

IS IT



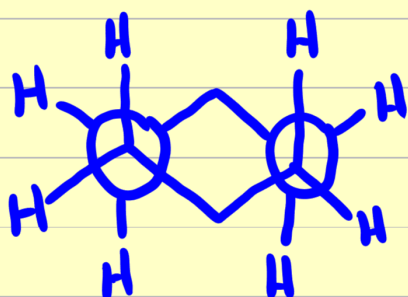
CHAIR

OR



??

BOAT



STAGGERED

∴ FAVOURED



ECLIPSED

∴ DISFAVOURED

DIFFERENCE IS $\sim 6.5 \text{ kcal/mol}$ (27 kJ/mol)

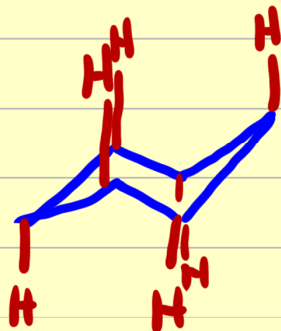
- IN FACT, THERE'S A TWISTED BOAT STRUCTURE ACTUALLY BETTER THAN THE BOAT BY $\sim 1.5 \text{ kcal}$

- CONCLUSION - WE ONLY HAVE TO WORRY ABOUT CHAIR CONFORMATIONS OF CYCLOHEXANES

- BOAT WILL EXIST TRANSIENTLY,
BUT IT WON'T STAY.

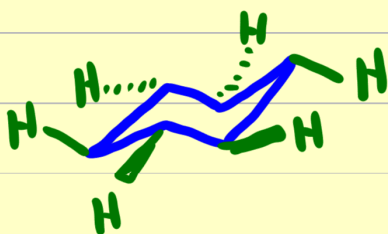
- SUBSTITUENTS ON CYCLOHEXANE

- TWO TYPES



- ALTERNATE STRAIGHT UP,
AND STRAIGHT DOWN.

CALLED AXIAL

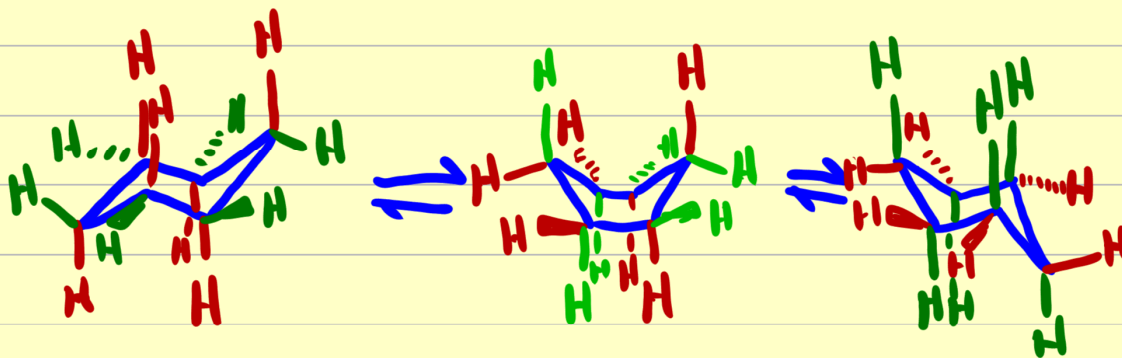


- ALTERNATING A BIT UP
AND A BIT DOWN, BUT
MOSTLY NEAR THE AVERAGE
'PLANE' OF CYCLOHEXANE

- CALLED EQUATORIAL.

- THESE ARE EXCHANGING AT ROOM TEMP

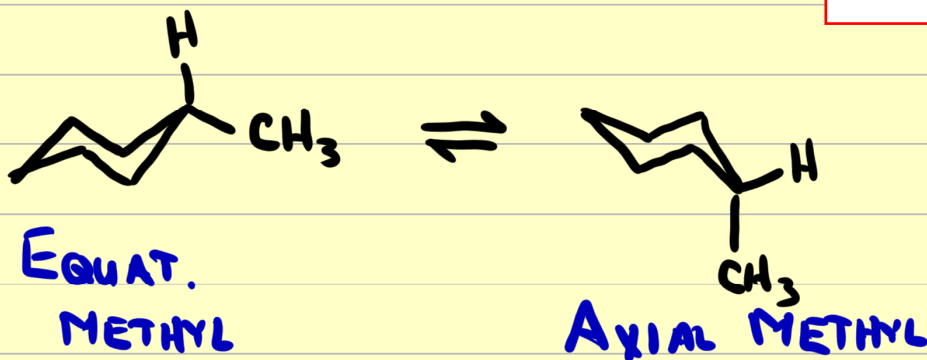
- AXIAL ONES BECOMING EQUATORIAL
AND VICE-VERSA



∴ ALL 12 H'S IDENTICAL.
 (BARRIER 10-11 kcal, 45 kJ/mol)

molecule can easily overcome this at room temperature, so this equilibration is happening >100 times per second

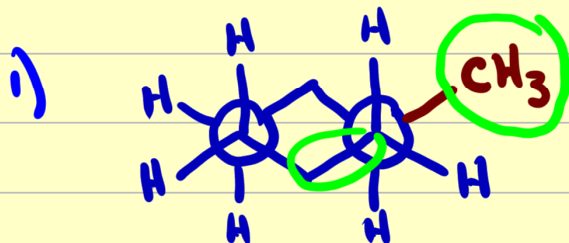
MONOSUBSTITUTED CASES.



that's 1.7 kcal/mol

THIS ONE IS MORE STABLE BY 1.7 kcal/mol
 (7 kJ/mol) ~ 20:1 AT RT.

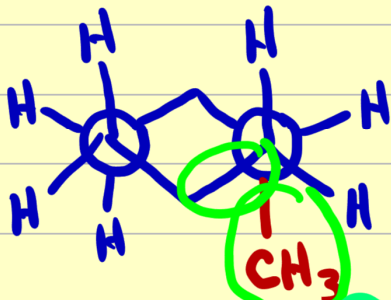
- TWO REASONS.



- ANTIPERIPLANAR RELATIONSHIP
 - BEST POSSIBLE

in equatorial conformation

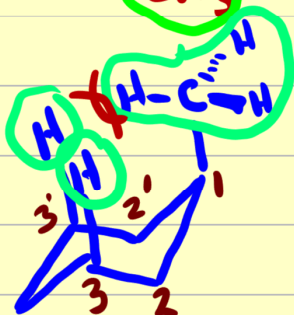
but, in the axial conformation



- SYNCLINAL (OR GAUCHE) RELATIONSHIP

- NOT QUITE AS STABLE

2)



- THERE ARE SLIGHT REPULSIVE 1,3-DIAXIAL INTERACTIONS

-all groups >H in size favour being equatorial, but not to the same degree

· DIRECTION IS THE SAME, BUT ENERGY DIFFERENCE DEPENDS ON GROUP SIZE

- Br (0.5 kcal/mol)

about 2.3:1 at room temp

- C(CH₃)₃ (4.5 kcal/mol) > 3000:1

∴ THE LARGER THE GROUP, THE MORE IT 'WANTS' TO BE EQUATORIAL.