Chiral Derivatizing Agents for Absolute Stereochemistry Determination ("Mosher's Method")

1-phenylethanol:
$$R$$
 or S ?

H₃C
Ph
H
O

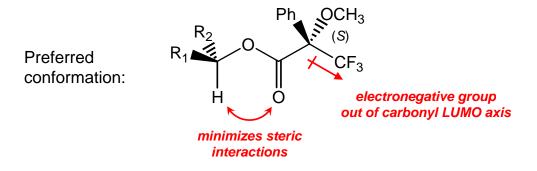
CI
Ph
OCH₃
Ph
CF₃
Ph
OCH₃
Ph
OCH₃
Ph
OCH₃
R,S)

 R,S

indistinguishable by NMR

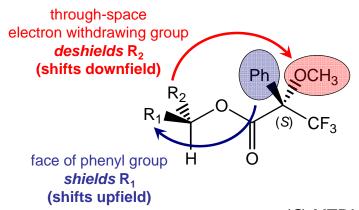
1-phenylethanol: R or S ?

MTPA Esters as NMR-Distinguishable Chiral Derivatives



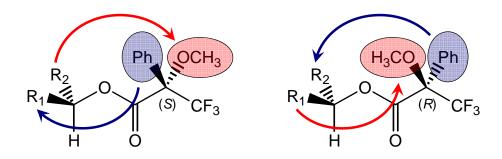
(Works best for secondary alcohols.)

MTPA Esters as NMR-Distinguishable Chiral Derivatives



(S)-MTPA ester group alters chemical shifts of R₁, R₂ in a predictable way.

MTPA Esters as NMR-Distinguishable Chiral Derivatives



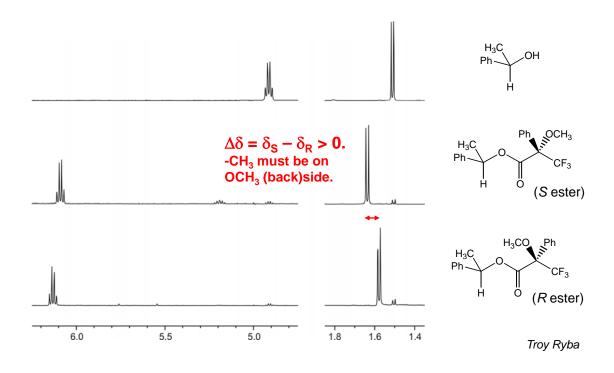
(*R*)-MTPA ester group has opposite effect on chemical shift.

So, if we define $\Delta \delta = \delta_S - \delta_R$,

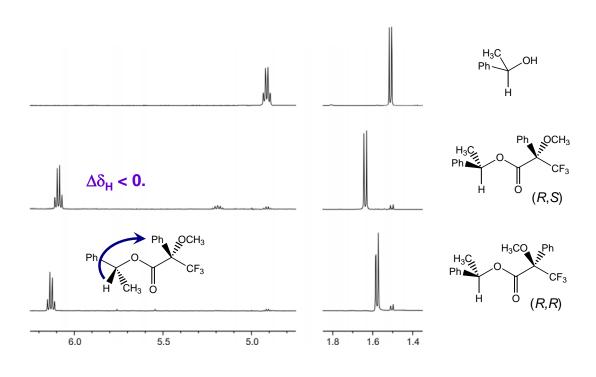
If a nucleus shows $\Delta\delta > 0$, must be R₂.

 $\Delta\delta$ < 0, must be R₁.

MTPA Esters as NMR-Distinguishable Chiral Derivatives



MTPA Esters as NMR-Distinguishable Chiral Derivatives



MTPA Esters as NMR-Distinguishable Chiral Derivatives

$$\Delta \delta = \delta_{S} - \delta_{R}$$

+0.19

+0.47, +0.40

H

-0.06

-0.06

H

-0.05

H

H

OCH₃

Ph

OCH₃

CF₃

(S ester)

-0.07

ottelione A (?)

Hollie Lewis

Other Chiral Derivatives and Complexing Agents

(There are lots.)