Conformational analysis of cyclohexane ppt

You should be able to quickly draw cyclohexane rings where axial and equatorial ties are easily identifiable and distinguishable. . Until now we have not described in detail the rotational path of the cyclohexane and what is the final result. We know that the best route (the lowest energy path) available goes through the half chair and requires an energy input of 10 kcal/mol. This transition state proceeds to a minimum of energy of the torsion boat, but this is not highly populated and generally plays little or no role in the structure or chemistry of the cyclohexan. However, the torsion boat can interconvert with another boat torsion equivalent (through the true conformation of the boat as a transition state) to give another structure of the chair, in which the sense of the ring puckering is reversed. This is significant in the cycloes themselves, because in this process axial and equatorial hydrogens are interconverted. Since this interconversion or ring quickly turns to room temperature, all hydrogen spend 50% of their time as axial hydrogen and 50% of their time as equatorial hydrogen, so that in average time all C-H ties of cyclohexane are equivalent. However, at any given instant, there are always two types of hydrogen. Since axial and equatorial ties are not equivalent, there are two positions not equivalent in which to place any substituent. We use the metilic group as an example, but the same concept applies to any substituent. Equatorial methyl cycloxia is the most stableWhen the flip ring occurs, however, it converts into axial methylcyclohexane. These two conformations are quickly balanced at room temperature, but can be frozen as compounds distinct to -78 degrees. Equatorial conofrmation is favoured in balance by a modest quantity because the axial isomer has about 1.8 kcal/mol of steric strain. This variety derives from the interaction of one of the hydrogen of the axial metilic group with each of the other two axial hydrogen on the same side of the ring, as illustrated above. Each of these sterical interactions is approximately equivalent to a gauche butane interaction of 0.9 kcal/mole, so the total is 1.8 kcal/mol. The point of the gauche butane comparison is that the H/H distance of hydrogen stericamente hindered is almost exactly the same in butane glacia as with axial methyl cyclohexane, except that there are two H/H interactions of this case. The disteric interactions in axial methylcyclohexane are called "1,3 diaxial interactions", because the interactions involve two atoms or axial groups (an H and a CH3 and the carbons carrying these atoms or groups are 1.3 related. The "primitive of EQUATORIALITY" demonstrates that any substitute pretext for occupying the EXTERNAL VALUE, if at all levels. In the case of POLY-SUBSTITUTED SOCIETY CICLOHEXAN NOT ALL PUBLICATIONS AND AQUATORIAL OGNI ISOMER, but the ISOMER will be the STABLE MOST IN WHO ALLOCCUPY EQUATORIAL POSITIONS (see examples below). Note that with the model of 1.4-disubstitution, the diequatorial agreement (most stable) is what we call "trans" isomer. in it, a substitute is "slant up" and a "slant down". The reversal of the ring gives a conformation in which the methyl substituents are anti (hehedron angle of 180) to each other, but this is still trans, and thisconformation is less stable because it has two axial substituents. There is another isomer of 1.4-dimethylcyclohexane, the issomero cis. We remember that cys and trans issomers are diastereoisomeri, they are not different conformations of the same isomer and can not be easily interconverted by a simple rotational process (a bond should be broken). In the isomro cis, here, a methyl group is equatorial and axial, and the pinball ring simply gives another equivalent conformation. Since a metilic is axial, this costs 1.8 kcal of steric strain. As a result, cys isomro is less thermodynamically stable than trans, which has no steric strain in the more stable conformation. The difference in energy is again, 1.8 kcal/mol. In the cys isomro, a substitute is vertically up (or down) and the other tilt (or down). So both bet, in general, in the same direction, that is, both up and down. 1,3-Dimethylcycloethane In the 1.3-disubstitution model (both it is dimethyl or any other 1.3-dibsubstitution), both groups can be equatorial only when they are both cys. So the issomero cis ismore stable isomer in this case. Flipping ring gives a conformation of the issomero cis which has both axial methylenes. Worse than this, they are both on the same part of the ring, so it is no longer an axial methyl/axial hydrogen interaction longer, it is an axial methyl/axial methyl interaction, which is sterically much worse. As a result, this ring lap is too energeticly difficult, and this conductor can be overlooked in him conformative analysis. The trans-1,3-dimethylcyclohexane isomer, on the other hand, has a methyl axial in both the rings-flipane conformers, so that it is less stable than the issomero cis from 1.8 kcal/mol. Both trans-1,4-dimethylcycloxane and cys-1,3-dimethylcycloxane essentially have the same energy, since none of them has any tension at all. The 1.2-disubstitution model is very similar to model 1.4, as the two groups can be equatorial only if they are trans, so the trans isomer is more stable than the cys. The diaxial trans conformer has 3.6 kcal of steric strain, of course and is much less favored than the diequatorial conductor. The issomero cis is less stable than the trans because in it, a metilic must be axial. The cis isomer is therefore less stable than the 1.8 kcal trans. The key difference between models 1.2 and 1,4, is that in the diequatorial 1.2 conformation, the methyl groups are gauches as in butane gauches (remember that the gauche essentially implies a dihedral angle of 60 degrees). As a result, this diequatorialis no longer free from strains, such as diequatorial conformation 1.4-trans, where methylenes are far away. Isomero 1,2-diequatorial is 0.9 kcal/mol less stable than the isomer 1.4-diequatorial, because of this gauche-like butane interaction (refer that the issomero gauche in butane is destabilized exactly by this amount.) return to the top of the page on the next return page to the bauld home page conformational analysis of disubstituted cyclohexane ppt

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