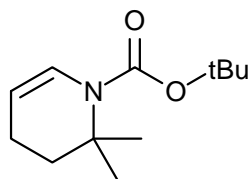


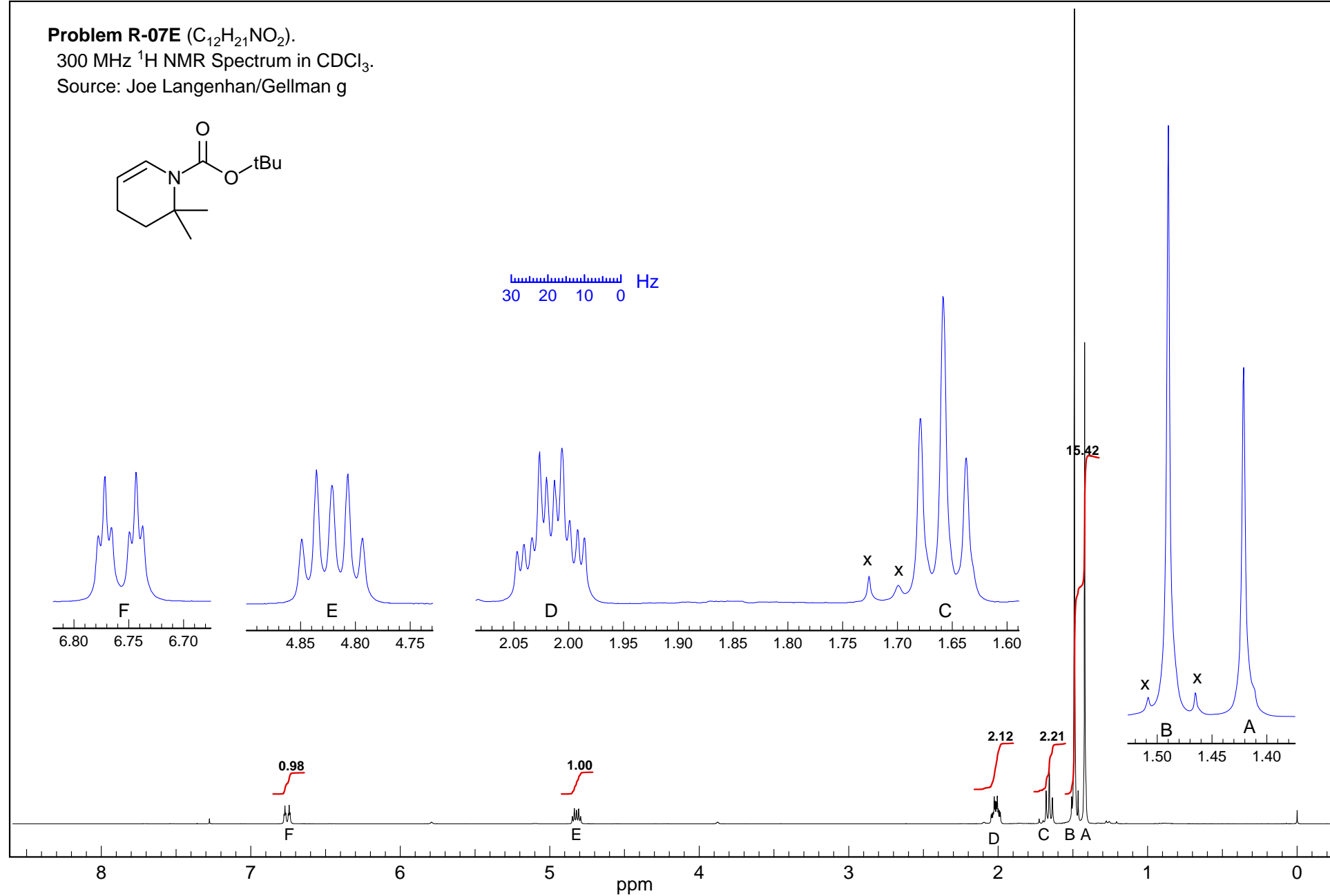
Problem R-07E (C₁₂H₂₁NO₂).

300 MHz ¹H NMR Spectrum in CDCl₃.

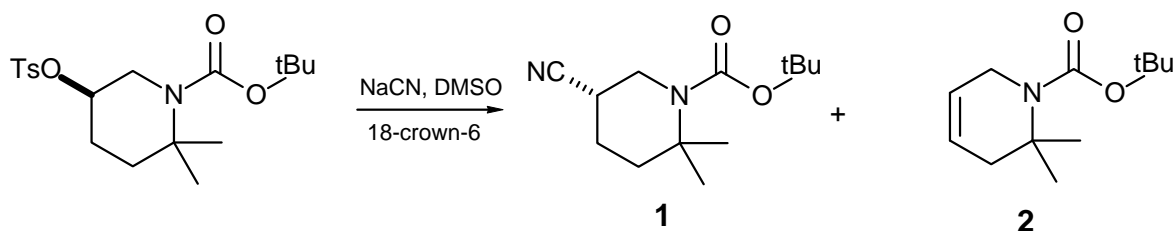
Source: Joe Langenhan/Gellman g



30 20 10 0 Hz

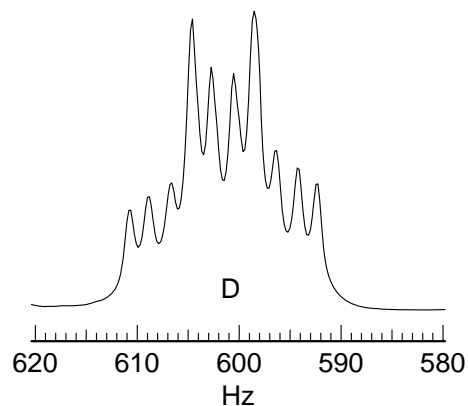


Problem R-07E. A chemist at UW prepared the nitrile **1**. In addition to the expected product he obtained a by-product initially assigned structure **2**. Carefully examine the proton NMR spectrum of **R-01E** to determine if the structure of **2** was correctly assigned, or if another isomer was formed.



(a) Interpret the multiplet at δ 2.0 (D) reproduced below, and draw a "coupling tree." Report multiplicity and coupling constants. Suggest a part structure.

D δ _____



(b) Interpret the multiplets at δ 4.8 and 6.7 (E and F). Report multiplicity and coupling constants, and a part structure

E δ _____

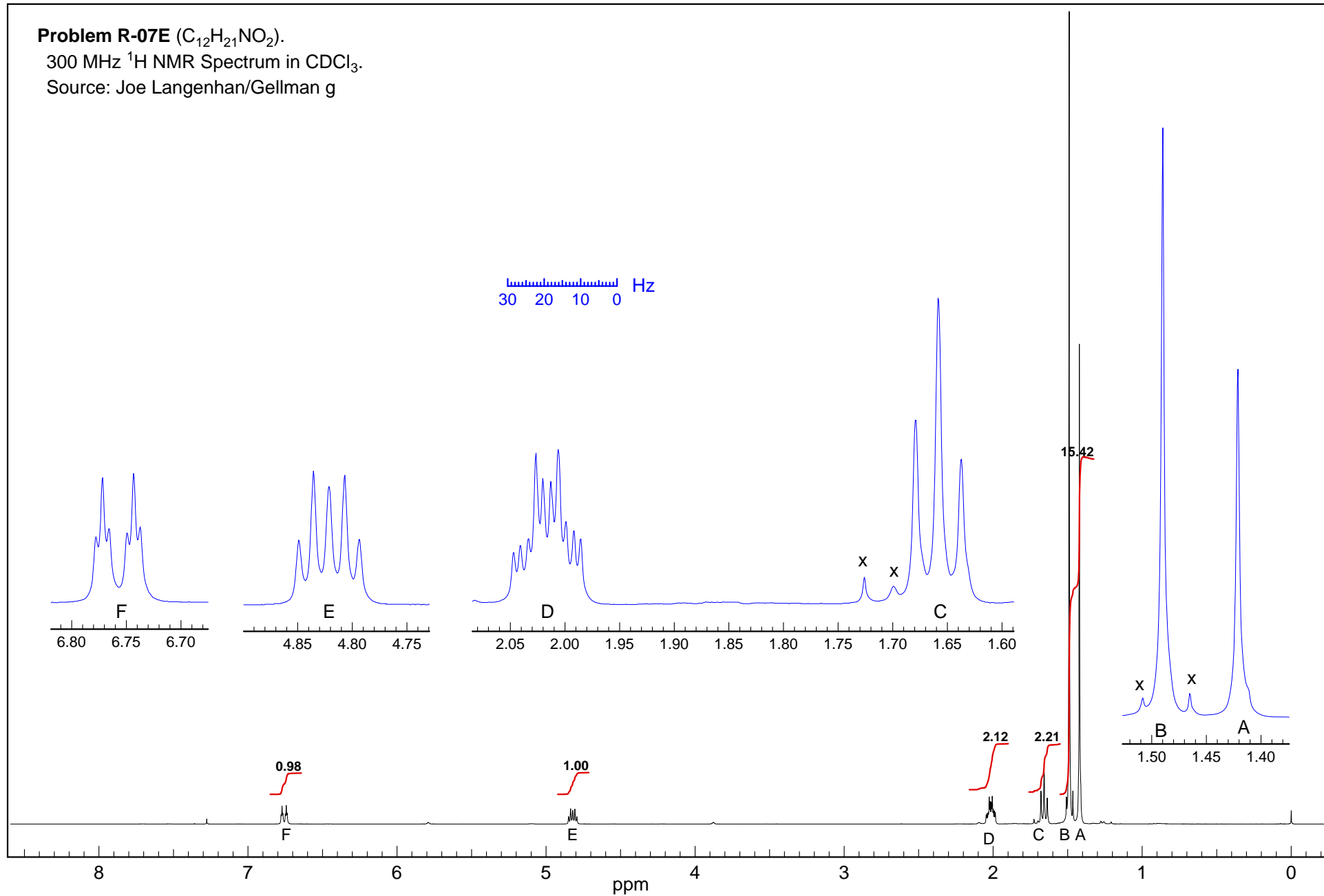
F δ _____

(b) Draw the correct structure below. If you prefer an alternative structure, briefly explain what features of the NMR spectrum are inconsistent with structure **2**. On your structure label each of the protons with the appropriate assignment (A, B, C ..)

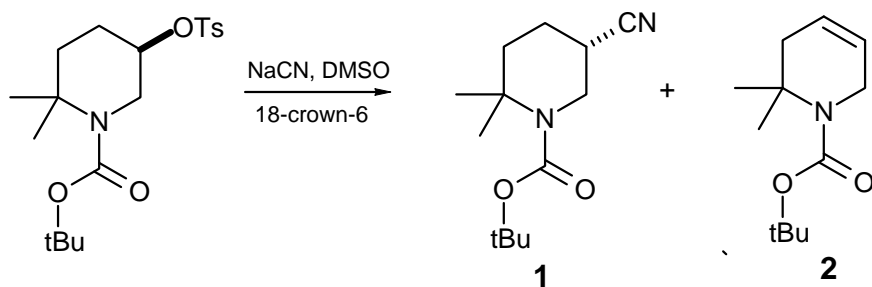
Problem R-07E ($\text{C}_{12}\text{H}_{21}\text{NO}_2$).

300 MHz ^1H NMR Spectrum in CDCl_3 .

Source: Joe Langenhan/Gellman g



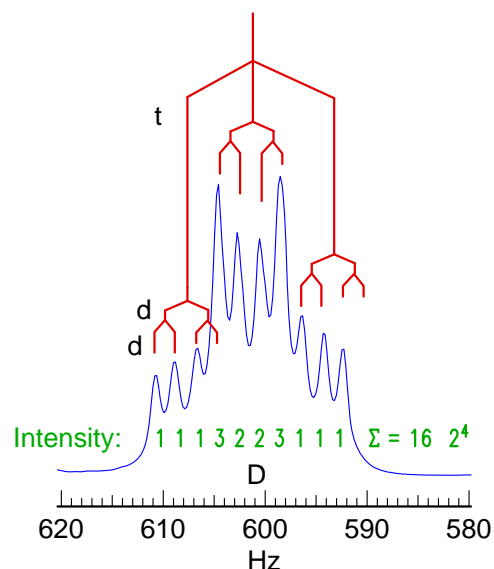
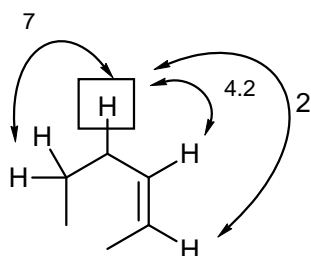
Problem R-07E. A chemist at UW prepared the nitrile **1**. In addition to the expected product he obtained a by-product initially assigned structure **2**. Carefully examine the proton NMR spectrum of **R-01E** to determine if the structure of **2** was correctly assigned, or if another isomer was formed.



(a) Interpret the multiplet at δ 2.0 (D) reproduced below, and draw a "coupling tree." Report multiplicity and coupling constants. Suggest a part structure.

4

D δ 2.02, tdd, $J = 7, 4.2, 2$ Hz, 2H

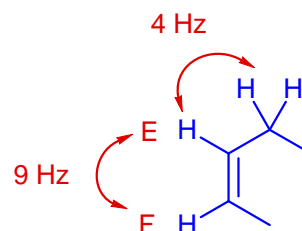


(b) Interpret the multiplets at δ 4.8 and 6.7 (E and F). Report multiplicity and coupling constants, and a part structure

4

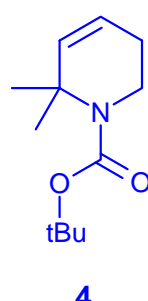
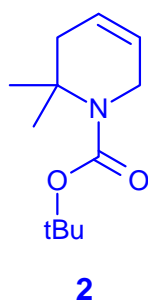
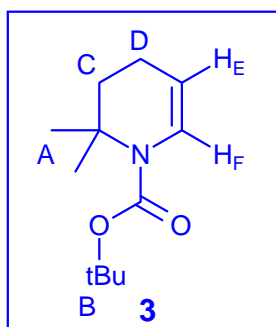
E δ 4.82, dt, $J = 9, 4$ Hz, 1H

F δ 6.76, dt, $J = 9, 2$ Hz, 1H



(b) Draw the correct structure below. If you prefer an alternative structure, briefly explain what features of the NMR spectrum are inconsistent with structure **2**. On your structure label each of the protons with the appropriate assignment (A, B, C ..)

7



The most distinguishing features are the chemical shifts of E and F, which should be quite close and around δ 5.5 for **2** and the other isomer **4**. The almost 2 ppm difference between the vinyl protons requires a strong electron-donating group (N) on the double bond. The vinyl protons in compound **2** should also be much more heavily coupled than what is observed.