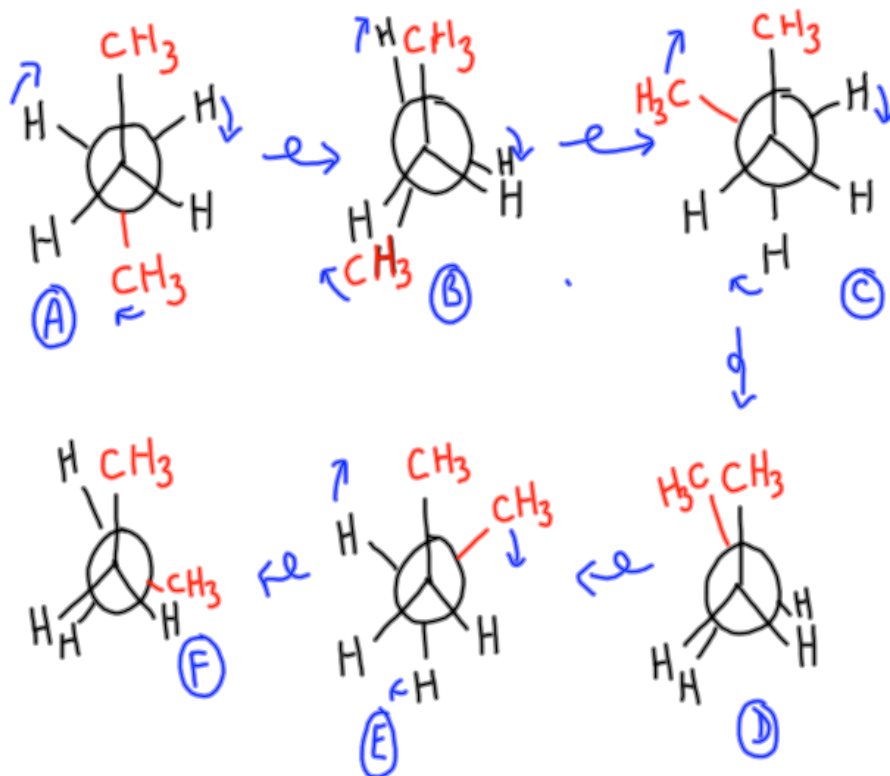


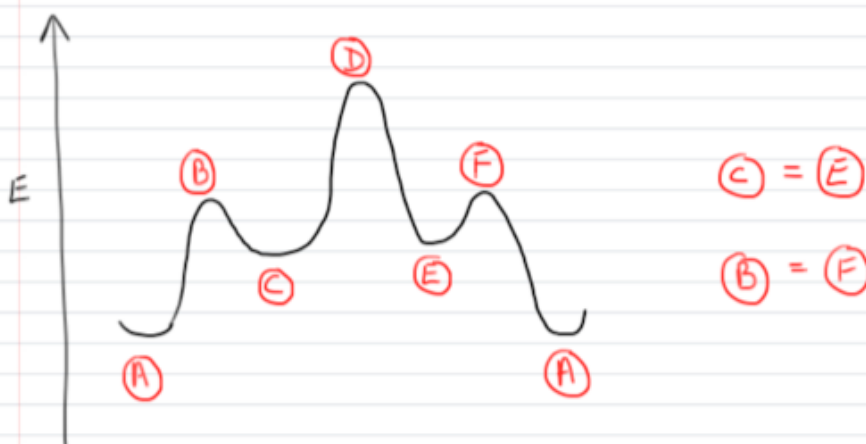
CHM 1321

Problem set 4 - ANSWERS

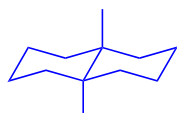
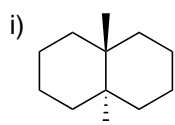
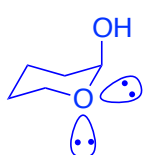
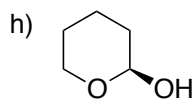
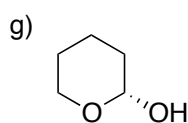
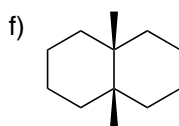
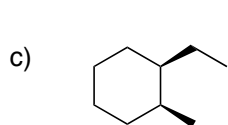
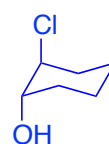
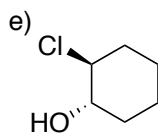
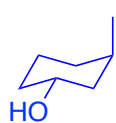
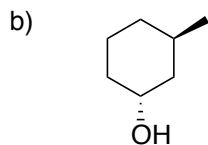
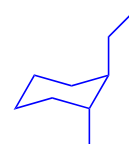
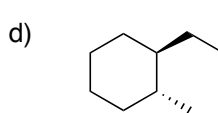
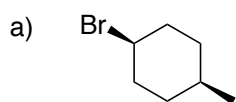
- 1) Draw all the conformations of butane in a Newman projection looking down the C2-C3 bond. Draw an energy diagram with all of these conformations.



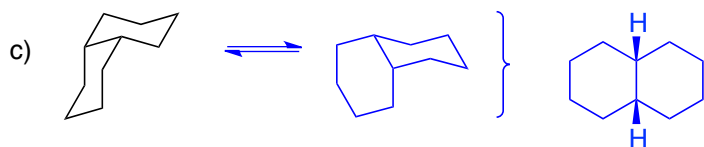
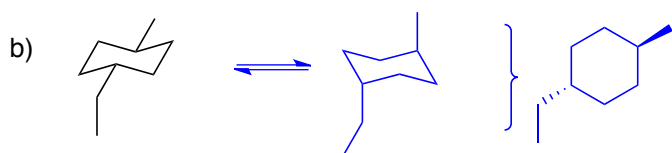
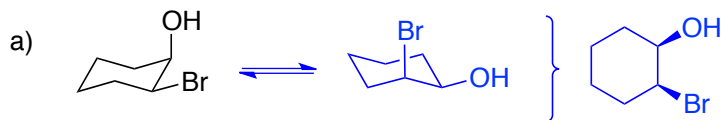
Representation in an energy diagram

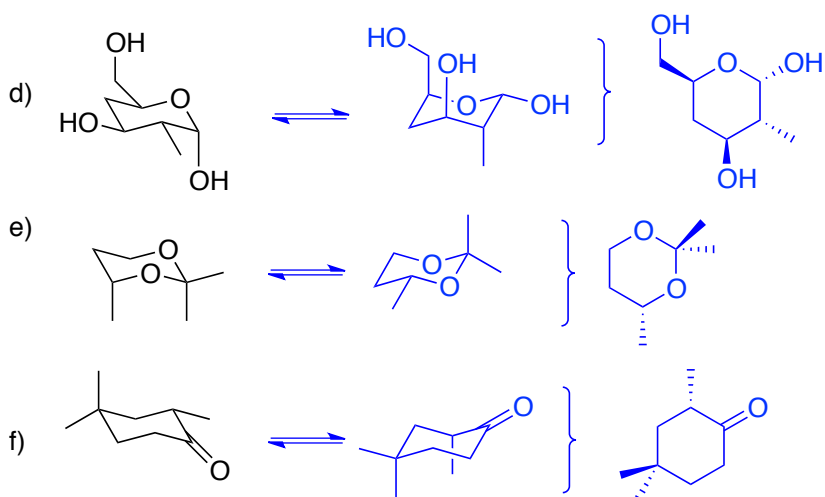


2) Draw the following line structures in 3D (chairs). For parts g and h, also draw in the lone pairs on the oxygen in the appropriate orbital.

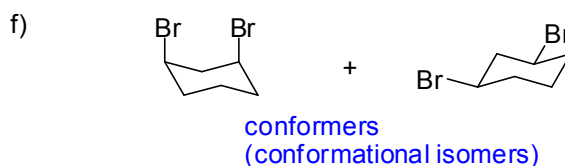
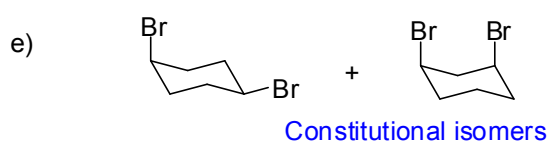
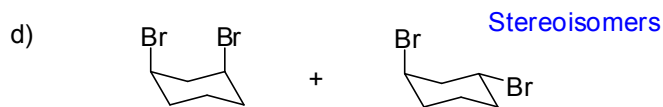
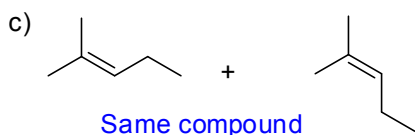
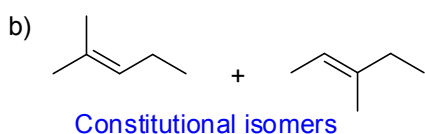
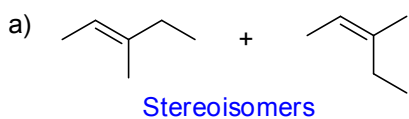


3) First, draw the other chair conformation (i.e., flip the chair). Then, draw the chairs as line structures.



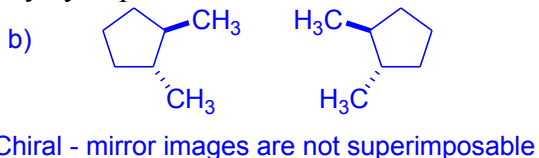
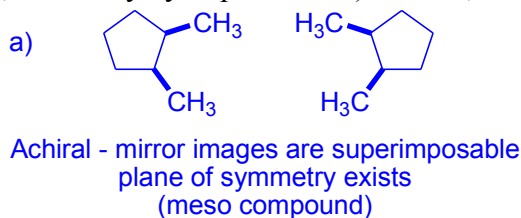


4) Identify each of the following pairs as constitutional isomers, stereoisomers (configurational isomers), or conformers.

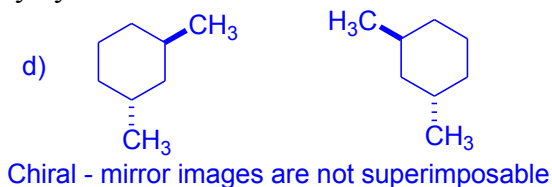
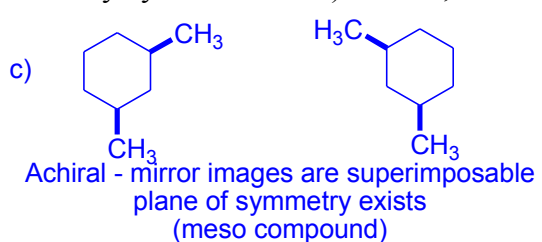


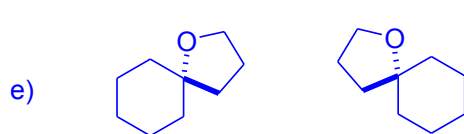
5) Draw each structure below along with its mirror image. Indicate whether the compound is chiral or achiral.

a) *cis*-1,2-dimethylcyclopentane. b) *trans*-1,2-dimethylcyclopentane

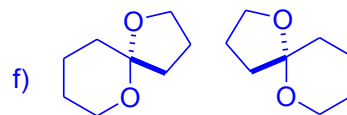


c) *cis*-1,3-dimethylcyclohexane d) *trans*-1,3-dimethylcyclohexane



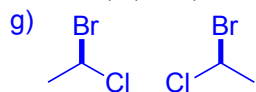
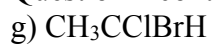


Achiral - mirror images are superimposable
 - no stereogenic centre, 2 identical groups on
 tetrasubstituted carbon
 Plane of symmetry exists

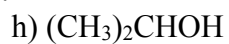


Chiral - mirror images are not superimposable

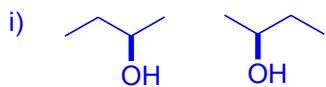
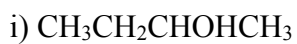
Question 2 cont'd:



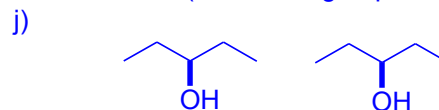
Chiral - mirror images not superimposable



Achiral - mirror images superimposable
(2 identical groups on central carbon)



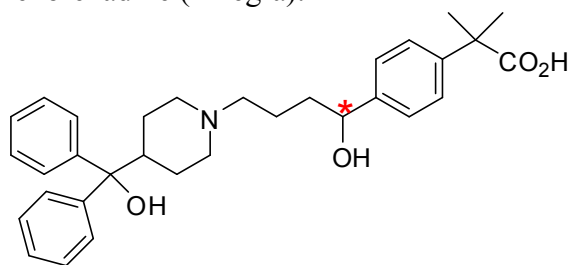
Chiral - mirror images not superimposable



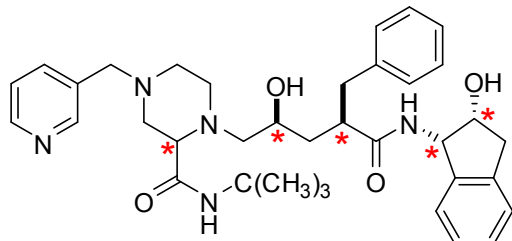
Achiral - mirror images superimposable
(2 identical groups on central carbon)
Plane of symmetry exists

6) Identify the stereogenic centres in the following molecules: (indicated with a *)

a. fexofenadine (Allegra):



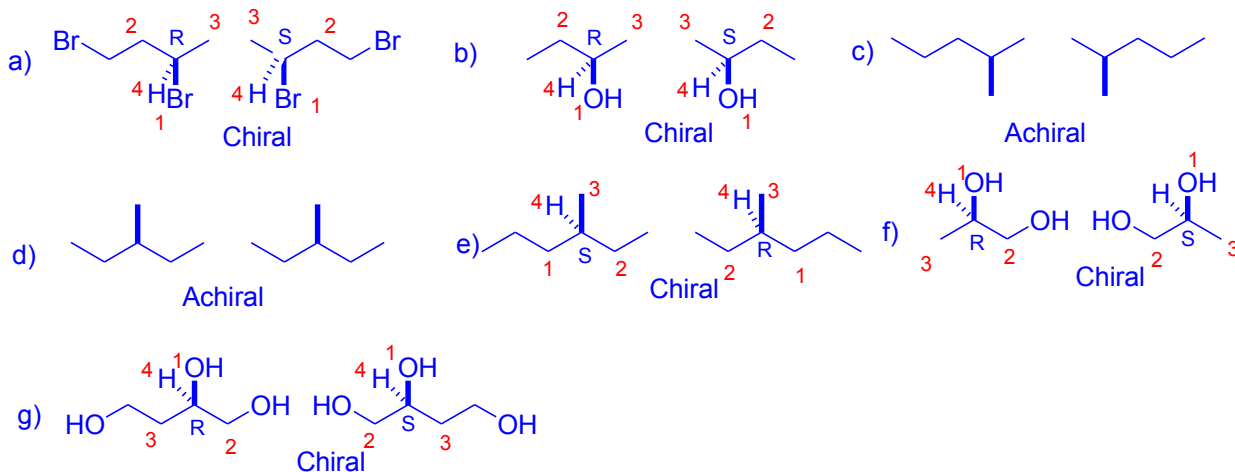
b. Indinavir (Crixivan):



7) Draw each of the following compounds in three dimensions. Draw the mirror image of each and determine whether the compounds are chiral. For all chiral compounds, determine whether the configuration of each stereogenic centre is R or S.

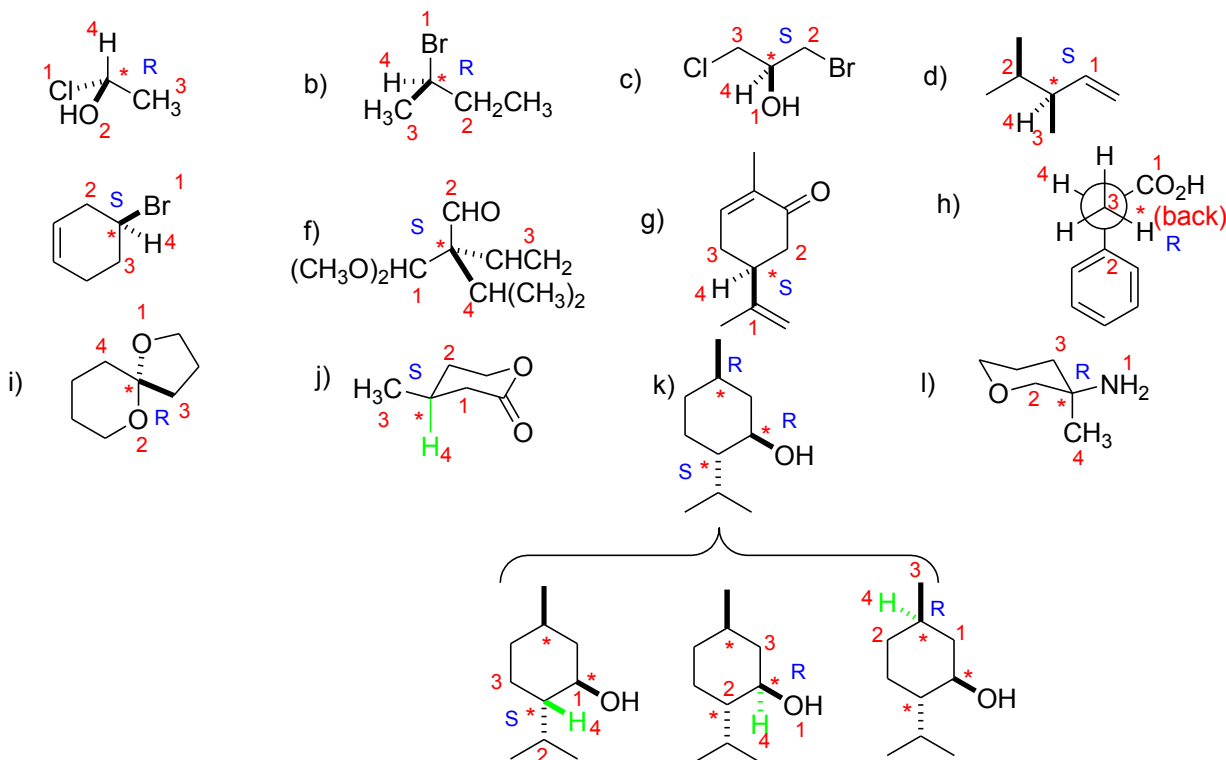
- a) 1,3-dibromobutane b) 2-butanol c) 2-methylpentane d) 3-methylpentane
 e) 3-methylhexane f) 1,2-dihydroxypropane g) 1, 2, 4-trihydroxybutane

(Priorities in red)



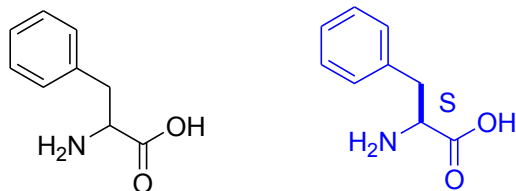
8) For the following compounds, show the stereogenic center(s) by labeling them with a star (*) and determine the configuration of each centre (R or S).

Priorities in red



- 9) Phenylalanine has the following structure, given that the configuration is S, what is the proper way to draw the compound?

One way to approach this problem is to draw the chiral center in your favourite conformation (arbitrary) and assign R or S to it. If you've drawn the S conformer, you've answered the question. If not, switch any two groups to obtain the opposite conformer.



- 10) Give the stereochemical relationship between each pair of isomers (enantiomers, diastereomers, meso compounds). **USE A MODEL!**
- Same compound
 - Enantiomers
 - Same compound
 - Diastereomers
 - Enantiomers
 - Enantiomers

- 11) Which of the following pairs of compounds could be separated by a method such as distillation or recrystallization?

Enantiomers (cyclohexanes) – not separable
 Diastereomers (salts) – separable