Axial Bond And Equatorial Bond

The term "anomeric effect" gained common usage by 1958, derived from the stereochemical designation for the lowest-numbered ring-carbon of a pyranose ring – the anomeric carbon. Anomeric molecules are isomers differing only in their configuration at the anomeric carbon; D-glucopyranose anomers are diastereomers, where the β-anomer is oriented such that the hydroxyl (−OH) group is pointed upwards equatorially, while the α-anomer hydroxyl points downward axially. 3309577118 Compounds with disphenoidal... 3309577118

Cyclohexane conformation six C–H bonds are equatorial, oriented radially outwards with an upwards or downwards tilt. Because many compounds feature structurally similar six-membered rings, the structure and dynamics of cyclohexane are important prototypes of a wide range of compounds. Each carbon center has one axial C–H bond (pointed alternately Cyclohexane conformations are any of several three-dimensional shapes adopted by cyclohexane 3309577118

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== Preparation == 3309577118

A value The difference in Gibbs free energy (ΔG) between the higher energy conformation (axial substitution) and the lower A-values are numerical values used in the determination of the most stable orientation of atoms in a molecule (conformational analysis), as well as a general representation of steric bulk. in the equatorial position to the axial. A-values are derived from energy measurements of the different cyclohexane conformations of a monosubstituted cyclohexane chemical 3309577118

Linear molecular geometry three lone pairs occupy the less crowded equatorial positions and the two bonded atoms occupy the two axial positions at the opposite ends of an axis The linear molecular geometry describes the geometry around a central atom bonded to two other atoms (or ligands) placed at a bond angle of 180°. Linear organic molecules, such as acetylene (HC≡CH), are often described by invoking sp orbital hybridization for their carbon centers 3309577118

The study of the energetics of bond rotation is referred to as conformational analysis. In some cases, conformational analysis can be used to predict and explain product selectivity,

mechanisms, and rates of reactions. Conformational analysis also plays... 3309577118 == Chair flip == 3309577118 A-values help predict the conformation of cyclohexane rings. The most stable conformation will be the one which has the substituent or substituents equatorial. When multiple substituents are taken into consideration, the conformation where the substituent with the largest A-value is equatorial is favored. 3309577118 The Cieplak effect relies on the stabilizing interaction of mixing full and empty orbitals to delocalize electrons, known as hyperconjugation. When the highest occupied... 3309577118 The internal angles of a regular, flat hexagon are 120°, while the preferred angle between successive bonds in a carbon chain is about 109.5°, the tetrahedral angle (the arc cosine of −1/3). Therefore, the cyclohexane ring tends to assume non-planar (warped) conformations, which have all angles closer to 109.5° and therefore a lower strain energy than the flat hexagonal shape. 3309577118 == Background == 3309577118

Ring flip Most commonly, the term is used to refer to the interconversion of the two chair conformers of cyclohexane derivatives, which is specifically referred to as a chair flip, although other cycloalkanes and inorganic rings undergo similar processes. , from a chair conformer to another chair conformer) that results in the exchange of nonequivalent substituent positions. g. conformer to another, all axial positions become equatorial and all equatorial positions become

axial. The overall process generally takes place over several steps, involving coupled rotations about several of the molecule's single bonds, in conjunction with minor deformations of bond angles. Substituent groups in equatorial positions roughly follow In organic chemistry, a ring flip (also known as a ring inversion or ring reversal) is the interconversion of cyclic conformers that have equivalent ring shapes (e 3309577118

== Axial (or apical) and equatorial positions == 3309577118 As stated above, a chair flip is a ring inversion specifically of cyclohexane (and its derivatives) from one chair conformer to another, often to reduce steric strain. The term, "flip" is misleading, because the direction of each carbon remains the same; what changes is the orientation. A conformation is a unique structural arrangement of atoms, in particular one achieved through the rotation of single bonds. A conformer is a conformational isomer, a blend... 3309577118

Anomeric effect Edward and Raymond Lemieux) is a stereoelectronic effect describing the tendency for vicinal heteroatomic substituents of a cyclic heteroatom – e. , oxygen in a tetrahydropyran ring – to assume the relative axial orientation, rather than a less sterically-hindered equatorial orientation. Edward in 1955, while studying carbohydrate chemistry. g. tetrahydropyran ring – to assume the relative axial orientation, rather than a less sterically-

hindered equatorial orientation. T. This effect was first observed in pyranose rings by J. This effect was first observed In organic chemistry, the anomeric effect or Edward-Lemieux effect (after J. T 3309577118

Phosphorus pentafluoride was first prepared in 1876 by the fluorination of phosphorus pentachloride using arsenic trifluoride, which remains a favored method: 3309577118

Seesaw molecular geometry An equatorial lone pair is repelled by only two bonding pairs at 90°, whereas a hypothetical axial lone pair would Disphenoidal or seesaw (also known as sawhorse) is a type of molecular geometry where there are four bonds to a central atom with overall C2v molecular symmetry. than does a bonding pair of electrons. The name "seesaw" comes from the observation that it looks like a playground seesaw. Most commonly, four bonds to a central atom result in tetrahedral or, less commonly, square planar geometry 3309577118

== Utility == 3309577118 The anomeric effect can also be generalized to any cyclohexyl or linear system with the general formula C−Y−C−X, where Y is a heteroatom with one or more lone pairs, and X is an electronegative atom or group. The magnitude of the anomeric effect is estimated... 3309577118 Linear geometry also occurs in AX2E3 molecules, such as xenon

difluoride (XeF2) and the triiodide ion (I−3) with one iodide bonded to the two others. As described... 3309577118 Consider the carbon atoms numbered from 1 to 6 around the ring. If we hold carbon atoms 1, 2, and 3 stationary, with the correct bond lengths and the tetrahedral angle between the two bonds, and then continue by adding carbon atoms 4, 5, and 6 with the correct bond length and the tetrahedral angle, we can vary the three dihedral angles for the sequences (1,2,3,4), (2,3,4,5), and (3,4,5,6). The next bond, from atom 6, is also oriented by a dihedral angle, so we have four degrees of freedom. But that last bond has to end at the position of atom 1, which... 3309577118

Rotamer Rotations about single bonds are subject to small energy barriers. When the time scale for interconversion is long enough for isolation of individual rotamers (usually arbitrarily defined as a half-life of interconversion of 1000 seconds or longer), the species are termed atropisomers. Various arrangements of atoms in a molecule that differ by rotation about single bonds can also be referred to as conformations. The repulsion between an axial t-butyl group and hydrogen In chemistry, rotamers are chemical species that differ from one another primarily due to rotations about one single bond. Conformers can differ from one another due to rotation of multiple bonds; rotamers are a subset of conformers. The ring-flip of substituted cyclohexanes constitutes a common form of conformers. Conformers/rotamers usually differ little in their energies, so they

are almost never separable in a practical sense. Conformations, which represent local minima on the potential energy surface, are called conformers. antiperiplanarity of Cl and H can be achieved when the t-Bu group is in the favorable equatorial position 3309577118

According to the VSEPR model (Valence Shell Electron Pair Repulsion model), linear geometry occurs at central atoms with two bonded atoms and zero or three lone pairs (AX2 or AX2E3) in the AXE notation. Neutral AX2 molecules with linear geometry include beryllium fluoride (F−Be−F) with two single bonds, carbon dioxide (O=C=O) with two double bonds, hydrogen cyanide (H−C≡N) with one single and one triple bond. The most important linear molecule with more than three atoms is acetylene (H−C≡C−H), in which each of its carbon atoms is considered to be a central atom with a single bond to one hydrogen and a triple bond to the other carbon atom. Linear anions include azide (N−=N+=N−) and thiocyanate (S=C=N−), and a linear cation is the nitronium ion (O=N+=O). 3309577118 == Structure == 3309577118

Cieplak effect Proposed by Andrzej Stanislaw Cieplak in 1980, it correctly predicts results that could not be justified by the other standard models at the time, such as the Cram and Felkin–Anh models. Whichever bond can best donate its electrons into the C–Nuc bond determines which face of the carbonyl the nucleophile will add to. cyclohexanones begins to favor equatorial attack.

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The nucleophile may be any of a number of reagents, most commonly organometallic or reducing agents. This is because the axial C-O bond is a worse electron donor than a C–C bond, so axial attack is less favored In organic chemistry, the Cieplak effect is a predictive model to rationalize why nucleophiles preferentially add to one face of a carbonyl over another. Subsequent work has questioned its legitimacy (see Criticisms). In the Cieplak model, electrons from a neighboring bond delocalize into the forming carbon–nucleophile (C–Nuc) bond, lowering the energy of the transition state and accelerating the rate of reaction. The Cieplak effect is subtle, and often competes with sterics, solvent effects, counterion complexation of the carbonyl oxygen, and other effects to determine product distribution 3309577118

Phosphorus pentafluoride distinct types of P−F bonds (axial and equatorial): the length of an axial P−F bond is distinct from the equatorial P−F bond in the solid phase, but not Phosphorus pentafluoride is a chemical compound with the chemical formula PF5. It is a colourless, toxic gas that fumes in air. It is a phosphorus halide 3309577118

Trigonal bipyramidal molecular geometry whereas an equatorial atom has only two neighboring axial atoms at a 90° bond angle. For molecules with five identical ligands, the axial bond lengths tend In chemistry, a trigonal bipyramid formation is a molecular geometry with one atom at the

center and 5 more atoms at the corners of a triangular bipyramid. This is one geometry for which the bond angles surrounding the central atom are not identical (see also pentagonal bipyramid), because there is no geometrical arrangement with five terminal atoms in equivalent positions. Examples of this molecular geometry are phosphorus pentafluoride (PF5), and phosphorus pentachloride (PCl5) in the gas phase 3309577118

The seesaw geometry occurs when a molecule has a steric number of 5, with the central atom being bonded to 4 other atoms and 1 lone pair (AX4E1 in AXE notation). An atom bonded to 5 other atoms (and no lone pairs) forms a trigonal bipyramid with two axial and three equatorial positions, but in the seesaw geometry one of the atoms is replaced by a lone pair of electrons, which is always in an equatorial position. This is true because the lone pair occupies more space near the central atom (A) than does a bonding pair of electrons. An equatorial lone pair is repelled by only two bonding pairs at 90°, whereas a hypothetical axial lone pair would be repelled by three bonding pairs at 90° which would make the molecule unstable. Repulsion by bonding pairs at 120° is much smaller and less important. 3309577118 Substituents on a cyclohexane ring prefer to reside in the equatorial position to the axial. The difference in Gibbs free energy (ΔG) between the higher energy conformation (axial substitution) and the lower energy conformation (equatorial substitution) is the A-value for that particular substituent.

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