Problem R-12C \((C_{12}H_{16}FNO_4)\).
100 MHz \(^{13}\text{C}\) 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 $\delta$ 155 ppm. Assign and explain these peaks.
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**ttc**

This must be either the ctc or ttt isomer, each of which has an axis of symmetry.

(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$_2$OH) on each side are cis to each other, and thus there is a $\gamma$-gauche interaction between them that is largely absent in the ttt isomer, so expect an upfield shift of the CH$_2$OH 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 $\delta$ 155 ppm. Assign and explain these peaks.

**F**

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