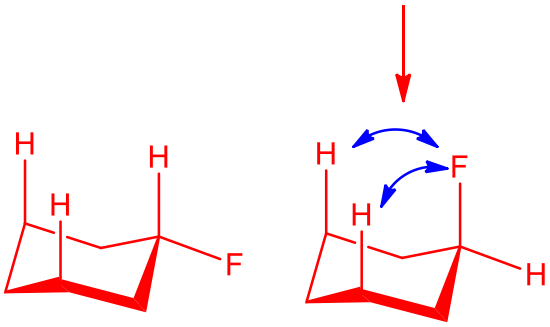
Exercise 8: - Conformational analysis and nomenclature of cyclohexanes

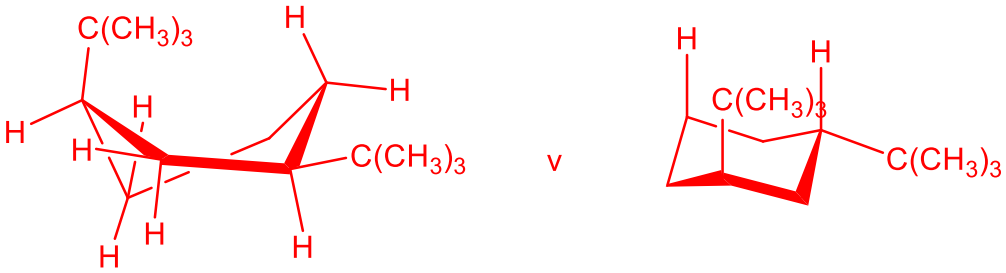
1. The axial conformation of fluorocyclohexane is 1.05 kJ/mol less stable than the equatorial conformation. What is the energetic cost of a 1,3-diaxial hydrogen-fluorine interaction?

2 1,3-diaxial interactions therefore
cost per H - F interaction = 1.05/2
= 0.525 kJ/mol



2. *trans*-1,3-Di-*tert*-butylcyclohexane is one of the few molecules that exists largely in a skew-boat conformation. Why?

The chair conformation would require an axial *tert*-butyl with at least 20 kJ/mol of steric strain. The skew-boat conformation reduces this strain:

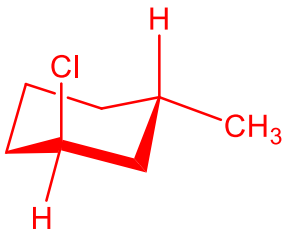


3. The following table lists the steric strain due to one hydrogen - substituent 1,3-diaxial interaction in some monosubstituted cyclohexanes:

Substituent	Strain (kJ/mol)	Substituent	Strain (kJ/mol)
Cl	1.09	CH_3	3.56
Br	1.15	CH_3CH_2	3.66
OH	1.96	$(CH_3)_2CH$	4,61

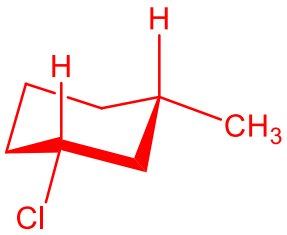
CH_3O	1.57	$(CH_3)_3C$	~10

a. Draw the most stable conformation of *trans*-1-chloro-3-methylcyclohexane:



b. Justify your decision using the principles of conformational analysis.
Both possible conformations are free of angle strain and of torsional strain. However the steric strain due to two H – Cl 1,3-diaxial interactions is 2.18 kJ/mol whereas that due to two H – CH_3 1,3-diaxial interactions is 7.12 kJ/mol

c. One of the two chair structures of *cis*-1-chloro-3-methylcyclohexane is more stable than the other by 15.5 kJ/mol. Draw the structure of the more stable structure.

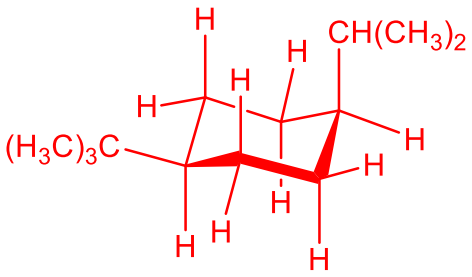


d. Calculate the energy cost of a 1,3-diaxial interaction between a chlorine and a methyl group.

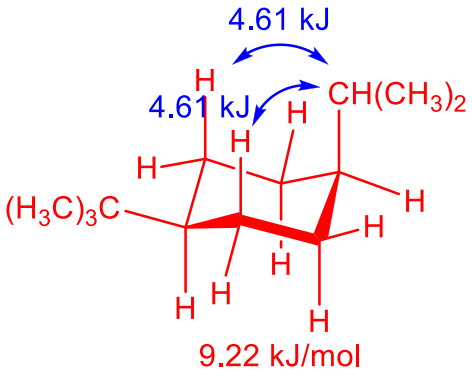
15,5 kJ/mol = 3,56 + 1,09 + (Cl – CH_3)

Thus the energy cost of a1,3 diaxial interaction between a chlorine and a methyl group is 10,96 kJ/mol.

e. Draw the most stable conformation of *cis*-1-*tert*-butyl-4-isopropylcyclohexane.



f. Calculate the strain in this molecule.

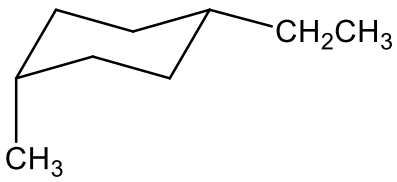


4. Name the following compounds :

a.

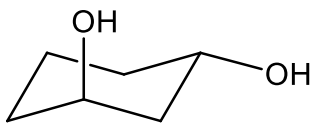
cis-3-isopropylcyclohexanol

b.



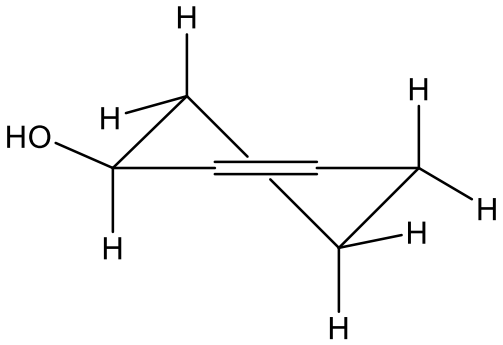
cis-1-ethyl-4-methylcyclohexane

c.



trans-1,3-cyclohexanediol

d.



2-cyclohexenol