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Baeyer strain theory

- Van't Hoff and Lebel proposed tetrahedral geometry of carbon.
- The bond angel is of 109° 28′ (or 109.5°) for carbon atom in tetrahedral geometry (methane molecule).
- On this basis, he proposed angle strain theory.

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Conformations of Cycloalkanes

- The bond angles in straight chain alkanes is normally 109.5°. This is expected for a tetrahedral arrangement of bonds that are not restricted.
- However, when the carbon atoms form part of a ring, the angle will be controlled by the requirements of the ring.

BOND ANGLE=

 $(n - 2) \times 180^{\circ}$

[where **n** is no of carbon in ring]

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BOND ANGLES in some cycloalkanes are as follows:

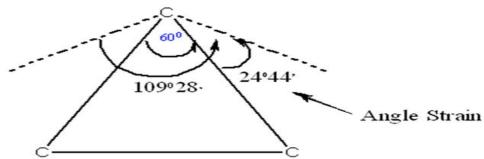


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Stability of Cycloalkanes

- ™ Bayer (1885) postulated a theory of angle strain for cycloalkanes in which the difference between a tetrahedral angle (109.5 °) and an internal angle of the appropriate polygon is used as a measure of stability.
- The deviation of bond angles from the tetrahedral angle causes the molecule to be strained and hence unstable compared with molecules with tetrahedral bond angles



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ANGLE STRAIN is Angle through which each of valency bond was deflected from normal direction in formation of rings. This is called as angle strain which determine stability of the ring

Angle strain = $1/2 (109^{\circ}28' - x)$

where **X**= internal bond angle

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Table 1.2 : Angle Strain In CycloAlk	kanes
--------------------------------------	-------

Compound	Bond Angle	Angle Strain
Cyclopropane	60°	24°44
Cyclobutane	90"	9°44
Cyclopentane	108°	0°44
Cyclohexane	120°	-5°16

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STABILITY AND ANGLE STRAIN RELATION

(Stability)

Cyclopropane Cyclobutane Cyclopentane and goes on

(Angle strain)

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Cyclopropane reaction

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TYPES OF STRAINS

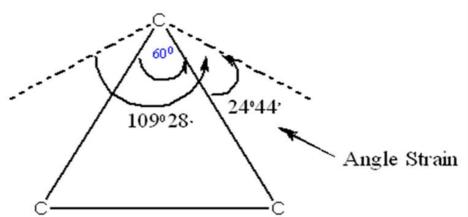
The stability of cycloalkanes are influenced by a combination of three factors:

- **Angle** strain
- CR Torsional strain
- Steric strain

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Angle strains

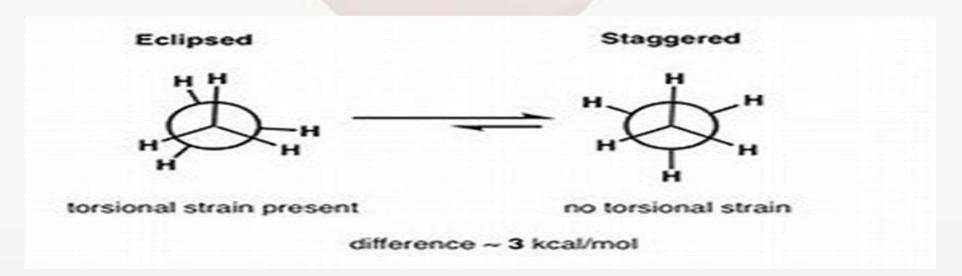
Angle through which each of valency bond was deflected from normal direction in formation of rings. This is called as angle strain which determine stability of the ring



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Torsional strain

The strain due to the eclipsing of bonds on neighbouring atoms. There is increase in energy when there are eclipsing interactions.

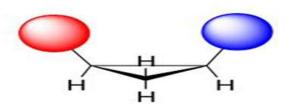


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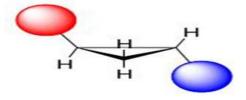
STERIC STRAIN

The strain due to the repulsive interactions when atoms approach each other too closely. There is increase in energy when atoms are forced too close to one another

 Steric strain focuses on the strain of functional groups bound due to size onto the cyclic ring. Because rings don't rotate freely in space like linear chains then energy is higher when they are on the same side. For example: cyclopropane



Higher Energy



Lower Energy

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Why does Baeyer theory fails?

The Baeyer theory fails for larger rings because:

- The angles that Baeyer used for each ring were based on the assumption that the rings of all cycloalkanes are planar.
- In fact, all cycloalkanes except cyclopropane are not planar (flat).
- The reality is that cycloalkanes tend to adopt puckered three dimensional conformations that allow all the bond angles to be nearly tetrahedral.

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