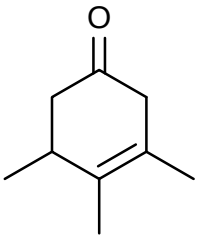
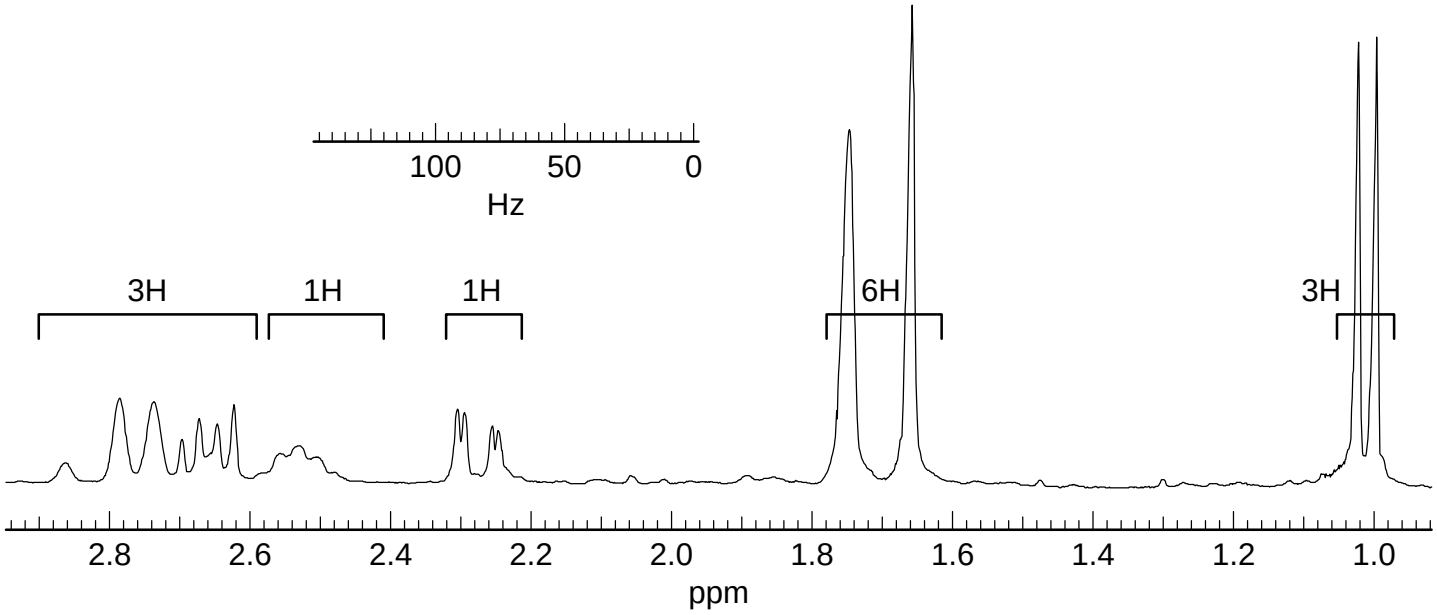
Problem N-104 ($C_9H_{14}O$)

270 MHz ^1H NMR spectrum in $CDCl_3$

Source: Steve Nelsen

IR: 2960, 2915, 2860, 1716, 1638, 1500, 1374, 1350, 1312, 1253, 1247, 1200, 1142, 1085, 850 cm^{-1}





PLT pn-080-to-373.plt

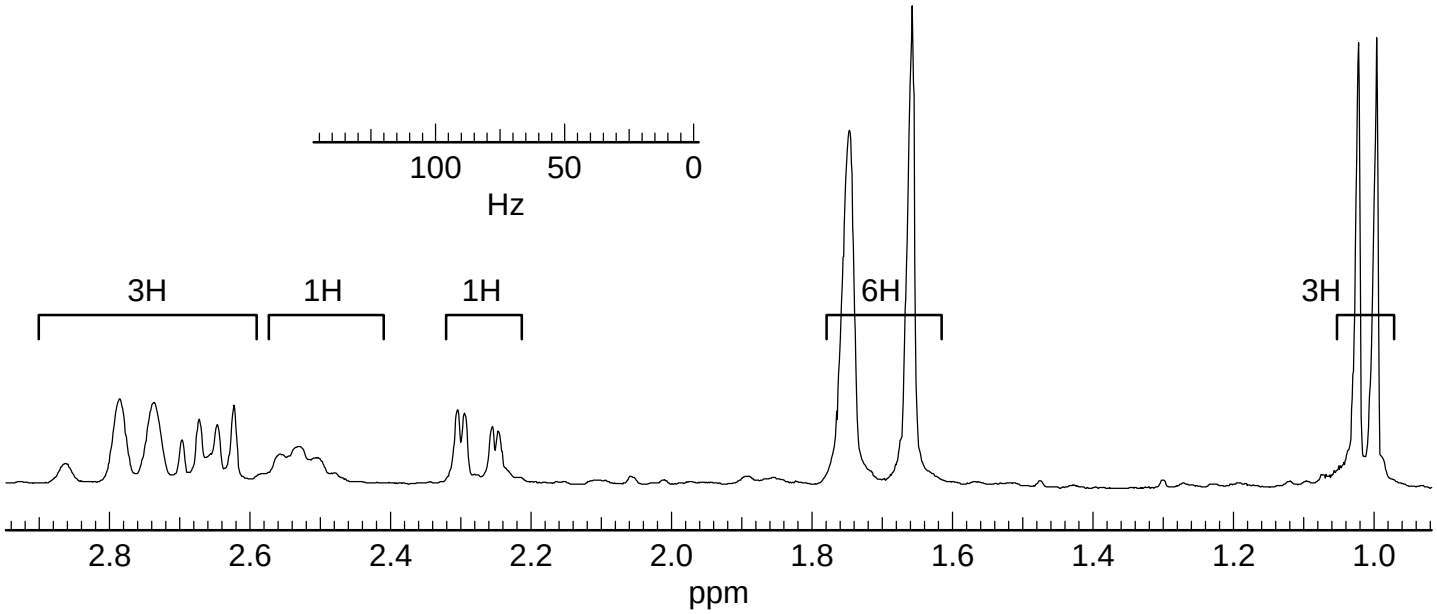
Problem N-104 ($C_9H_{14}O$). Determine the structure and assign the major conformation from the ^1H NMR coupling constants.

MS: 138.105

IR: 2960, 2915, 2860, 1716, 1638, 1500, 1374, 1350, 1312, 1253, 1247, 1200, 1142, 1085, 850 cm^{-1}

HMR: 270 MHz, $CDCl_3$ solvent

Analysis: 78.3% C, 10.2% H



PLT pn-080-to-373.plt

Problem N-104 ($C_9H_{14}O$). Determine the structure and assign the major conformation from the ^1H NMR coupling constants.

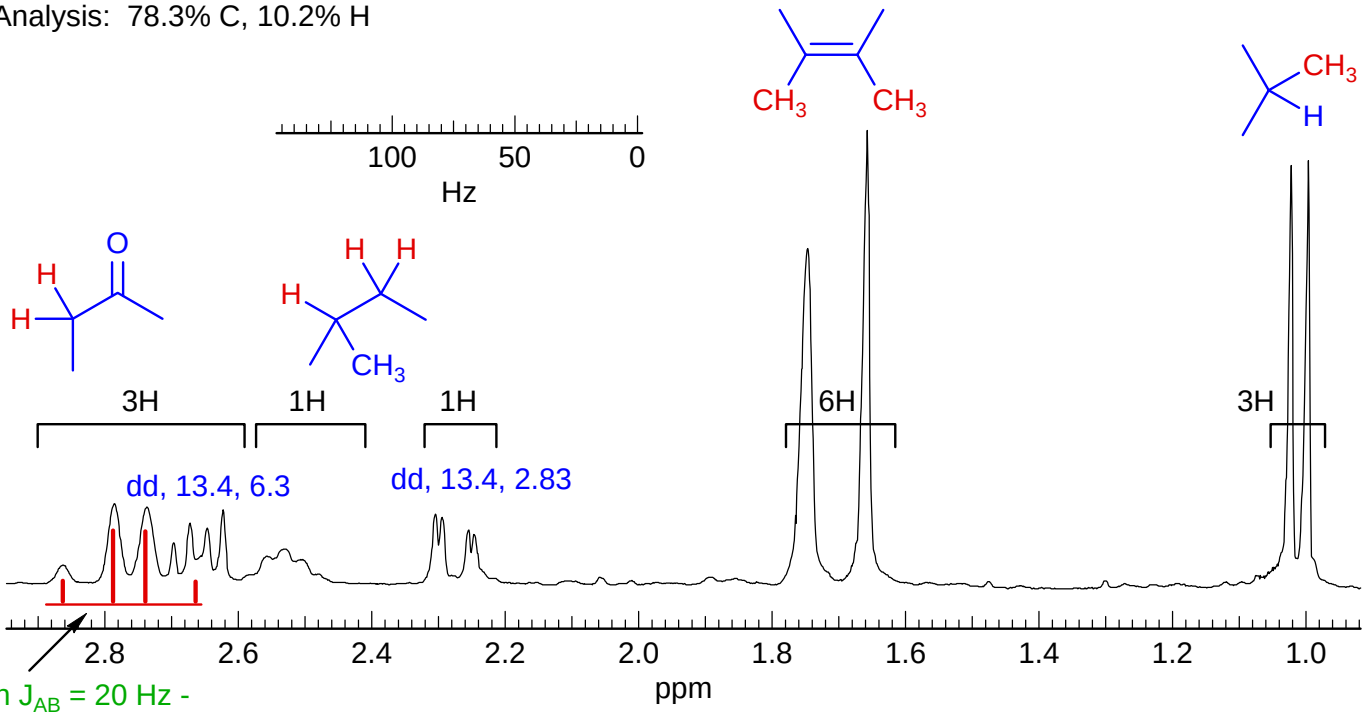
Unconjugated ketone C=O stretch
Three DBEs - ketone, double bond, plus one ring

MS: 138.105

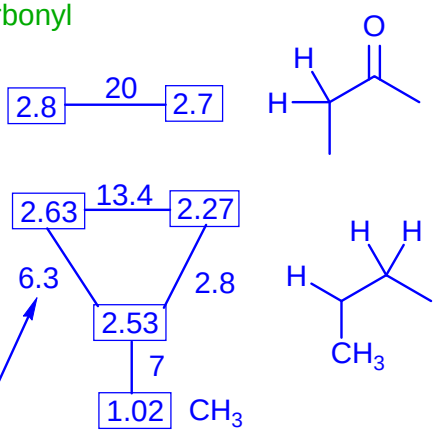
IR: 2960, 2915, 2860, 1716, 1638, 1500, 1374, 1350, 1312, 1253, 1247, 1200, 1142, 1085, 850 cm^{-1}

HMR: 270 MHz, $CDCl_3$ solvent

Analysis: 78.3% C, 10.2% H

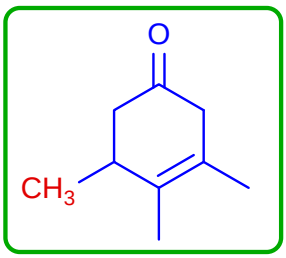


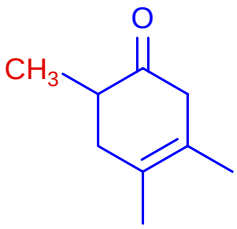
AB q with J_{AB} = 20 Hz - must be CH_2 α to a carbonyl



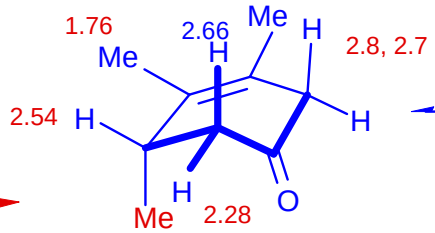
This coupling too small to be a Jax-ax, so the proton on the $CHCH_3$ carbon must be equatorial, CH_3 axial. Why?

In this isomer the CH_3 group should be mostly equatorial

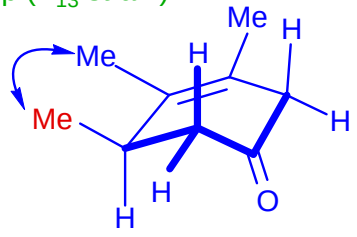




1.64



Severe buttressing interaction in the conformation with equatorial CH_3 group (A_{13} strain)



Main conformation
The axial Me group
has no 1,3-diaxial interactions

PLT pn-080-to-373.plt