Conformational Analysis

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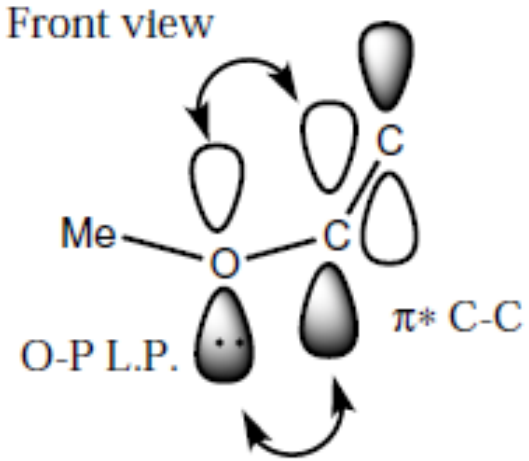
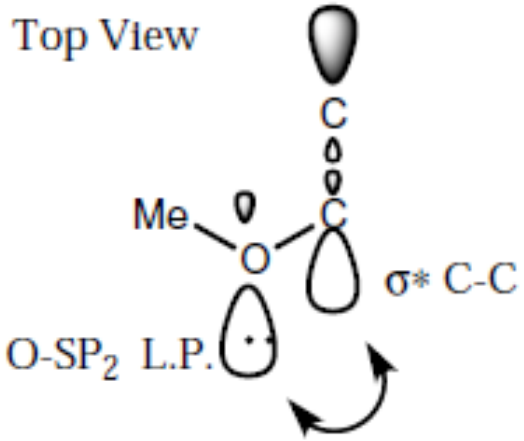
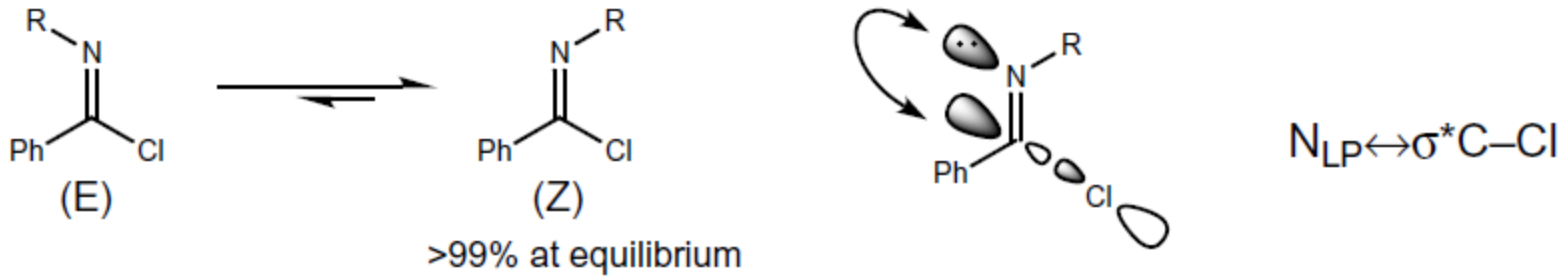
30/03/2016

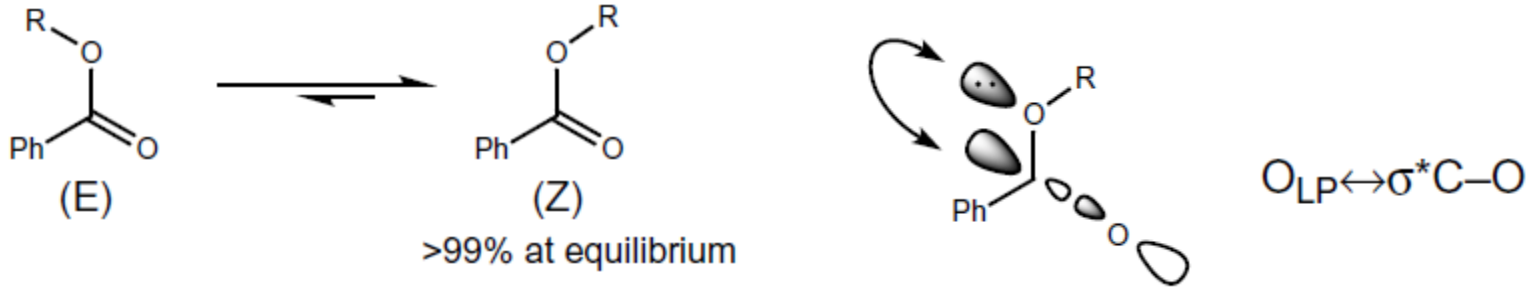
Conformational analysis



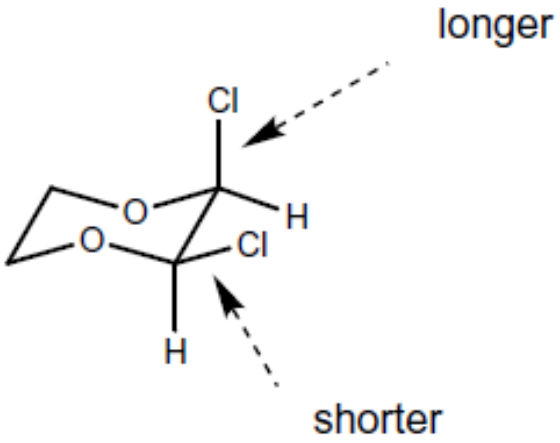


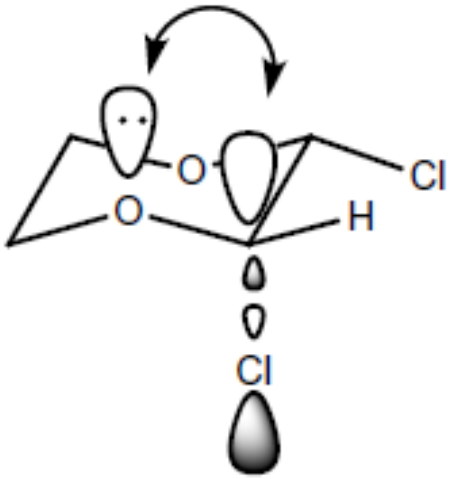
Conformational analysis



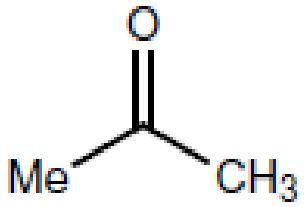


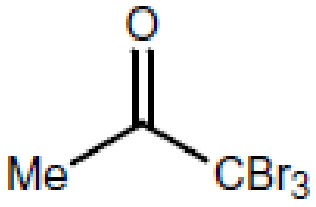
Lone pair – σ* interaction

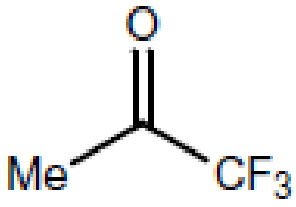




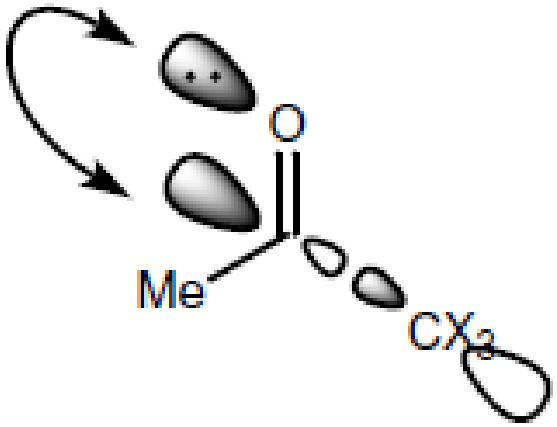
Lone pair – σ* interaction





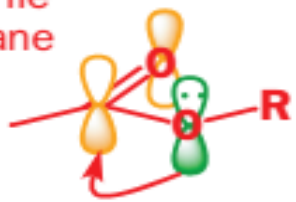


$\bar{\nu}_0$ (cm $^{-1}$) 1720 1750 1780

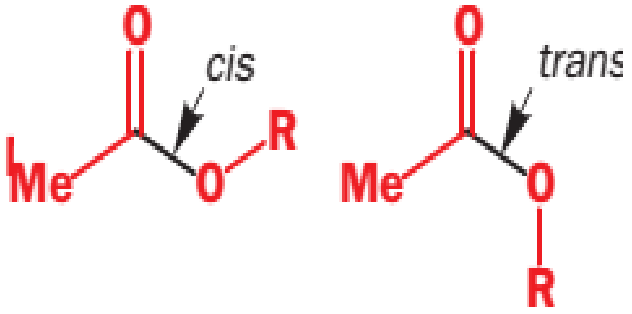


Lactones are distinctly more reactive than esters

all bonds shown lie in a plane



donation from lone pair of O into π* keeps ester planar



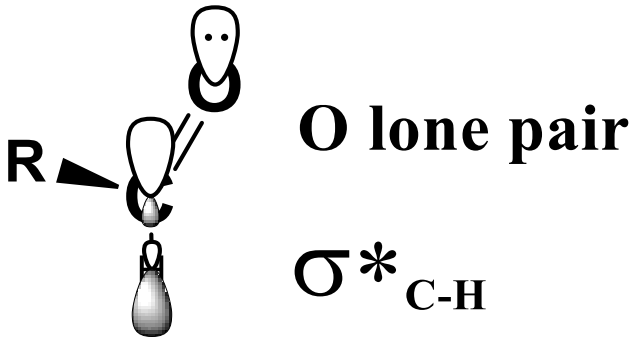
cis about C–O

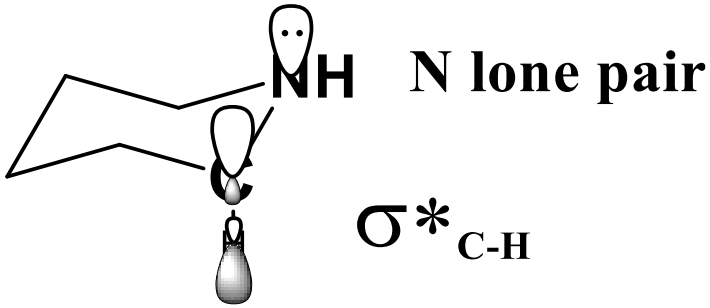
in this conformation, additional stabilization is possible as second lone pair of O donates into C–O σ*

trans about C–O

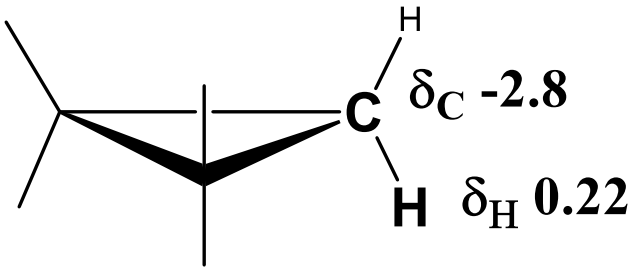
in this conformation, no additional stabilization is possible. Second lone pair of O cannot donate into C–O s*

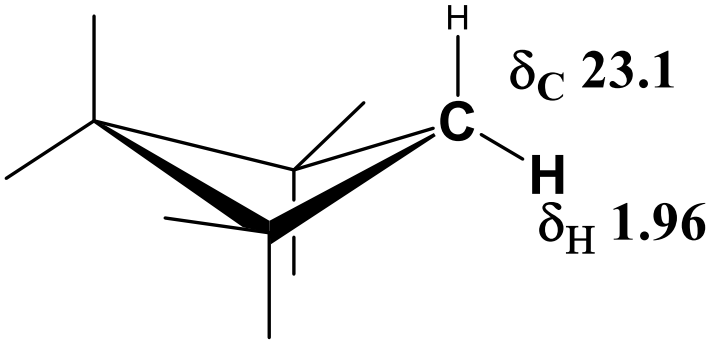
$\nu_{C\text{-}H}$ stretching

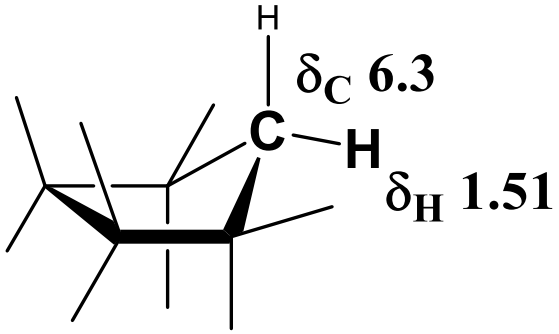




NMR chemical shifts of cycloalkanes







Baldwin's Rules