoms of molecule A in order of **decreasing** electronegativity. If two atoms have equal electronegativity, write them in the same blank and leave the next blank empty.

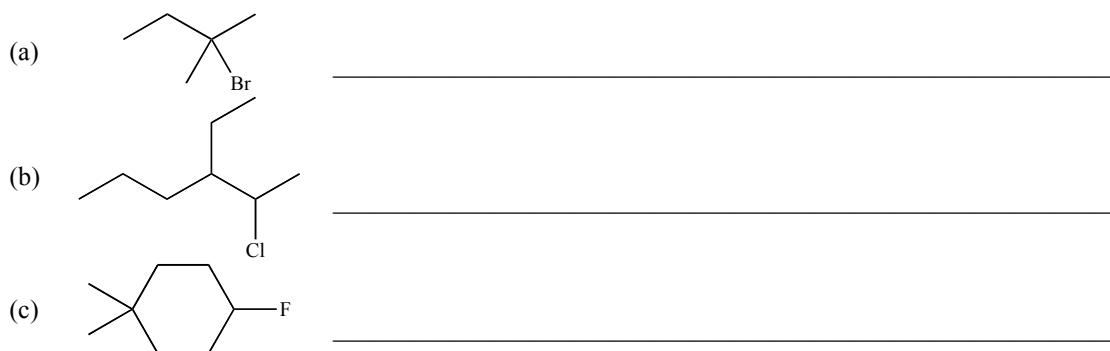
_____ > _____ > _____ > _____
Highest EN *Lowest EN*

- (2) Circle the bond of molecule A which has the largest δ^+ : C-H C-O C=O O-H C-N C=C
- (4) Write the names of all of the functional groups present in molecule A.
- (2) Write the name of a functional group that always has at least one *sp* atom.
- (6) Write numbers in the blanks: Molecule A has _____ lone pair(s), _____ sp^2 carbon(s), and _____ sp^3 carbon(s).
- (4) Write numbers in the blanks. Molecule A has _____ sp^3 carbon stereocenter(s). Of these stereocenter(s), _____ has/have an *R* configuration and _____ is/are *S*.
- (8) Circle one choice from each set that best completes each sentence concerning the nitrogen of molecule A.
 - How many electron groups around this nitrogen atom? 0 1 2 3 4 5
 - Our first guess at the geometry of the nitrogen atom is...

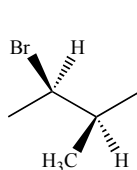
linear T-shaped trigonal planar square planar tetrahedral trigonal bipyramidal
 - To achieve this geometry, the nitrogen uses... atomic orbitals sp^3 orbitals sp^2 orbitals sp orbitals
 - This bonding results in a C–N–C bond angle that is (circle one adjective phrase and one number)...

a bit less than almost exactly a bit more than 90° 120° 109.5° 180°

9. (6) Write a correct name in the blank next to each molecule. You may use IUPAC or any other accepted nomenclature system.



10. (6) Draw in each box an isomer of the indicated type of molecule **B**.



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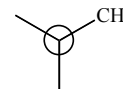
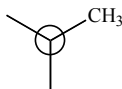
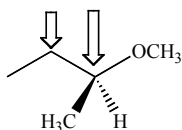
Molecule **B**

Constitutional isomer

Conformational isomer

Stereoisomer

11. (6) Complete the following drawings of conformations along the bond indicated with the arrows. *Place the atom indicated with the shortest arrow in the front of your drawing.*

Most stable conformationLeast stable conformation

12. (2) List the type(s) of strain that is (are) present in the least stable conformation in question 11.

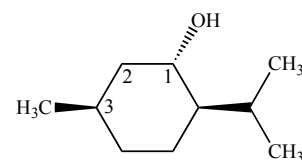
Here are some strain energies (in kcal mol⁻¹) that you will find useful for questions 13 and 14: H/H gauche = 0.0, H/CH₃ gauche = 0.0, CH₃/CH₃ gauche = 0.9, H/H eclipse = 1.0, H/CH₃ eclipse = 1.4, and CH₃/CH₃ eclipse = 2.5.

13. (2) Write a number. Based on the given strain energies, the barrier to rotation in butane is _____ kcal mol⁻¹.
14. (5) The best estimate for the strain (in kcal mol⁻¹) caused by eclipsing two fluorine atoms is (circle one):

0.0 0.9 1.0 1.4 2.5

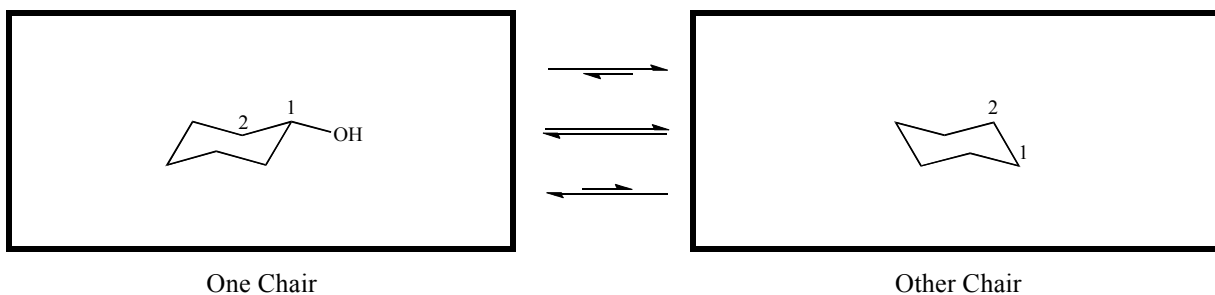
Complete this sentence by adding *no more than 25 words*: I chose this number for the strain caused by the eclipsing of two fluorine atoms because...

Questions 15–20 refer to the conformational isomers of isomenthol. *Note the numbering of the ring atoms.*



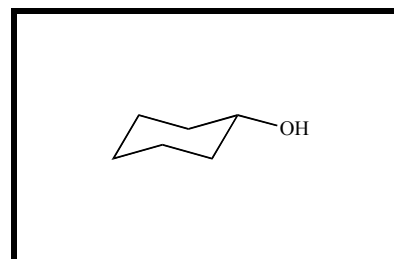
Isomenthol

15. (3) In the box below labeled ‘One Chair’ complete the drawing of isomenthol’s chair conformation. *Note the numbering of the ring atoms.*
16. (3) In the box below labeled ‘Other Chair’ draw the other chair conformation of isomenthol. Note the numbering of the ring atoms.
17. (2) Between the boxes below circle the equilibrium arrow set that properly indicates the position of the isomenthol chair flip equilibrium.

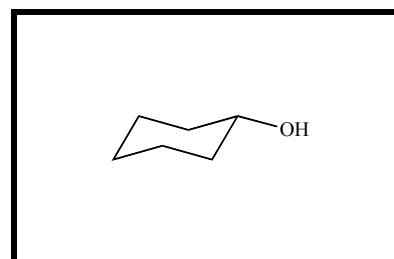


18. (4) Write numbers in the blanks. There is/are _____ enantiomer(s) and _____ diastereomer(s) of the structure in the ‘One Chair’ box.

19. (2) In the box complete this drawing of an enantiomer of the structure in the ‘One Chair’ box. If this is not possible write ‘not possible’.



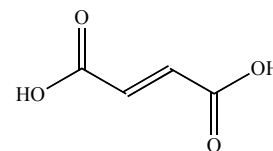
20. (2) In the box complete this drawing of a diastereomer of the structure in the ‘One Chair’ box. If this is not possible write ‘not possible’.



21. (2) Draw in the box a meso compound with chemical formula $C_5H_{11}BrO_2$. If this not possible write ‘not possible’.

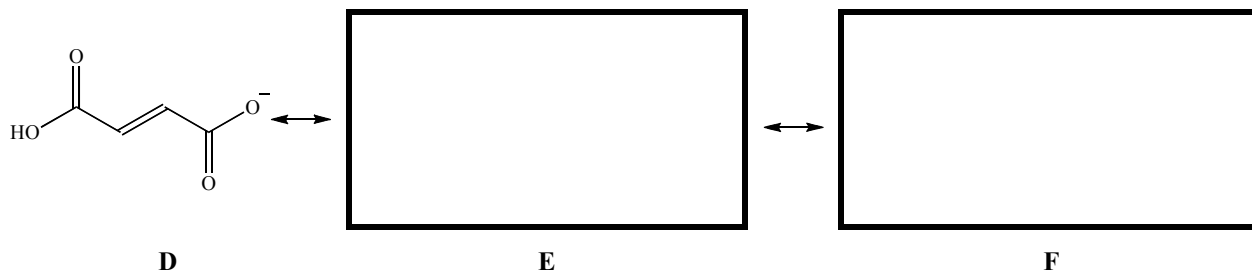


Toviaz is formed by the reaction of molecule **C** (an acid) with molecule **A** (a base). Molecule **C**'s resonance (the main reason it is an acid of moderate strength) is the subject of questions 22–24.



Molecule C

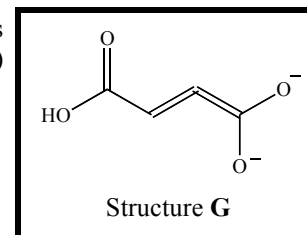
22. (6) In boxes **E** and **F** draw two additional resonance contributors for molecule **D** (the conjugate base of molecule **C**). *Select the most significant contributors possible. Less significant contributors may earn less credit. Include all lone pairs and formal charges. Curved arrows are optional.*



23. (5) Of the structures in question (previous) which is *least* significant? Circle one: **D** **E** **F**

Complete this explanation by adding *no more than twenty words*: This is the least significant contributor because...

24. (3) Complete this sentence by adding *no more than twenty words*: Structure **G** is not a legitimate resonance contributor for the conjugate base (structure **D**) because...



Structure G

25. (9) Provide precise but concise definitions for the following terms.

(a) Functional group:

(b) Constitutional isomer:

(c) Strain:

26. (2) Under what circumstances can an *R* enantiomer be converted into an *S* enantiomer by rotation around one or more single bonds? Describe (using *no more than twenty words*), or give an example. If it is not possible to achieve this conversion, write 'not possible'.