

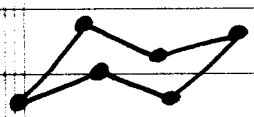
- ① CYCLOHEXANE
- ② PROPERTIES OF ALKANES
- ③ REACTIONS/SOURCES/IMPORTANCE
- ④ STEREOCHEMISTRY

READ 2.9, 2.10, 3.1, 3.2

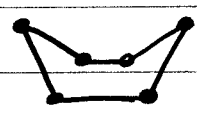
PROBLEMS 2.12-2.15, 2.38-2.61

+ web worksheets

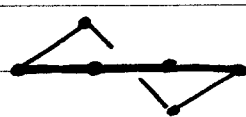
① CYCLOHEXANE - conformations



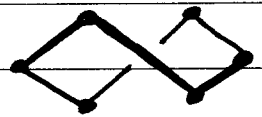
CHAIR



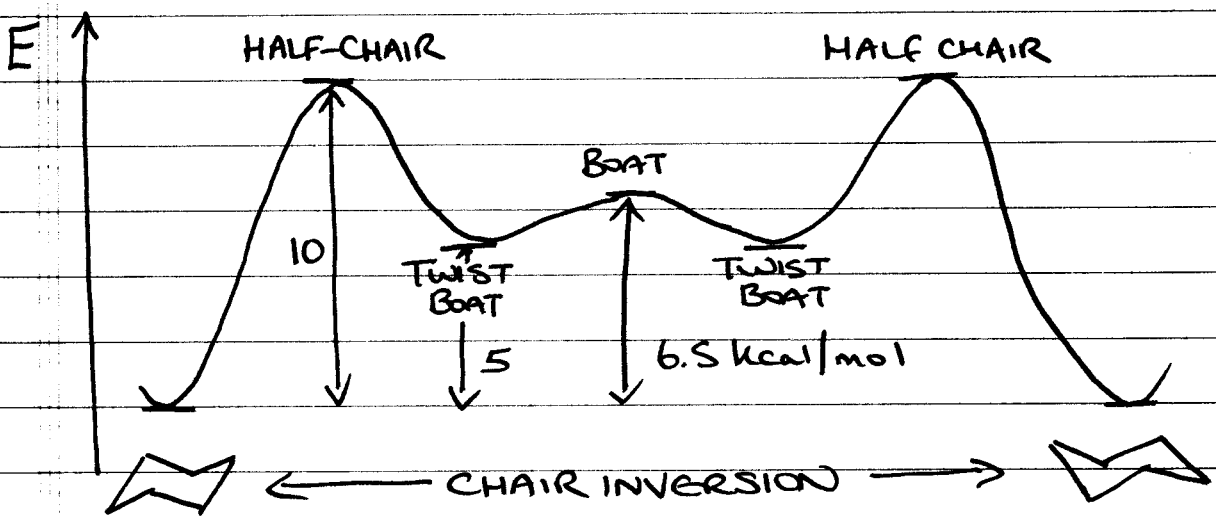
BOAT



TWIST CHAIR



TWIST BOAT

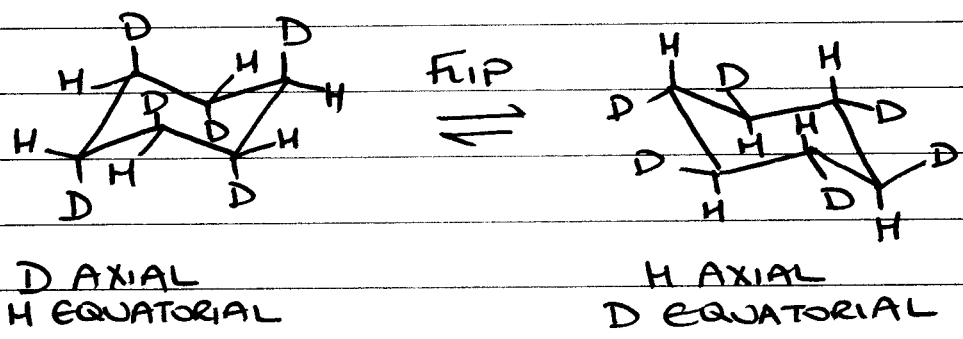


AT RT, CHAIR > 99.99% of EQUILIBRIUM MIXTURE

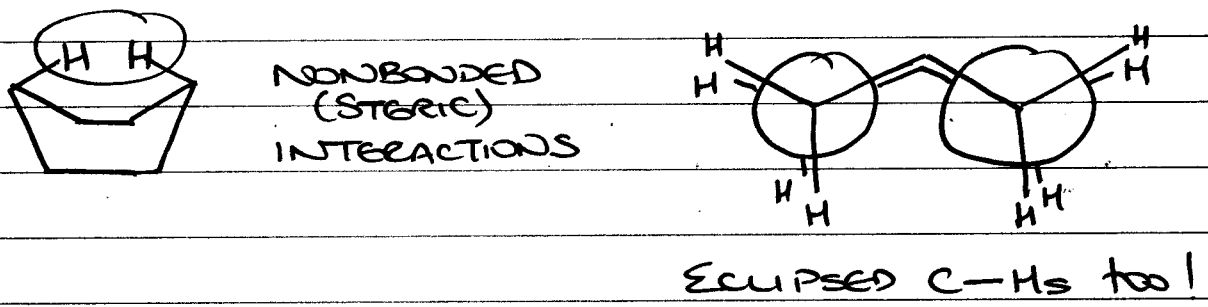
CHAIR FLIP



### SWITCHES AXIAL & EQUATORIAL POSITIONS

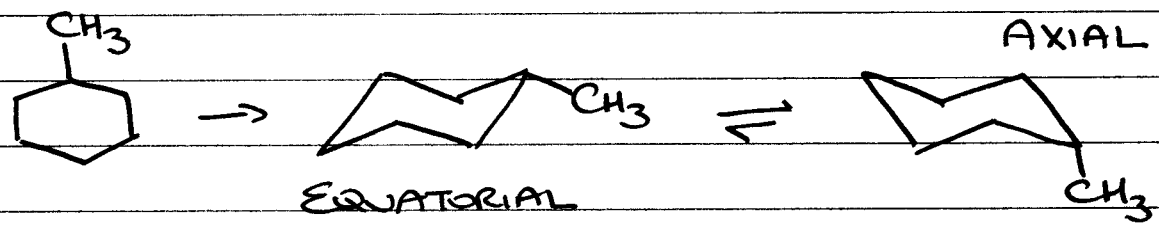


### A CLOSER LOOK AT THE BOAT CONFORMATION



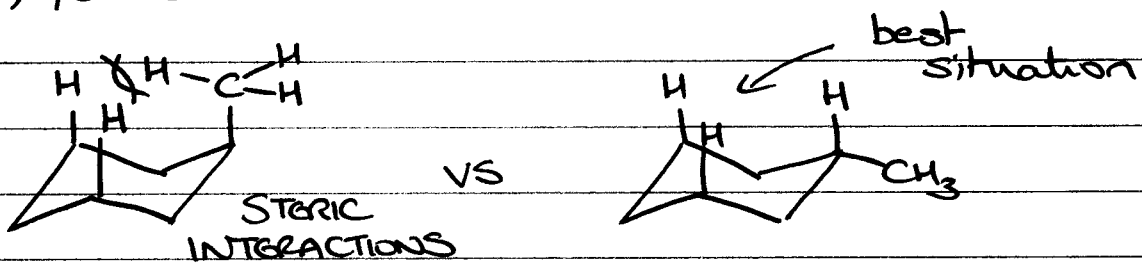
### - SUBSTITUTED CYCLOHEXANES

consider methylcyclohexane

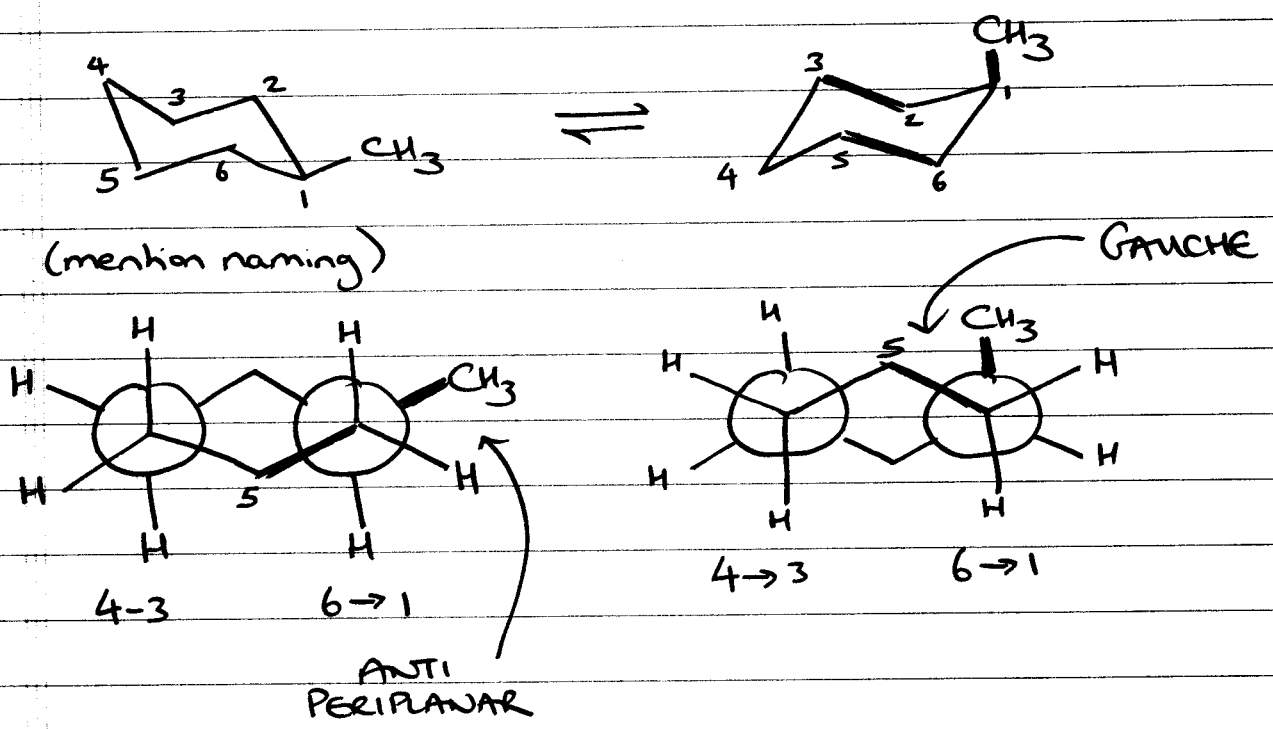


Which is more stable?

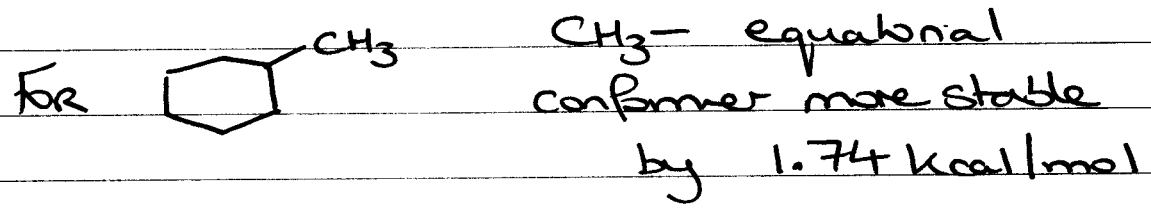
### (i) 1,3-DIAXIAL INTERACTIONS



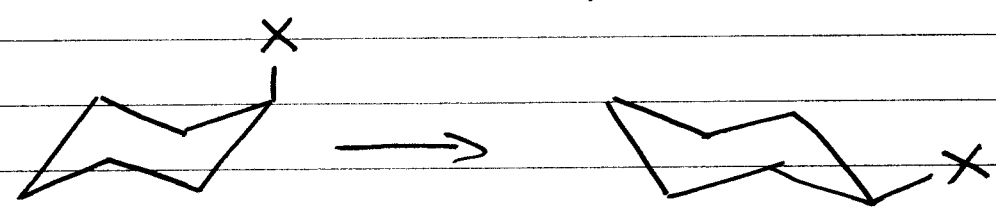
(ii) GAUCHE INTERACTIONS



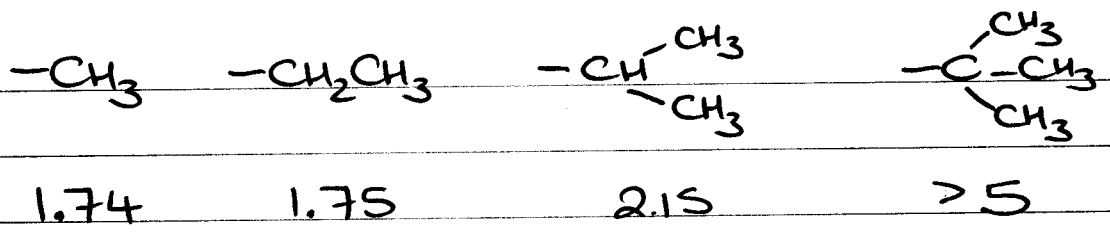
In general, conformer in which largest substituent is equatorial will be the most stable.



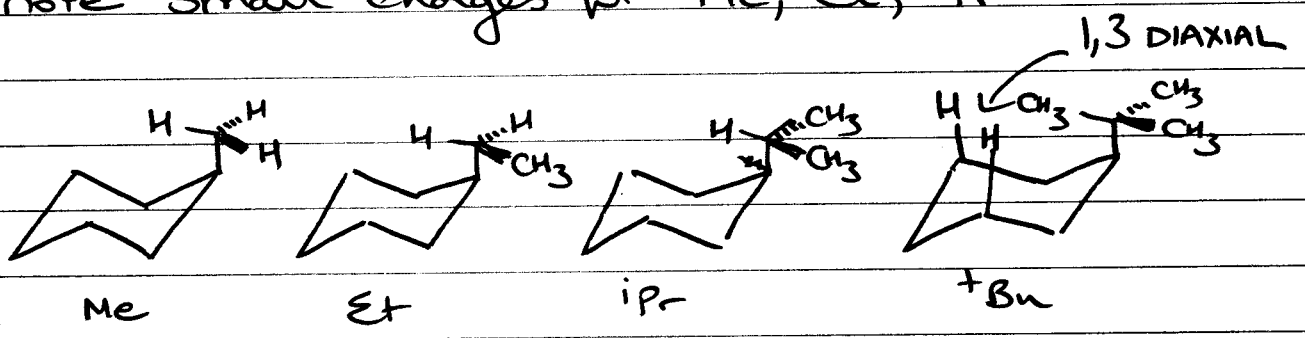
A VALUES → measure of thermodynamic preference for equatorial position.



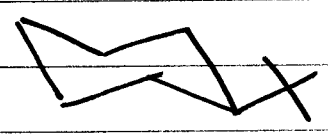
NEGATIVE of  $\Delta G$  change for AXIAL → EQUATORIAL, so A values are usually positive



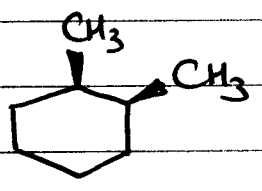
note small changes for Me, Et, iPr



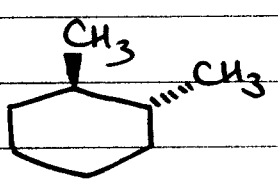
tBu ⇒ LOCKING GROUP  
overwhelming pref for equatorial position



- DISUBSTITUTED CYCLOHEXANES



same side cis  
cis-1,2-dimethylcyclohexane

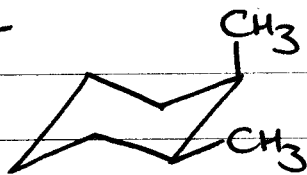


opposite side trans  
trans-1,2-dimethylcyclohexane

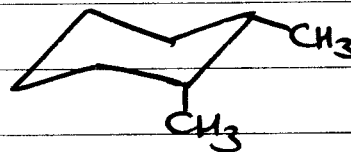
NOTE: when converting to CHAIR form I e<sup>iii</sup>  
have nothing to do with AXIAL/EQUATORIAL  
or UP/DOWN

5

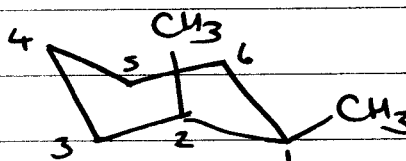
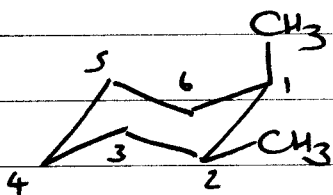
cis



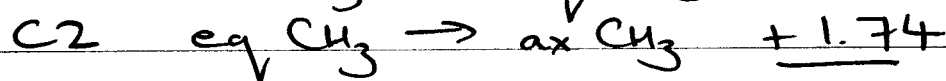
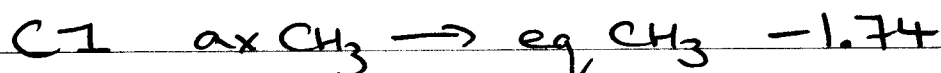
same as



RING-FLIP



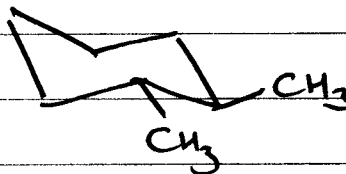
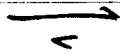
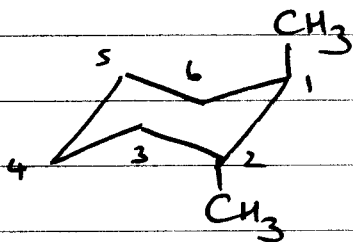
What is  $\Delta G$  for this equilibrium?



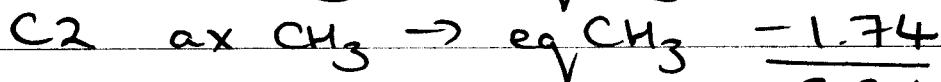
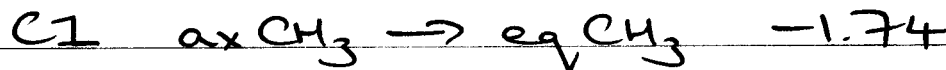
0 kcal/mol

So, 50:50 mixture.

trans



What is  $\Delta G$  for this equilibrium?



-3.5 kcal/mol

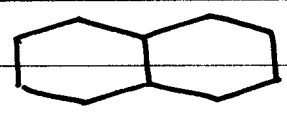
(actually -2.6 kcal/mol)

(A values generally ADDITIVE)

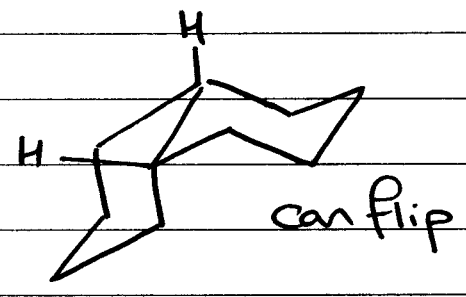
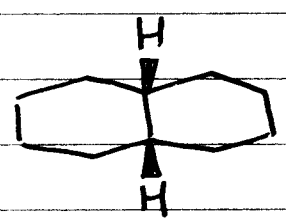
So, conformer with two equatorial methyls is favored.

Do same for 1,3- and 1,4- cis & trans dimethylcyclohexanes

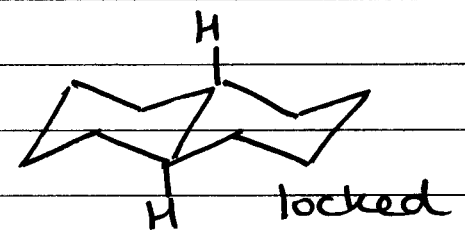
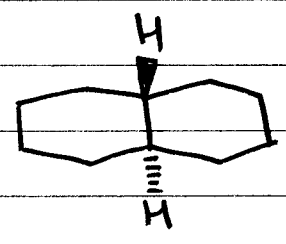
- DECALINS



cis-decalin



trans-decalin



② PROPERTIES OF ALKANES

as MW increases, m.p. & b.p. increases

INTERMOLECULAR INTERACTIONS

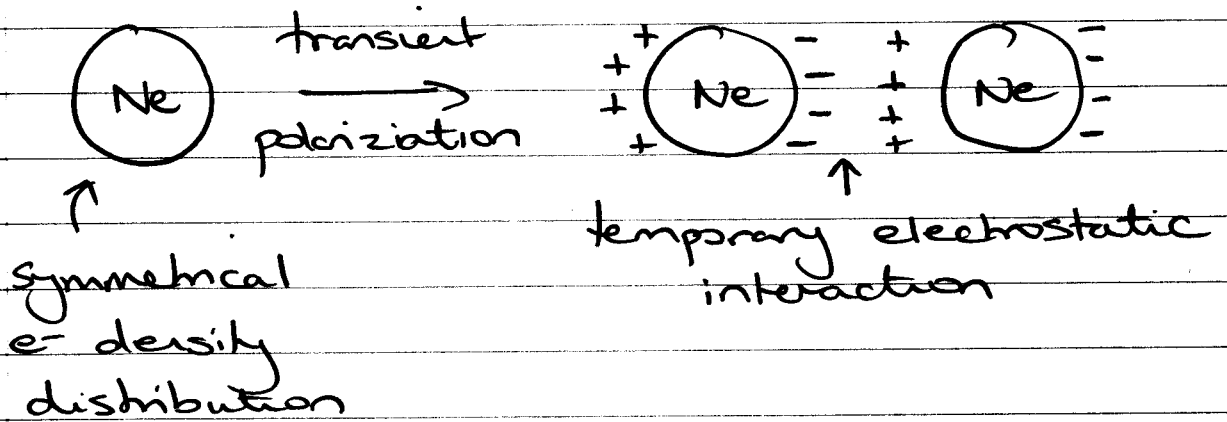
- ionic
  - hydrogen bonding
  - dipole-dipole
  - dipole-induced dipole
  - induced dipole-induced dipole
- ↓ decreasing strength

also called DISPERSION / LONDON forces

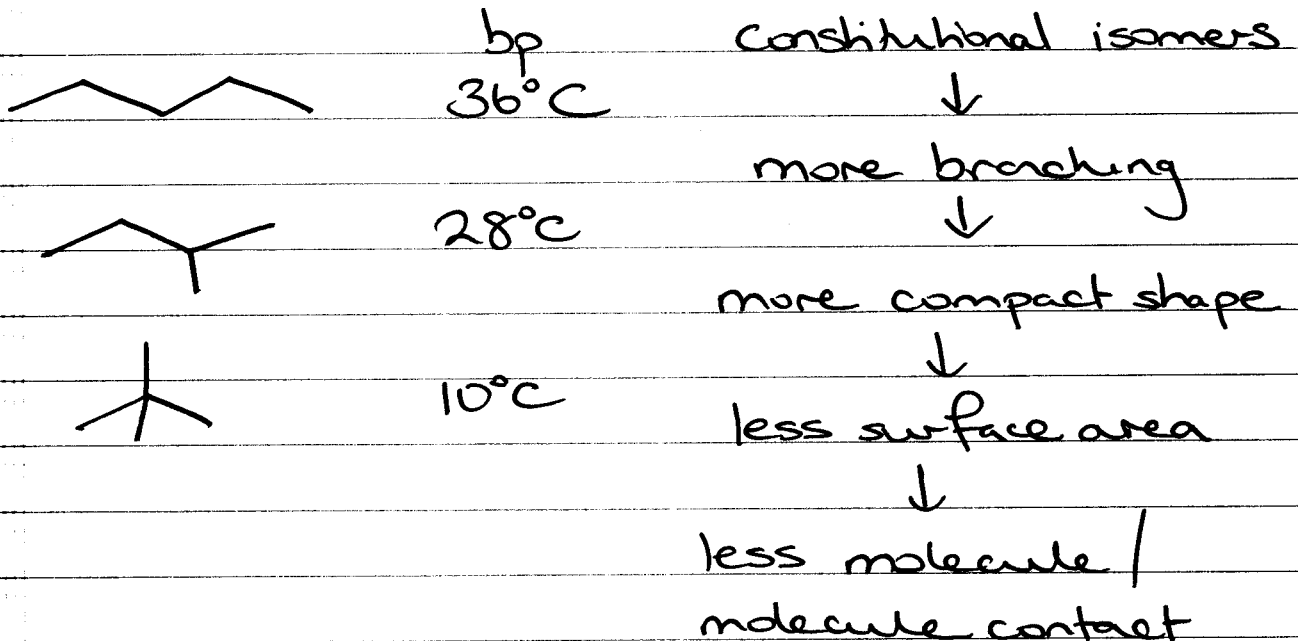
Reason why low MW non-polar substances can be liquified.

He 4K , Ne 27K

Bigger e<sup>-</sup> clouds, stronger forces



consider:



8

③ Reactions / Sources / Importance

↳ read sections 2.9, 2.10  
(and look over associated questions)

④ STEREOCHEMISTRY

next time....