Carey Chapter 3 – Conformations of Alkanes and Cycloalkanes

Figure 3.5

Conformational Analysis

Cytosine (C) (from TGCA alphabet in DNA)

Hemoglobin

Thymidine – incorporated into DNA as “T”

Zidovudine (AZT) – incorporated into DNA instead of T – stops chain growth
3.1 Conformational analysis of Ethane

Since single bonds can rotate around the bond axis, different conformations are possible - conformational analysis.

Figure 3.1
(use SpartanModel)

3.1 Conformational analysis

Different 3-D depictions of Ethane

Wedge/dash  Sawhorse  Newman Projection

Rotation around the central C-C bond will cause the hydrogens to interact - rotamers or conformers.

Definitions

Gauche  Eclipsed  Anti
torsion angle 60°  torsion angle 0°  torsion angle 180°

Both gauche and anti conformers are staggered.

Eclipsed conformers are destabilized by torsional strain.
3.1 Conformational analysis of Ethane

3.2 Conformational analysis of Butane

3.3 Conformations of higher alkanes

Applicable for any acyclic molecule
3.4 Cycloalkanes – not planar

Cyclohexane

3.5 Cyclopropane and Cyclobutane

3.6 Cyclopentane
3.7 Conformations of Cyclohexane

Conformationally flexible (without breaking bonds)

Chair ↔ Boat ↔ Chair

3.7-3.8 Cyclohexane – axial and equatorial positions

3.9 Conformational inversion – ring flipping
3.10 Conformational analysis of monosubstituted cyclohexanes

Based on unfavourable 1,3-diaxial interactions

3.11 Disubstituted cycloalkanes - Stereoisomers

Cis-1,2-dimethylcyclopropane is less stable than the trans isomer

Cis-1,2-dimethylcyclohexane is less stable than the trans isomer

Cis-1,3-dimethylcyclohexane is more stable than the trans isomer

Cis-1,4-dimethylcyclohexane is less stable than the trans isomer

All based on interactions between substituents and other groups on the ring

3.11 Disubstituted Cyclopropanes
3.12 Disubstituted Cyclohexanes

Consider 1,2-; 1,3-; and 1,4-disubstituted isomers

*trans*-1,2-dimethylcyclohexane is more stable than the *cis* isomer.
*cis*-1,3-dimethylcyclohexane is more stable than the *trans* isomer.
*trans*-1,4-dimethylcyclohexane is more stable than the *cis* isomer.

3.13 Medium and large rings – not covered

3.14 – Polycyclic compounds – covering bicyclics

- Bicyclo[3.2.0]heptane
- Bicyclo[2.2.2]octane

3.15 Heterocyclic compounds

- Tetrahydrofuran
- Pyrrolidine
- Piperidine
- Morphine
- Ritalin
- Librium