PHARMACEUTICAL ORGANIC CHEMISTRY-II- BP301T

UNIT: 5 Cycloalkanes

CLASS: 4

TOPIC: Cycloalkanes

STABILITY OF CYCLO-ALKANES

A stable organic compound means it is very less reactive. By the term stability we get an idea about chemical reactivity of a compound. To describe stability of cycloalkanes some very famous theoretical concepts are there viz.
Bayer Strain Theory
Sachse Mohr Concept
Coulson and Moffitt's modification

Bayer Strain Theory

Adolf von Baeyer, a German chemist and a Nobel prize winner from university of Munich, Germany in 1885 proposed a theory to explain the relative stability of the first few cycloalkane. The theory based on following facts. . Cyclo-alkanes are saturated compounds. So all the carbons should have normal tetrahedral angle of 109.5^0 . . Any deviation of bond angles from the normal tetrahedral value would, impose a condition of internal strain on the ring called angle strain. . More the value of angle strain less stable the compound is. . He assumes that all the cyclo-alkanes are flat and coplanar that means they are two dimensional and present in one plane.	 A.V. Baeyer

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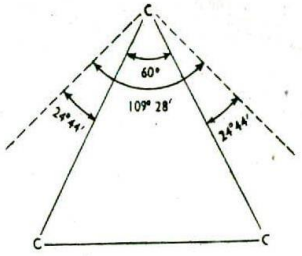
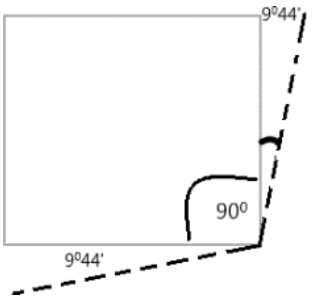
Case-Study:-

1.Cyclopropane:-



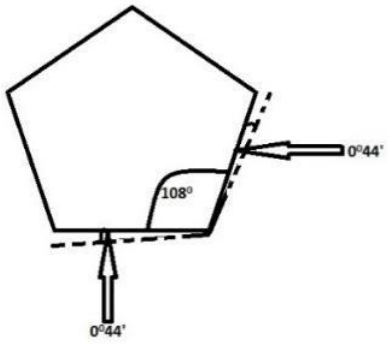
In cyclopropane, the three carbon atoms occupy the corners of an equilateral triangle. Thus cyclopropane has C—C—C bond angles of 60°. This implies that the normal tetrahedral angle of 109.5° between any two bonds is compressed to 60°, and that each of the two bonds involved is pulled in by 1/2(109°28'—60°)=24°44'.
The value 24°44' then represents the *angle strain* or the deviation through which each bond bends from the normal tetrahedral direction.

2. Cyclo-butane:-



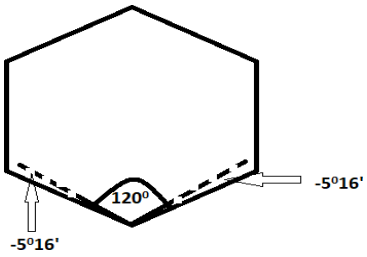
Here the four carbon atoms occupy the corners of a square. So it has C—C—C bond angles of 90° & angle strain on each bond is 1/2(109°28'-90°) = 9°44'.

3. Cyclo-Pentane:-



Here the five carbon atoms lie at the corners of a regular pentagon. Thus cyclopentane has C—C—C bond angles of 108°. The angle strain which each bond fills is 1/2(109°28'— 108°) = $0^0$44'.

4. Cyclo-hexane:-



In cyclohexane the six carbon atoms occupy the corners of a regular hexagon. Thus cyclohexane has C—C—C bond angles of 120°. The angle strain will be 1/2(109°28'— 120^0)= -5°16'

Similarly, in the case of cyclo-heptane the deviation from the normal tetrahedral angle is -$9^0$33'. In the case of cyclooctane it is - 12°46'.

Derivation:-

Sl.No	Name	Angle strain
1	Cyclo-propane	+24°44'
2	Cyclo-butane	+9°44'.
3	Cyclo-pentane	+$0^0$44'.
4	Cyclo-hexane	-5°16'
5	Cyclo-heptane	-$9^0$33'
6	Cyclo-octane	- 12°46'

1. The + sign indicates that the C—C bonds have to be compressed to satisfy the geometry of the ring. The - sign indicates that the C—C bonds have to be widened to satisfy the geometry of the ring. *Whether the angle strain is positive or negative, its magnitude determines the extent of strain in the ring.*
2. The deviation from the normal tetrahedral angle is *maximum* in the case of cyclopropane. So, it is most unstable and open up on the slightest provocation and thus releasing the strain within.
3. The deviation from the normal tetrahedral angle is *minimum* in the ease of cyclopentane. This implies that cyclopentane is under least strain and should be most stable
4. According to the Baeyer Strain Theory, cyclohexane and the higher cycloalkanes should become increasingly unstable and hence more reactive.

Drawbacks of Bayer-strain theory

1. The limitation of Bayer strain theory is that he assumed that all cycloalkanes are planar.
2. Baeyer was unable to explain the effect of angle strain in Larger Ring System.
3. According to Baeyer Cyclopentane should be much stable than cyclohexane but practically it is reversed.
4. Larger ring systems are not possible according to Baeyer as they have negative strain but they exist and much stable. - Larger ring systems are not planar but puckered to eliminate angle strain.