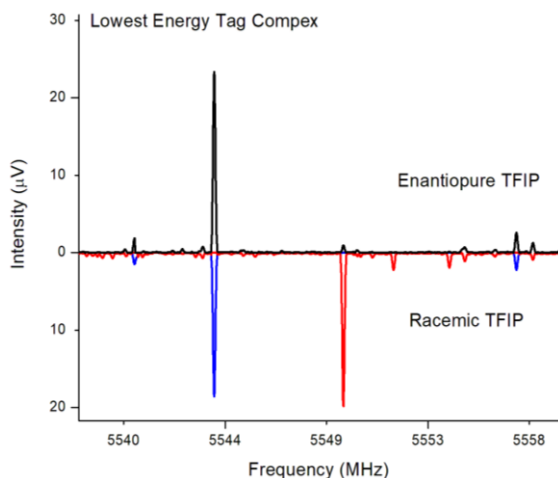


Chiral Tag Rotational Spectroscopy for the Chiral Analysis of Carboxylic Acids

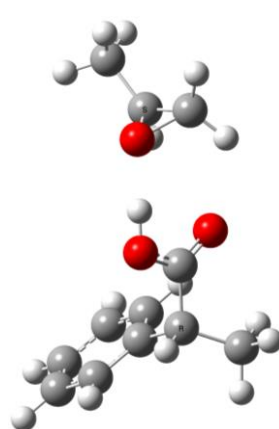
Chiral Tag Rotational Spectroscopy

Conversion of enantiomers in diastereomeric mixture

Non-covalent bonding – “tagging”



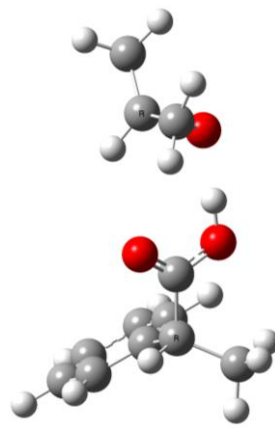
Heterochiral



A / MHz = 958.682
B / MHz = 287.032
C / MHz = 253.434

E / H = -692.90416
 $\Delta E / \text{cm}^{-1} = 0$

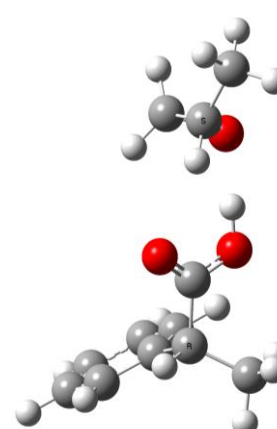
Homochiral “flip”



A / MHz = 945.353
B / MHz = 289.063
C / MHz = 254.705

E / H = -692.90294
 $\Delta E / \text{cm}^{-1} = 267.6454$

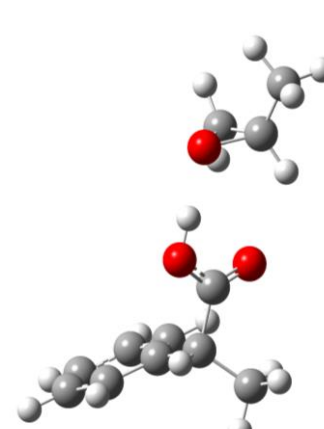
Heterochiral “flip”



A / MHz = 1168.001
B / MHz = 257.639
C / MHz = 241.080

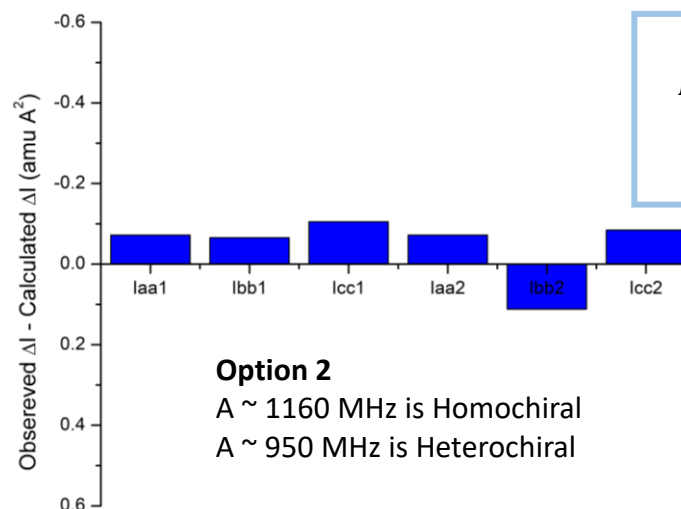
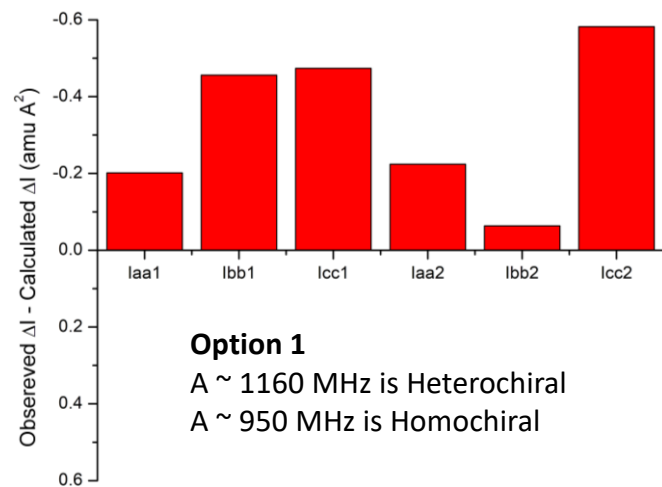
E / H = -692.90288
 $\Delta E / \text{cm}^{-1} = 280.8568$

Homochiral



A / MHz = 1162.163
B / MHz = 259.368
C / MHz = 241.516

E / H = -692.90404
 $\Delta E / \text{cm}^{-1} = 26.4935$



$$I_a = \frac{\hbar^2}{2A} \quad I_b = \frac{\hbar^2}{2B} \quad I_c = \frac{\hbar^2}{2C}$$

$$\Delta I = I_{\text{Theory}} - I_{\text{Experimental}}$$