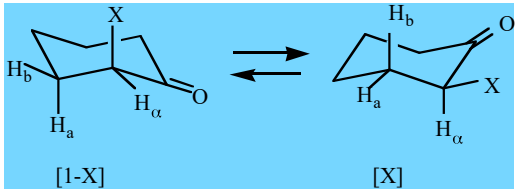
CALCULATING CONFORMATIONAL FREE ENERGY USING COUPLING CONSTANTS

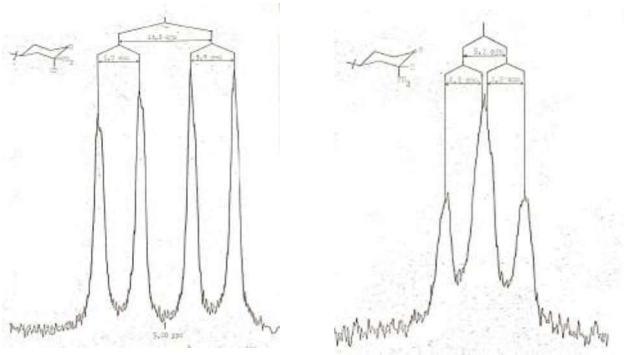


Average $J_{H\alpha Hb} = J_{aa}[X] + J_{ee}[1\text{-}X]$

Average $J_{H\alpha Ha} = J_{ae}[X] + J_{ea}[1\text{-}X]$

The values of J_{aa}, J_{ee}, J_{ae} and J_{ea} are determined from Conformationaly rigid cyclohexanone systems

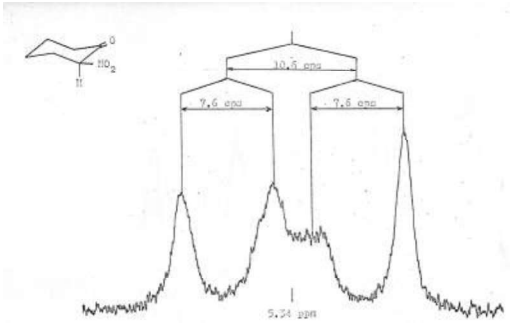
NMR OF 4-t-BUTYL-2-NITROCYCLOHEXANONE



$J_{aa} = 12.6$ Hz
$J_{ae} = 5.7$ Hz

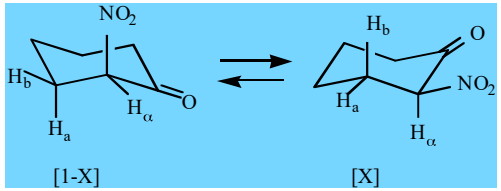
$J_{ea} = 5.2$ Hz
$J_{ee} = 4.3$ Hz

NMR OF 2-NITROCYCLOHEXANONE



Average $J_{H\alpha Ha} = 10.6$
Average $J_{H\alpha Hb} = 7.6$

CALCULATING THE CONFORMATIONAL FREE ENERGY OF 2-NITROCYCLOHEXANONE USING COUPLING CONSTANTS



Average $J_{H\alpha Hb} = J_{aa}[X] + J_{ee}[1\text{-}X]$
$10.6 = 12.6\,[X] + 4.3\,[1\text{-}X]$
$X = 0.76$
$K = [X]/[1\text{-}X] = 0.76/0.24 = 3.17$
$\Delta G^{\#} = -RT\ln K = -(2.3)(2)(298)\log 3.17 = 0.73$kcal/mol