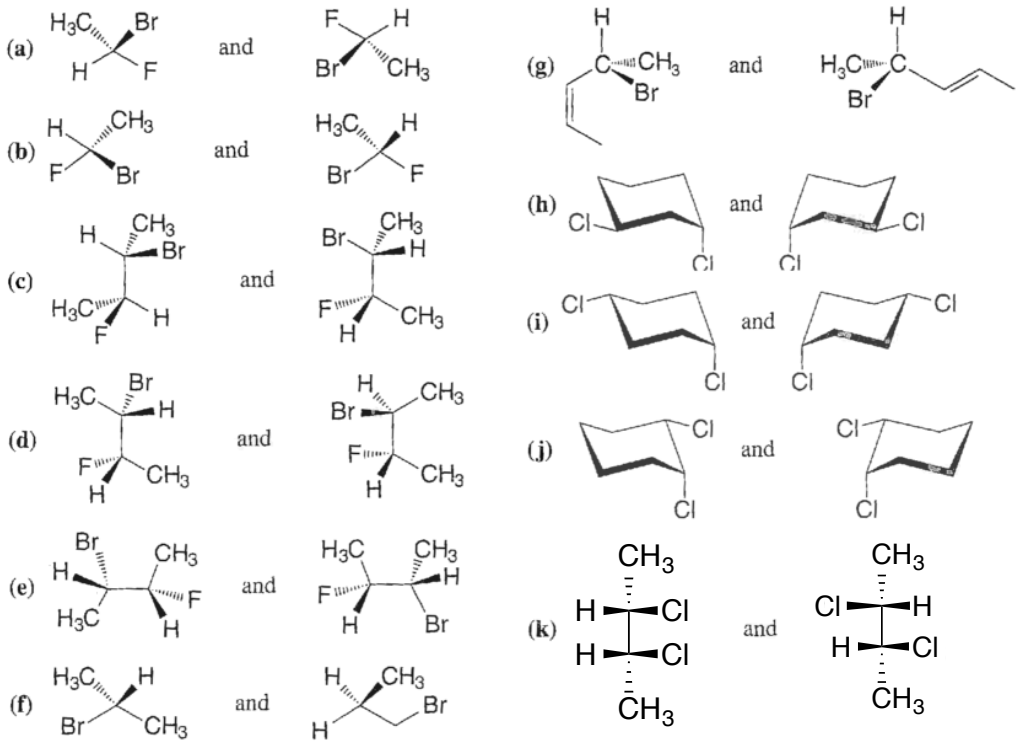
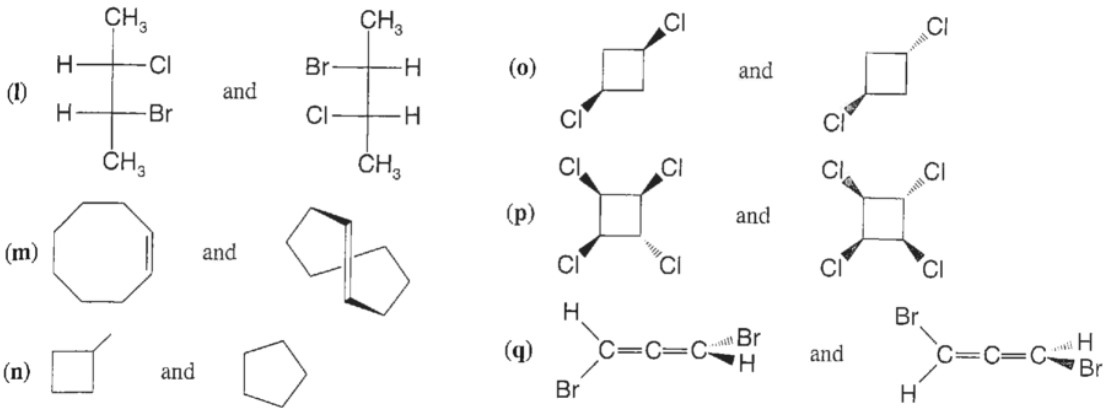
Example Questions



More Example Questions

See problem 5.62 Smith 4th edition



Optical Rotation and Enantiomers

Compounds that have an enantiomer are chiral

Enantiomeric compounds have identical physical properties
e.g. b.p., m.p., R_f, IR Spectra, density, $\Delta H_{combustion}$, etc.,

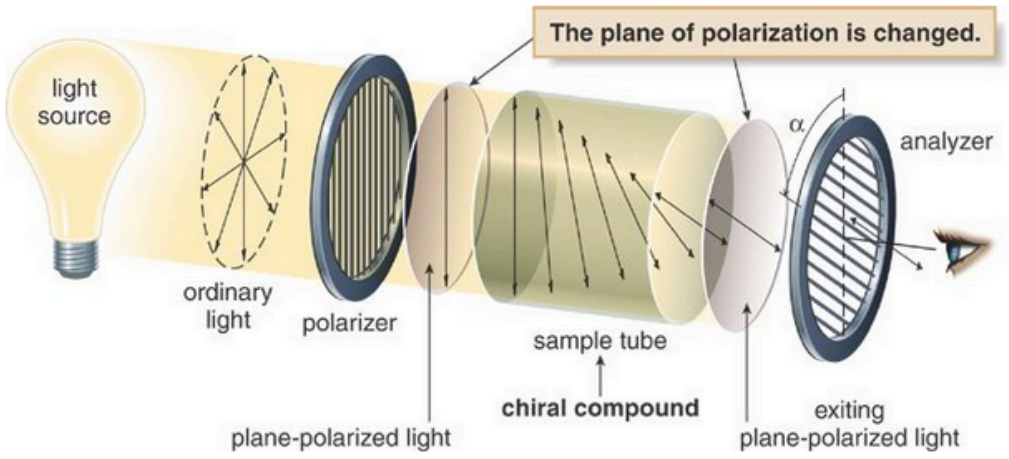
EXCEPT:
1) they react/interact with other chiral compounds differently

2) rotate plane-polarized light in equal but opposite directions

to the right (+) dextro *d*

to the left (–) levo *l*

Plane Polarized Light and Optical Rotation



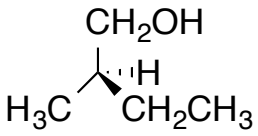
Specific Rotation

$$[\alpha]_D^{26} = \frac{\alpha}{l \times c}$$

589.6 nm

l = length of the sample tube (dm)

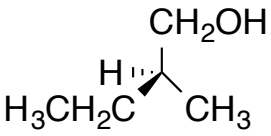
Stereochemical Descriptors



$[\alpha]_D^{26} = +5.75°$

(+)-(*R*)-2-methylbutan-1-ol

d-2-methylbutan-1-ol



$[\alpha]_D^{26} = -5.75°$

(–)-(*S*)-2-methylbutan-1-ol

l-2-methylbutan-1-ol

The direction of rotation (+/–) cannot be determined by looking at the structure.

Stereochemical Terms for Solutions

1) A solution is said to be **optically active** if it rotates plane polarized light. **Achiral compounds** will not be optically active.

2) A solution containing an unequal mixture of enantiomers is required to rotate plane polarized light.

3) An equal mixture of enantiomers is not optically active and the sample is called a **racemic mixture (racemate)** which is denoted with a "*dl*-" or "±"

4) Chirality is NOT equal to optical activity

5) A sample with only one enantiomer is **optically pure**

6) A sample that has an unequal mixture of enantiomers has an optically purity reported as **enantiomeric excess (e.e.)**

Enantiomeric Excess

$$\text{e.e.} = \frac{\text{observed rotation}}{\text{rotation of the pure compound}} \times 100 = \frac{[\alpha] - [\ell]}{[\alpha] + [\ell]} \times 100$$

A sample with 40% e.e. of the (+) isomer means:

The sample contains 40% more of the (+) enantiomer.

Thus, there is 40% of the (+) enantiomer + 60% of a 1:1 mixture of the (+):(–) isomers

Thus, there is 70% of the (+) enantiomer and 30% of the (–) enantiomer in solution

Example e.e. Questions

1) What is the e.e. of a solution containing 90% (+) and 10% (–)?

2) What is the e.e. of a solution with a specific rotation of –90 where the pure solution rotates at –135?

3) For the solution above (in question 2), how much of the (–) and (+) enantiomers are present?