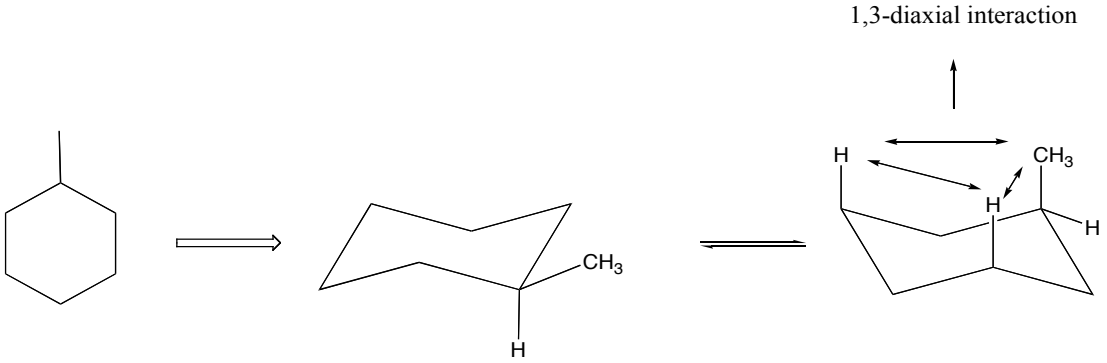
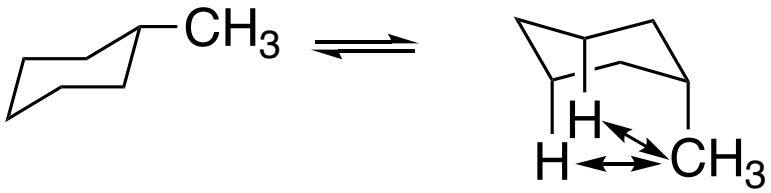
Substituted Cyclohexanes – Draw the most stable conformation



- Largest (bulkiest group close to ring) group placed equatorial – otherwise get unfavorable 1,3-diaxial interactions

- 1,3-diaxial interaction (steric effect) makes this conformation less stable.

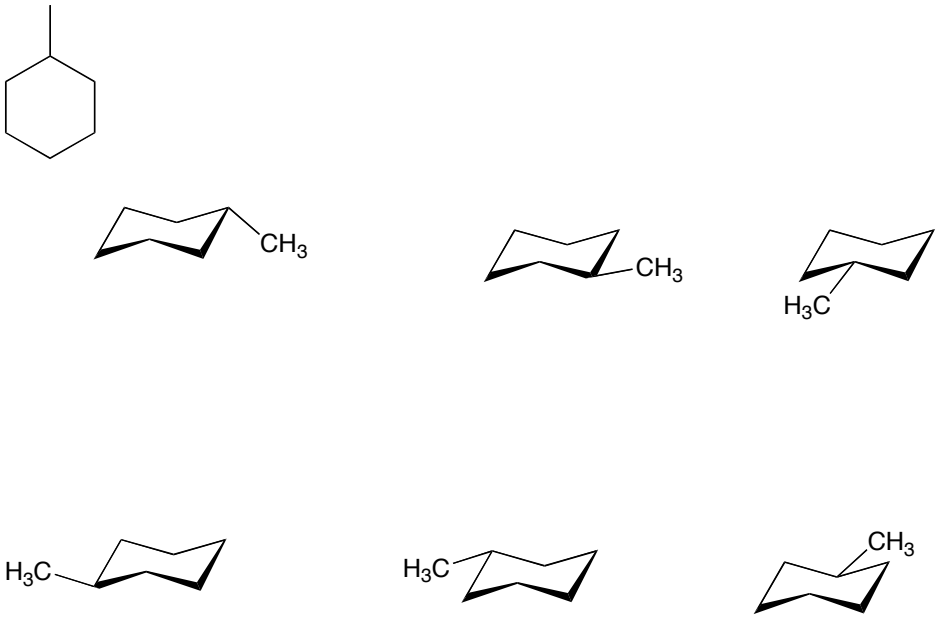


Equatorial methyl interaction
More stable

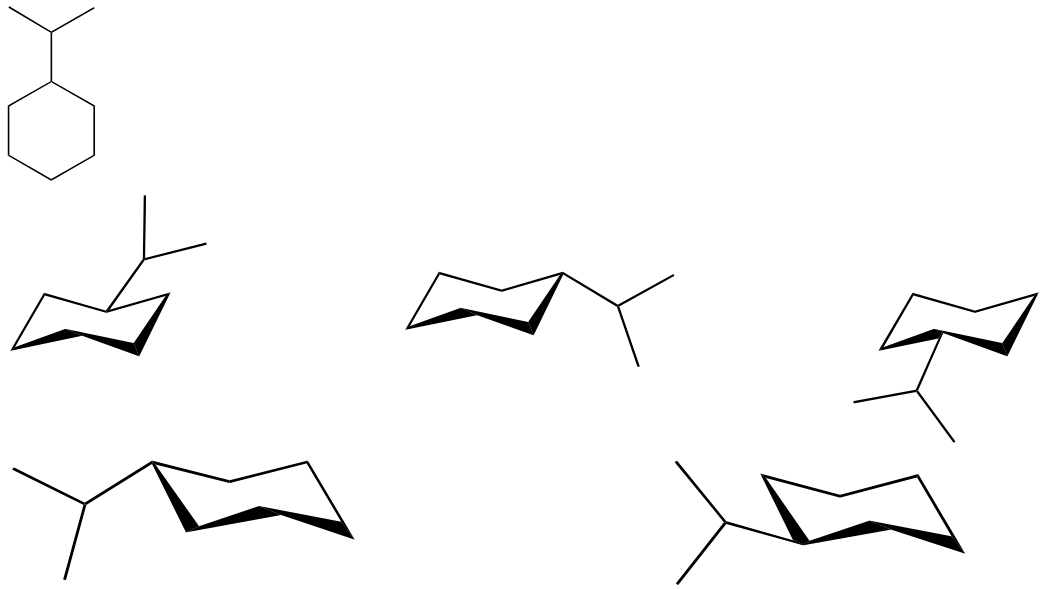
Axial methyl interaction
Less stable

Examples of Most Stable Conformation of Substituted Cyclohexanes :

1. Methylcyclohexane
   – 6 drawings of same molecule



2. Isopropylcyclohexane

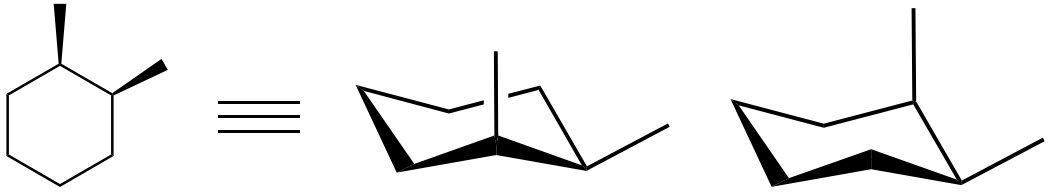


NB: For most stable conformation, largest group at equatorial position

Examples of Most Stable Conformation of Polysubstituted cyclohexanes:

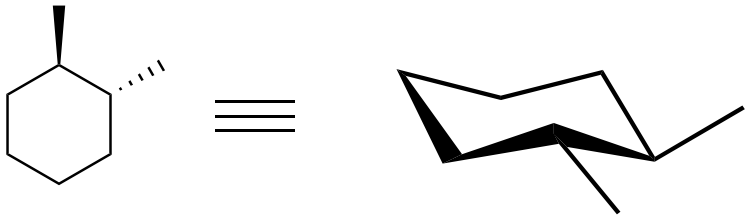
Examples:

1) cis-1,2-dimethylcyclohexane



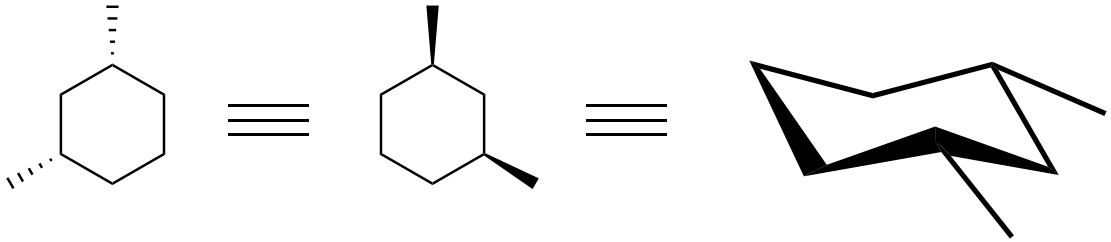
- One methyl group axial and one methyl group equatorial

2) trans-1,2-dimethylcyclohexane (a stereoisomer (diastereomer) of above structures)



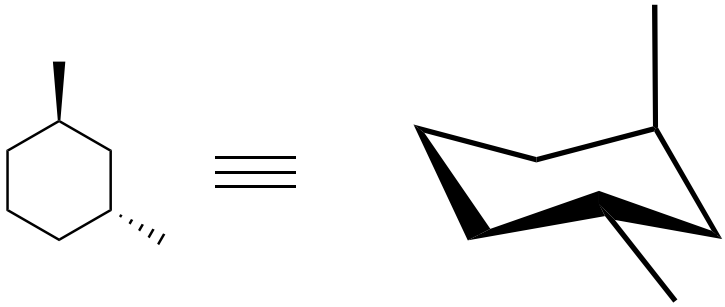
- Both methyl groups equatorial

3) cis-1,3-dimethylcyclohexane (a structural isomer of above structures)



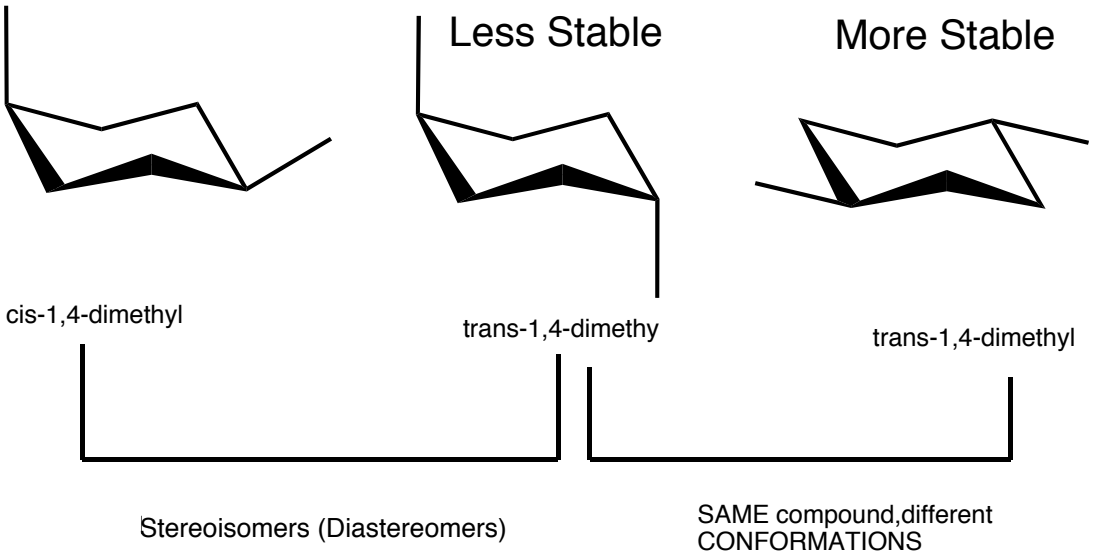
- Both methyl groups equatorial

4) trans-1,3-dimethylcyclohexane : a stereoisomer of above cis-1,3- dimethylcyclohexane

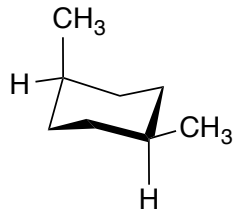


- One methyl group axial and one methyl group equatorial

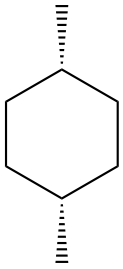
5) cis-1,4-dimethylcyclohexane and trans-1,4-dimethylcyclohexane:

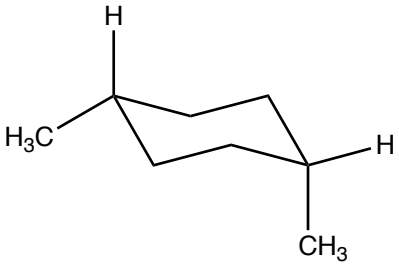


6) cis-1,4-dimethylcyclohexane:

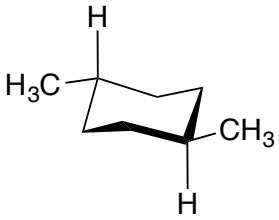


cis-1,4-dimethylcyclohexane

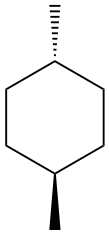


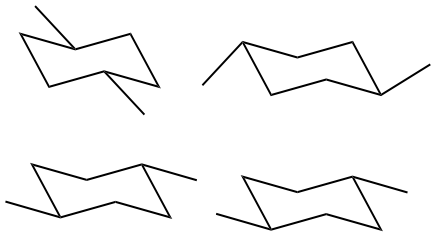


7) trans-1,4-dimethylcyclohexane:



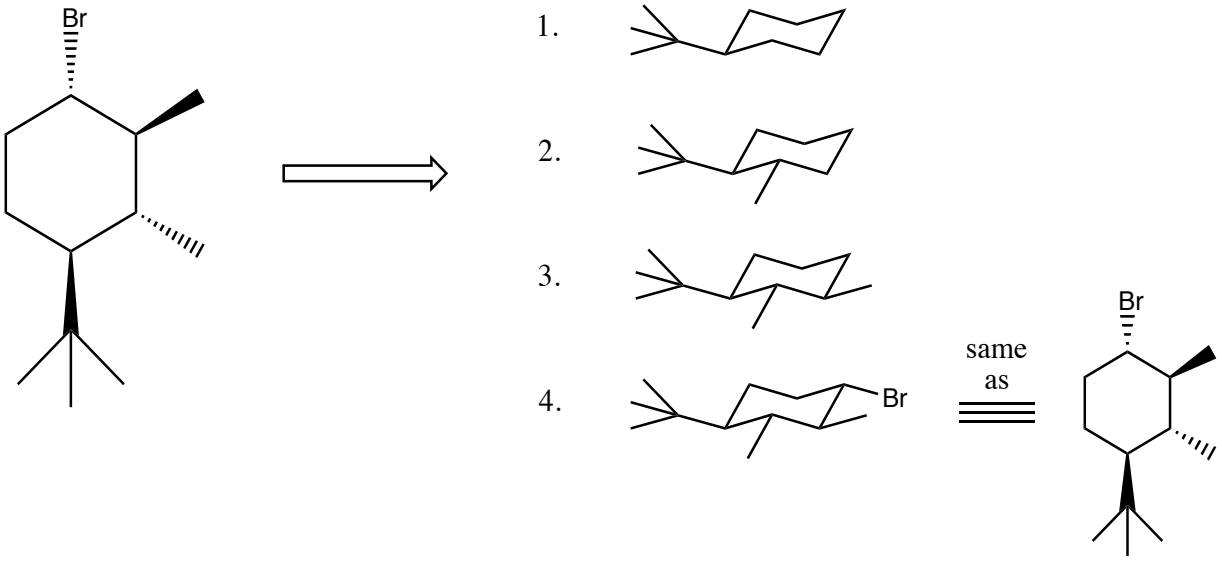
trans-1,4-dimethylcyclohexane





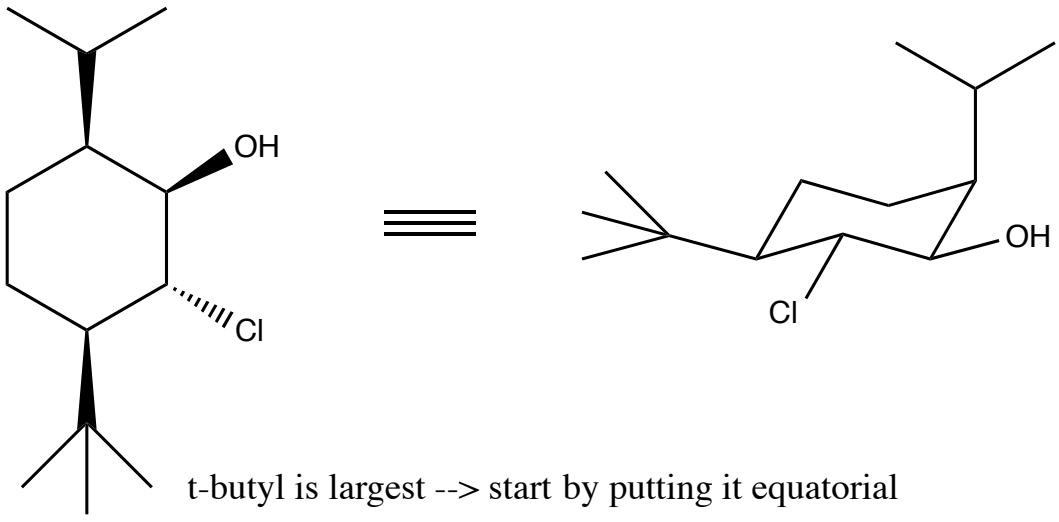
How to draw the most stable conformation of substituted cyclohexanes:

1. Start by drawing the chair conformation of cyclohexane
   Put the largest group in an equatorial position
2. Draw the next group(s) on the correct atom(s) with respect to the largest group in correct geometry



Note that the largest substituent (tertiary butyl) is placed in the equatorial position to avoid destabilizing 1,3-diaxial interactions

Another example:



t-butyl is largest --> start by putting it equatorial