Problem R-07E \((C_{12}H_{21}NO_2)\).

300 MHz \(^1\)H 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 $\delta$ 2.0 (D) reproduced below, and draw a "coupling tree." Report multiplicity and coupling constants. Suggest a part structure.

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

(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 ..)
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The most distinguishing features are the chemical shifts of E and F, which should be quite close and around $\delta$ 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.