Molecular modeling

[Science](), [Chemistry]()

MOLECULAR MODELING 1. Objectives â—� Predictthe shape of identified compounds; â—� Construct molecular models of identified compounds; and â—�Determine the molecular structure of identified compounds. 2. Theory Building models of molecules are useful for visualizing how atoms are connected in three-dimensional space called molecular geometry, which is best predicted by Valence-Shell Electron-Pair Repulsion (VSPER) theory. The following are the sets of rules summarizing thsi theory: â—� Consider molecules and ions where two or more atoms are bonded to a central atom. â—� The electron pairs in the valence shell of the central atom are assumed to position as far apart as possible because electron pair repels one another. The shape of the molecule or ion is a result of the electron-pair repulsion. â—� All the valence-shell electron pairs of the central atom are considered both the pairs that form covalent bonds (called bonding pairs) and the pairs that are unshared (called nonbonding pairs or lone pairs). â—� The nonbonding pairs help to determine the position of the atoms in the molecule or ion. Valence —Shell-Electron-Pair Repulsion (VSEPR) theory allows the chemist to predict 3-dimensional shape of molecules from knowledge of their Lewis Dot Structure. In VESPR theory, the position of bound atoms (ligands0 and electron pairs are described relative to a central atom. Once the ligands and lone pair electrons are positioned, the resulting geometrical shape presented by the atoms only (ignoring lone pairs) is used to describe the molecule. Electron Density and Molecular Geometry | d(Be-Cl) = 0, 117 nmï�¡ = 180 ° | | | Linear d(B-F) = 0, 130 nm ï�¡ = 120 ° Triangular Planar d(S-O) = 0, 150 nm ï�¡ = 109 . 5° Tetrahedral | | d(P-Cléq) = 0, 202 nmd(P-Clax) = 0, 214 nmï�¡(ClPCl) = 90 ° ; ï�¡ (ClPCl) = 120 ° | Triangular Biplanar | | d(Xe-F) =

0, 190 nmï�¡ = 90° | Octahedral 3. Apparatus and Materials 2- Modeling Clay (diff. colors) 1 — Wire (3mm. diameter, 5ft. long) 1- Protractor 4. Procedure 4. 1. Determine the molecular structure of the compounds listed in the table. 4. 2 Fill the table provided for the experiment. 4. 3 Construct the molecular models for each compound. 4. 3. 1 Use color for the central atom diff. from the attached atoms. Use one color for the attached atoms. 4. 3. 2 Make a 2-inch diameter central atom X and ½ inch diameter for the attached atoms Y. 4. 3. 3 Cut the wire into 3 inches long. 4. 3. 4 Attach the central atom X to the Y atoms based on the arrangement. 5. MolecularFormula | BondAngles | MolecularStructure | No. ofBond Pairs | No. ofLone Pairs | AngularGeometry | BeCl2 | 180° | | 2 | 0 | Linear | BF3 | 120° | | 3 | 0 | TrigonalPlanar | SO4 | 109. 5° | | 4 | 0 | Tetrahedral | PCl5 | 120° | | 5 | 0 | TriangularBipyramidal | XeF6 | 90° | | 6 | 0 | Octahedral | 6. Questions 1. What is valence electron? Give its importance. In chemistry, valence electrons are the electrons of an atom that can participate in the formation of chemica bonds with other atoms. Valence electrons are their " own" electrons, present in the free neutral atom, that combine with valence electrons of other atoms to form chemical bonds. In a single covalent bond both atoms contribute one valence electron to form a shared pair. For main group elements, only the outermost electrons are valence electrons. In transition metals, some inner-shell electrons are also valence electrons. Valence electrons can determine the element's chemical properties and if it will bond with others or not. When two atoms approach each other and react with each other, it is their outer shells that come into contact first, and it is therefore the electrons in their outer shells that are normally involved in any chemical reaction. So it is the number of electrons in an atom’s outer shell that determines, to a large extent, how that element will react chemically.