**Stereochemistry**: The study of properties of matter in 3D
**Constitutional isomers**: Different compounds with the same molecular formula. For example, $C_4H_{10}$ has two constitutional isomers

*n*-butane  *i*-butane

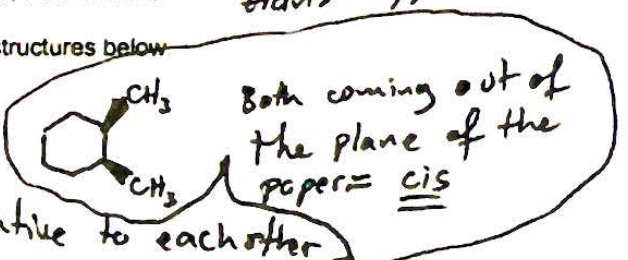
or 2-methylpropane.

**Stereoisomers**: Two or more compounds with identical molecular formula and arrangement of atoms in space. However, they differ from each other in the spatial orientation of groups

cis = same side
trans = opposite sides

For example: **1,2-dimethylcyclohexane** has two stereoisomers, *cis* and *trans*

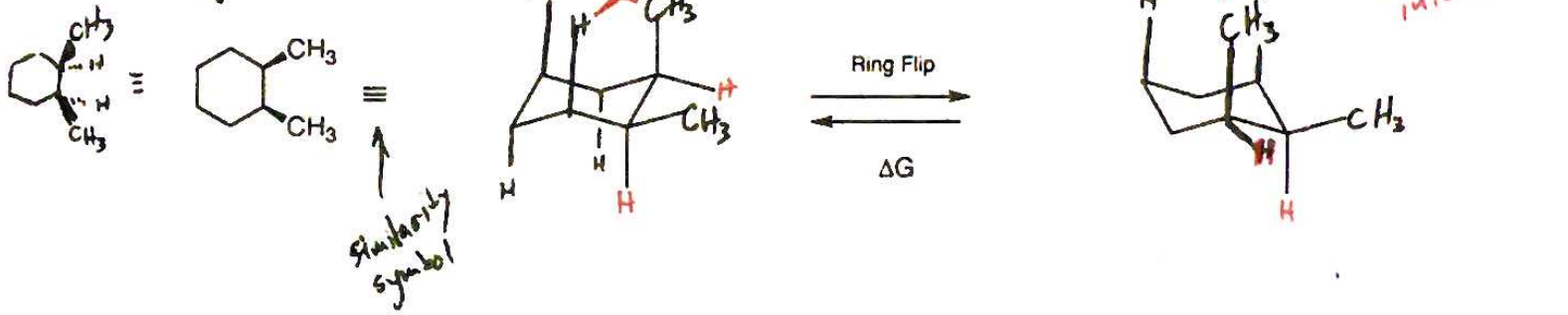
To differentiate the two isomers by name, consider one of the structures below




Name: cis-1,2-dimethylcyclohexane

prefix indicates position of $CH_3$ relative to each other

Fill in the missing H's and methyl groups to show the chair structures of the **1,2-dimethylcyclohexane** stereoisomer and its conformer, as they interconvert by a chair ring flip.




The *A* value for each H/$CH_3$ *1,3-diaxial* interaction is 0.9 kcal/mol, *i.e.* each 1,3-diaxial interaction raises the strain energy of the molecule due to steric hindrance

What is the strain energy of each conformational isomers?

$2 \times 0.9 = 1.8$ kcal/mol for both

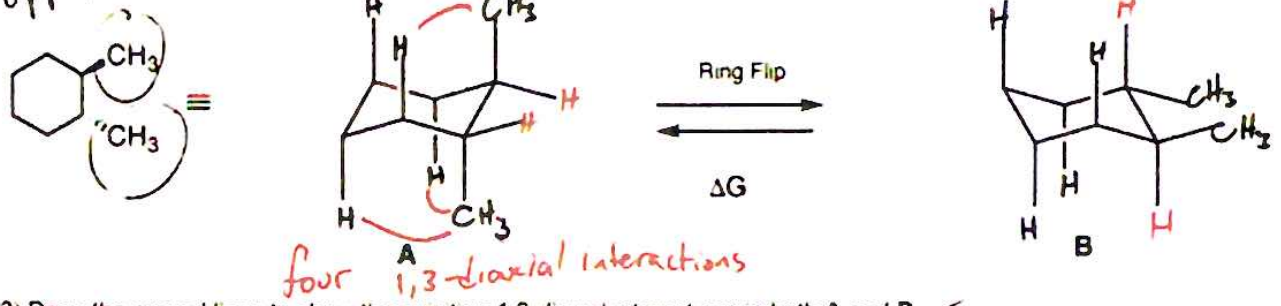
What is ΔG at equilibrium?

Zero

∴ At equilibrium, no preference for either conformer.

1) Fill in the missing H's and methyl groups to show the chair structures of *trans*-1,2-dimethylcyclohexane as they interconvert by a chair ring flip. Note: 3 equitonal H's are not shown for clarity

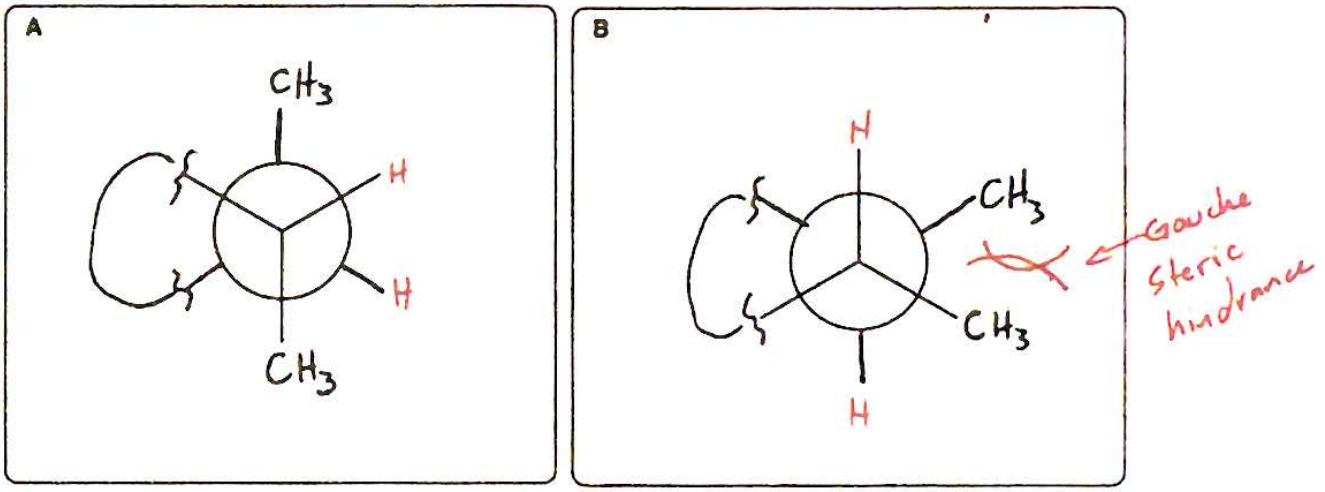
opposite sides.




four 1,3-diaxial interactions

2) Draw the curved lines to show the exisiting 1,3-diaxial interactions in both **A** and **B**. ✓

3) Draw the Newman Projection between carbons 1 and 2 in the ring (the ones bonded to the methyl groups) and identify any other sources of steric hindrance, if any




4) Consider the following Strain Values:
Each $CH_3/CH_3$ *gauche* interaction raises the internal energy by 0.9 kcal/mol
Each $H/CH_3$ *1,3-diaxial* interaction raises the internal energy by 0.9 kcal/mol
Each $CH_3/CH_3$ *1,3-diaxial* interaction raises the internal energy by 0.9 kcal/mol

What is the strain energy of **A** and **B**?

**A** = 3.6 kcal/mol

**B** = 0.9 kcal/mol

B is lower in energy & more favored @ equilibrium.

5) What is the relative energy difference between both chair conformational isomers above?

$\Delta G^\circ$ = −2.7 Kcal/mol