Lecture I

01-13-2020

CHEM 6394: STEREOCHEMISTRY

Discuss syllabus:
Introduce yourself, ask them class to introduce themselves
Discuss grading, 3D models
Textbooks:
- Eliel & Wilen: Stereochemistry of Organic Compounds
- Kagan: Organic Stereochemistry
- Kepert: Inorganic Stereochemistry

Stereochemistry is the study of spatial arrangements of molecules in a 3D space. It is not a branch of chemistry in a way organic or inorganic chemistry are. Instead, it is more of a way of looking at molecules and reactions in a manner that pays attention to spatial relationships.

History of stereochemistry

1848 Louis Pasteur separates two kinds of crystals of sodium-ammonium salt of tartaric acid, based on their optical isomerism—they looked like mirror images of each other

1874 van't Hoff (NP) and le Bel independently propose that the central carbon in many organic cpds has its groups pointing at the vertices of a tetrahedron — easy explanation of optical isomerism

1893 Werner (father of coordination chemistry) similarly proposes that six ligands in transition metal complexes point at the vertices of an octahedron
- This explained the observation that $M(NH_3)_4X_2$ and $M(NH_3)_3X_3$ have two isomeric forms

1899 Werner suggests that chiral coordination complexes could exist, calling them "mirror image isomers"

Plane-polarized light was discovered in 1809 by the French physicist Malus. Biot (1812-1815) discovered that quartz, as well as turpentine and sugar solutions will rotate the plane of that light, forming the basis for polarimetry.

Lord Kelvin first used the term "chiral" in 1884.

stereo (Greek) = solid, three-dimensional

Modern inorganic stereochemistry is richer, because of the greater variety of coordination geometries. However, organic stereochemistry is more developed.

Stereochemistry today is divided into organic and inorganic, but also into static and dynamic. . The first studies molecules, their shapes and their chirality. Dynamic stereo-chemistry studies chemical reactions and their stereochemica outcomes. Bridging the two is the field of conformationa <u>analysis</u>, which studies the dynamics of individual molecul

In this course, we will look at the methods of studying stere chemistry and try to be as general as possible in their application.

Molecular Representations

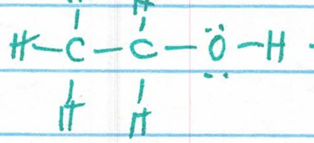
For each molecule, there are several equally correct—but not equally detailed—ways to represent it. Let's look at the example of ethanol:

C_2H_6O – useful when studying its combustion

C_2H_5OH – useful " " " deprotonation

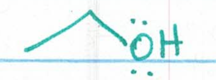
CH_3CH_2OH – condensed structural formula

$CH_3CH_2\ddot{\underset{..}{O}}H$ – showing lone pairs helps explain nucleophilicity

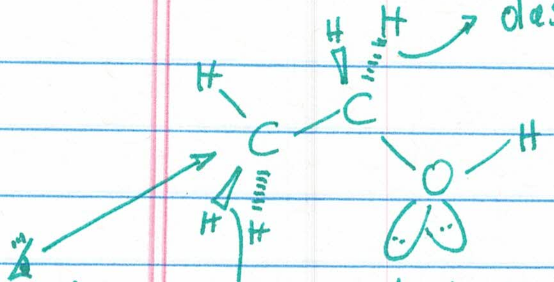


$$\begin{array}{ccccc} & H & H & & \\ & | & | & & \\ H- & C- & C- & \ddot{\underset{..}{O}}- & H \\ & | & | & & \\ & H & H & & \end{array}$$

– structural formula



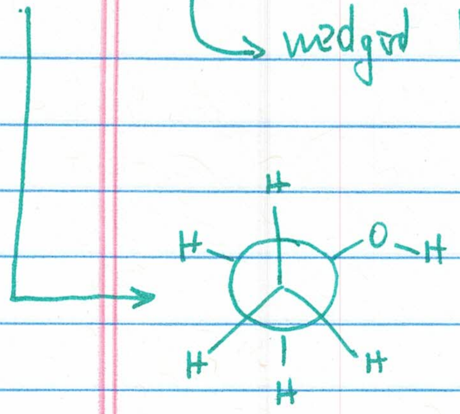
line-angle formula



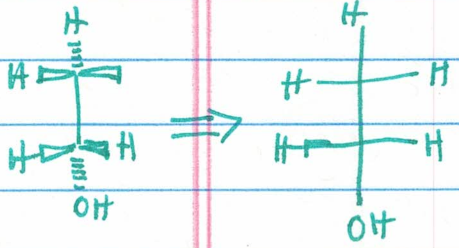
dashed lines - bonds behind the plane

sawhorse formulas show tetrahedral nature

wedged lines - bonds in front of the plane



Newman projection formula (useful for analyzing stereochemistry around a certain bond)

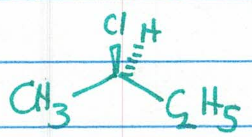


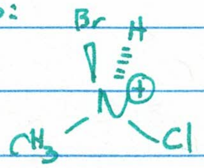
Fischer projection formula (always eclipsed)

While they all have their benefits, they are also all flawed -as they aim to represent a 3D object on a 2D plane. That is why sometimes molecular models - either physical or the ones constructed by a computer - are indispinsable in some complex cases.

You should practice converting between these formulas, and be very proficient in it. Also, review organic chemistry I - stereochemical aspects!

Practice molecules:





NEXT TIME: SHAPES OF MOLECULES