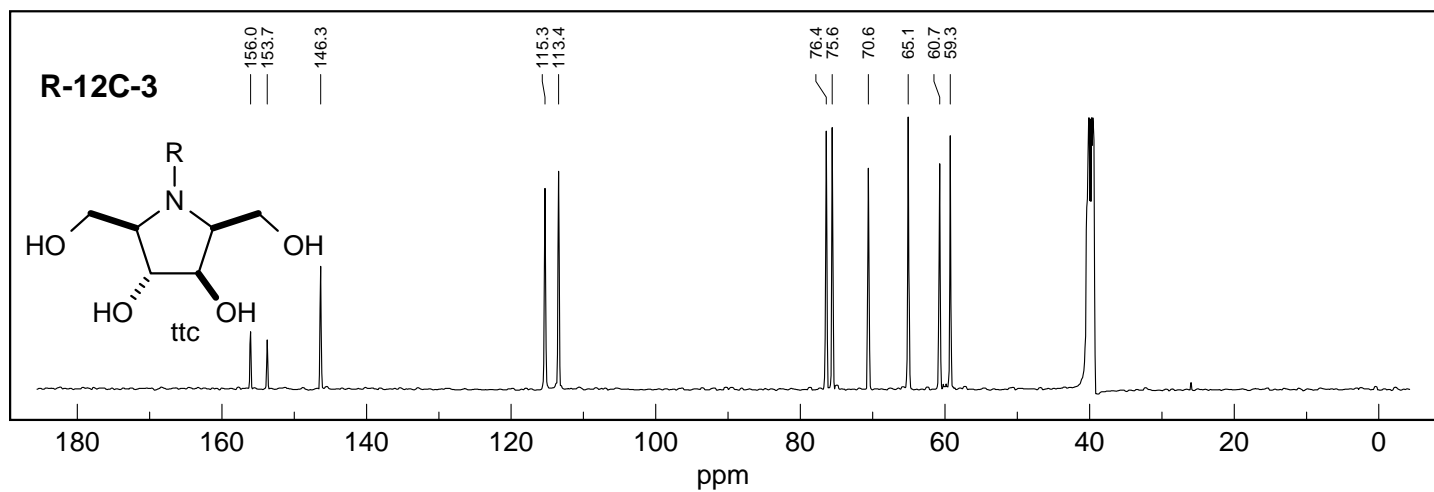
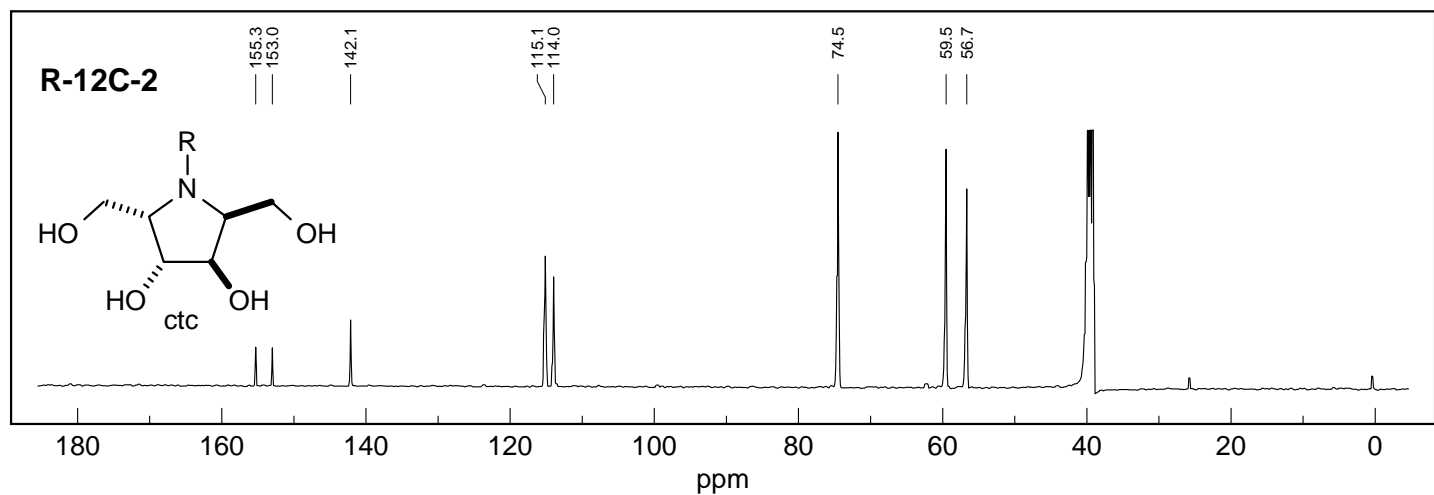
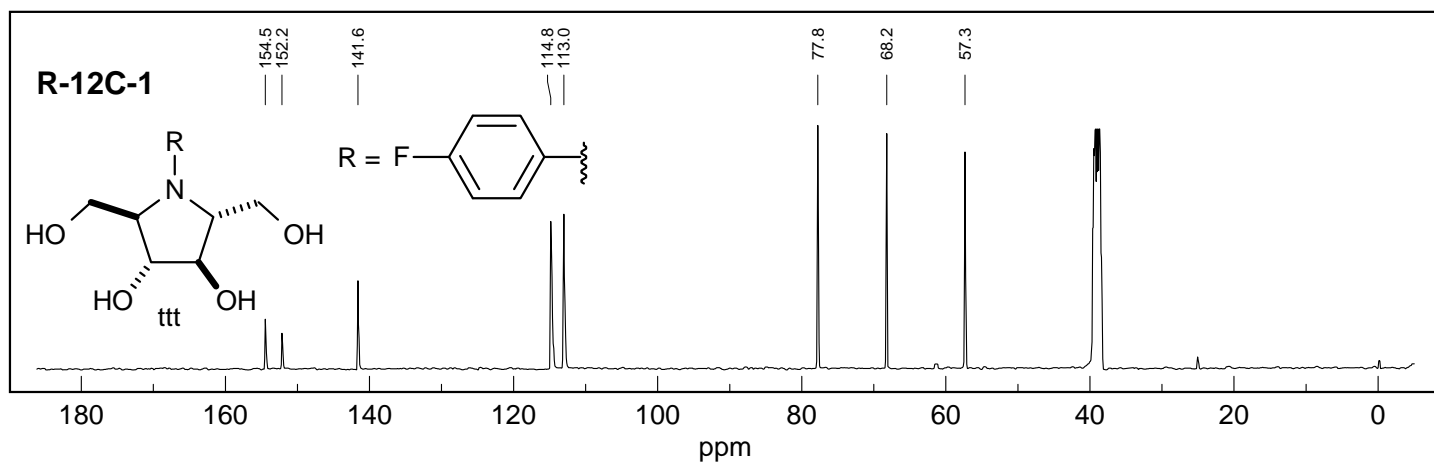


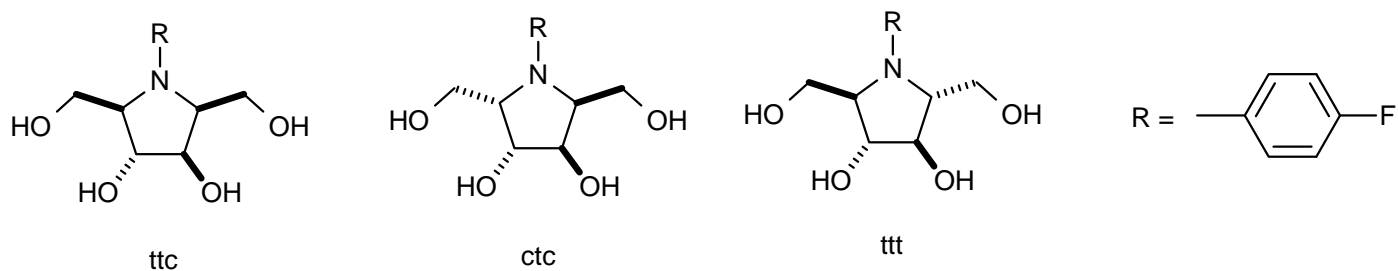
Problem R-12C (C₁₂H₁₆FNO₄).

100 MHz ¹³C NMR spectra in DMSO-d₆

Source: Allen B. Reitz, *JOC* **1994**, *59*, 3175 (digitized hard copy)



Problem R-12C The 100 MHz ^{13}C NMR spectra of three substituted pyrrolidines is shown on the next page. Their structures are shown below (ttc = trans-trans-cis). R = para-fluorophenyl.



(a) Identify the compound (ttc, ctc or ttt) which corresponds to spectrum **R-12C-1**. Give your reasoning.

(b) Identify the compound which corresponds to spectrum **R-12C-2**. Give your reasoning.

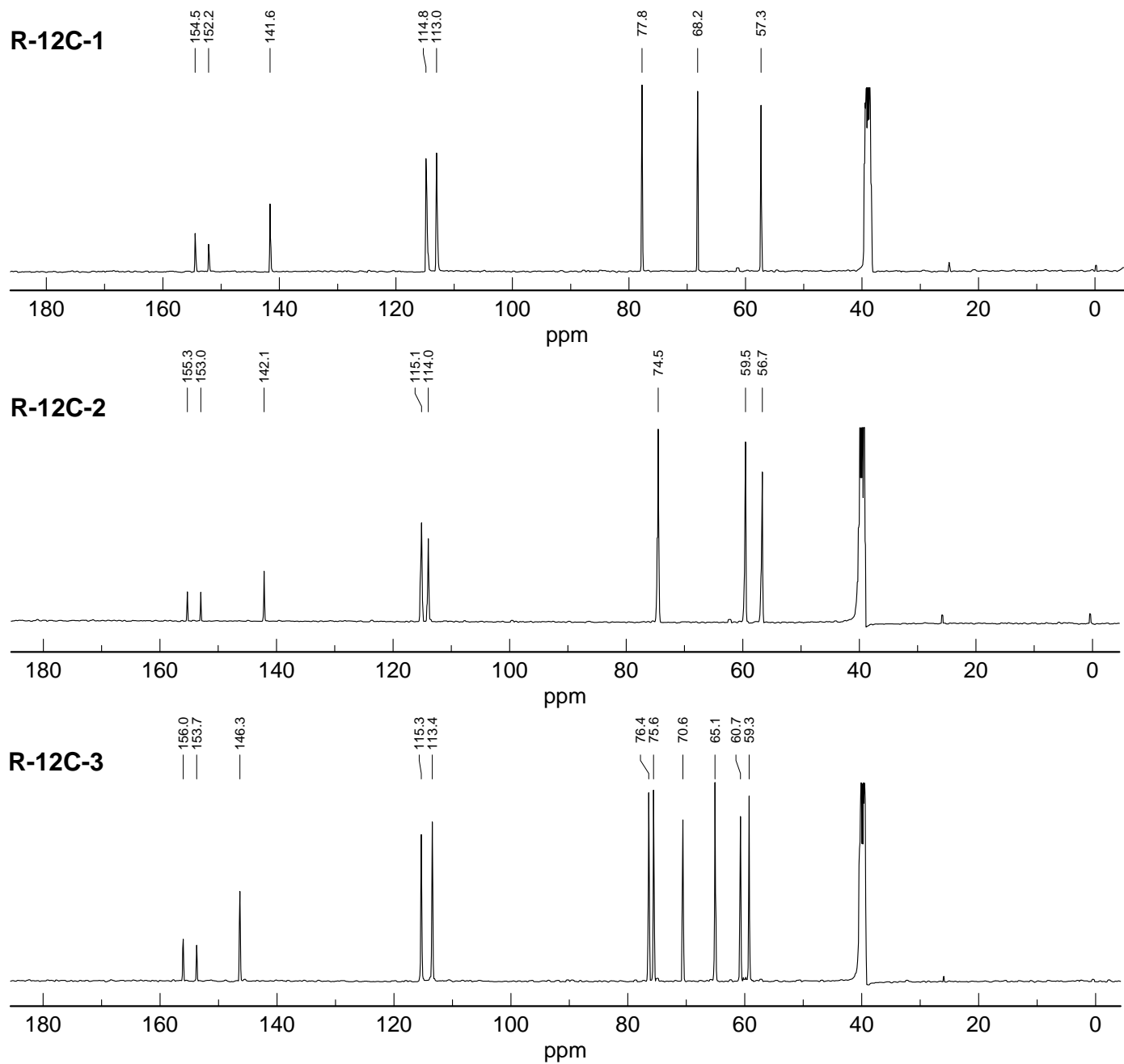
(c) Identify the compound which corresponds to spectrum **R-12C-3**. Give your reasoning.

(d) In each of the spectra there are two peaks at δ 155 ppm. Assign and explain these peaks.

Problem R-12C ($C_{12}H_{16}FNO_4$).

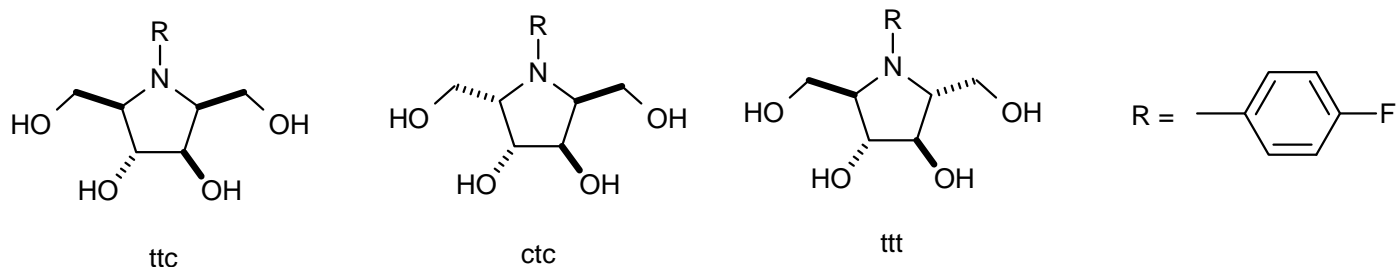
100 MHz ^{13}C NMR spectra in DMSO- d_6

Source: Allen B. Reitz, *JOC* **1994**, 59, 3175 (digitized hard copy)



20

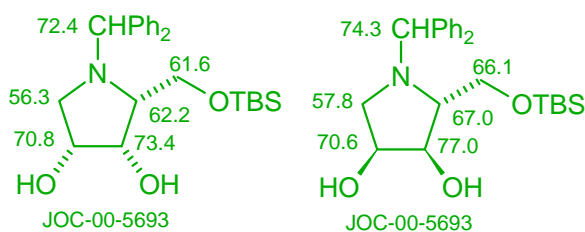
Problem R-12C The 100 MHz ^{13}C NMR spectra of three substituted pyrrolidines is shown on the next page. Their structures are shown below (ttc = trans-trans-cis). R = para-fluorophenyl.



(a) Identify the compound (ttc, ctc or ttt) which corresponds to spectrum **R-12C-1**. Give your reasoning.

ttt

This must be either the ctc or ttt isomer, each of which has an axis of symmetry. See part (b) for distinction between the isomers.



(b) Identify the compound which corresponds to spectrum **R-12C-2**. Give your reasoning.

ctc

This must be either the ctc or ttt isomer, each of which has an axis of symmetry. In the ctc isomer two of the groups (an OH and a CH_2OH) on each side are cis to each other, and thus there is a γ -gauche interaction between them that is largely absent in the ttt isomer, so expect an upfield shift of the CH_2OH carbon. So this must be the ctc isomers since all carbons are upfield of the ttt isomer

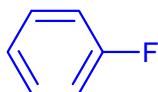
(c) Identify the compound which corresponds to spectrum **R-12C-3**. Give your reasoning.

ttc

This is the only isomer which has all carbons different (no symmetry), so must be ttc

(d) In each of the spectra there are two peaks at δ 155 ppm. Assign and explain these peaks.

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This is the C-F carbon, split into a doublet by J_{CF}