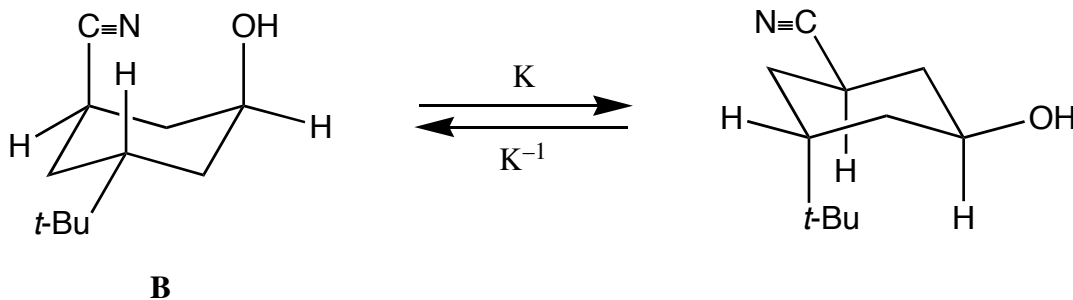
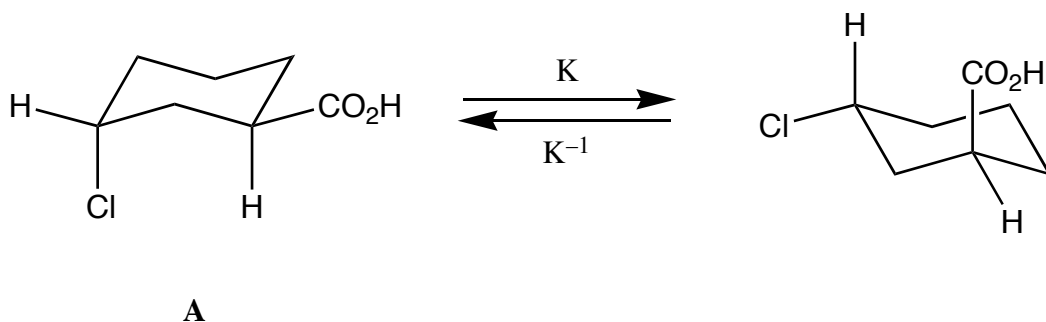


Supplemental Problems 2

CHEM 30A : Prof. Y. Rubin

Fall 2003

For the following substituted cyclohexanes, **A** and **B**, calculate the conformational energy differences, the equilibrium constant K , and the percentages of each conformer at room temperature. (NOTE : $25^\circ\text{C} = 298\text{ K}$).



For **B**: $DG^0 = (5.5 - 0.2 - 1.0) = +4.3$
 $K = 7.0 \times 10^{-4}$ ($K^{-1} = 1425$)
 99.93% (t-Bu equatorial; -OH, -CN axial)
 0.07% (t-Bu axial; -OH, -CN equatorial)
 (Note: A-value for t-Bu = 5.5)

For **A**: $DG^0 = -RT \ln K$
 $(1.4 - 0.5) = +0.9 = -RT \ln K$
 $K = e^{-0.9/RT}$
 $K = 0.22$ (i.e., $K^{-1} = 4.57$)
 82% (-CO₂H equatorial; -Cl axial)
 18% (-CO₂H axial; -Cl equatorial)

Answers