

Molecule essay



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Molecular geometry is the three-dimensional arrangement of the atoms that constitute a molecule.

It determines several properties of a substance including its reactivity, polarity, phase of matter, color, magnetism, and biological. The angles between bonds that an atom forms depend only weakly on the rest of molecule, i. e. They can be understood as approximately local and hence transferable properties. The specific three dimensional arrangement of atoms in molecules is referred to as molecular geometry. We also define molecular geometry as the sections of the atomic nuclei in a molecule.

There are various instrumental techniques such as X-Ray crystallography and other experimental techniques which can be used to tell us where the atoms are located in a molecule.

Using advanced techniques, very complicated structures for proteins, enzymes, DNA, and RNA have been determined. Molecular geometry is associated with the chemistry of vision, smell and odors, taste, drug reactions and enzyme controlled reactions to name a few. Molecular geometry is associated with the specific orientation of bonding atoms. A careful analysis of electron distributions in orbital will usually result in correct molecular geometry determinations.

In addition, the simple writing of Lewis diagrams can also provide important clues for the determination of molecular geometry. Molecular geometry, the bond lengths and angles, are determined experimentally.

Lewis structures can give us an approximate measure of molecular bonding. There is a simple procedure that allows us to predict overall geometry is the VESPER, Valence Shell Electron Pair Repulsion. The concept is that valence shell electron pairs are involved in bonding, and that these electron pairs will keep as far away from each other, due to electron-electron repulsion.

DETERMINING MOLECULAR GEOMETRY The molecular geometry can be determined by various spectroscopic methods and diffraction methods.

¹R, microwave and Raman spectroscopy can give information about the molecule geometry from the details of the vibrations and rotational absorbency detected by these techniques. X-ray crystallography, neutron diffraction and electron diffraction can give molecular structure for crystalline solids based on the distance between nuclei and concentration of electron density. Gas electron diffraction can be used for small molecules in the gas phase.

NMR and FRET methods can be used to determine complementary information including relative distances, dihedral angles, angles, and connectivity. Molecular geometries are best determined at low temperature because at higher temperatures the molecular structure is averaged over more accessible geometries (see next section). Larger molecules often exist in multiple stable geometries (conformational isomerism) that are close in energy on the potential energy surface.

Geometries can also be computed by ab initio quantum chemistry methods to high accuracy.

The molecular geometry can be different as a solid, in solution, and as a gas. The position of each atom is determined by the nature of the chemical bonds by which it is connected to its neighboring atoms. The molecular geometry can be described by the positions of these atoms in space, evoking bond lengths of two joined atoms, bond angles of three connected atoms, and torsion angles (dihedral angles) of three consecutive bonds. Principle: Electron pairs around a central atom arrange themselves so that they can be as far apart as possible from each other.

The valence shell is the outermost electron-occupied shell of an atom that holds the electrons involved in bonding. In a covalent bond, a pair of electrons is shared between two atoms. In a polyatomic molecule, several atoms are bonded to a central atom using two or more electron pairs. The repulsion between negatively charged electron pairs in bonds or as lone pairs causes them to spread apart as much as possible. The idea of "electron pair repulsion" can be demonstrated by tying several inflated balloons together at their necks. Each balloon represents an electron pair.

The balloons will try to minimize the crowding and will spread as far apart as possible. When two groups try to get as far away from each other as possible, a linear shape is formed. The M represents the central atom. The pairs of dots (:) represent two pairs of valence electrons forming bonds to the central atom. The angle between the lone pairs and the central atom is 180°. When three electron pairs get as far apart from each other, a trigonal planar structure is formed, as shown below.

The bond angle in this structure is 120°.

Four electron pairs form a tetrahedron when they are separated as far as possible from each other. The bond angle in a tetrahedron is 109.5° .

Five electron pairs form a trigonal bipyramid when they are separated in space. This shape consists of a triangle with two electron pairs directly above and below it. The bond angles of the middle, triangular portion are 120° . The groups above and below the central triangle are at a 90° angle to the triangle. Six pairs of electrons separated in space will form an octahedron, with 90° between all of the valence electrons.