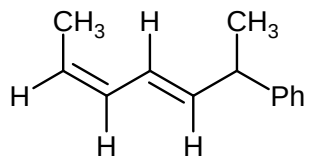
Problem N-152 ($C_{13}H_{16}$)

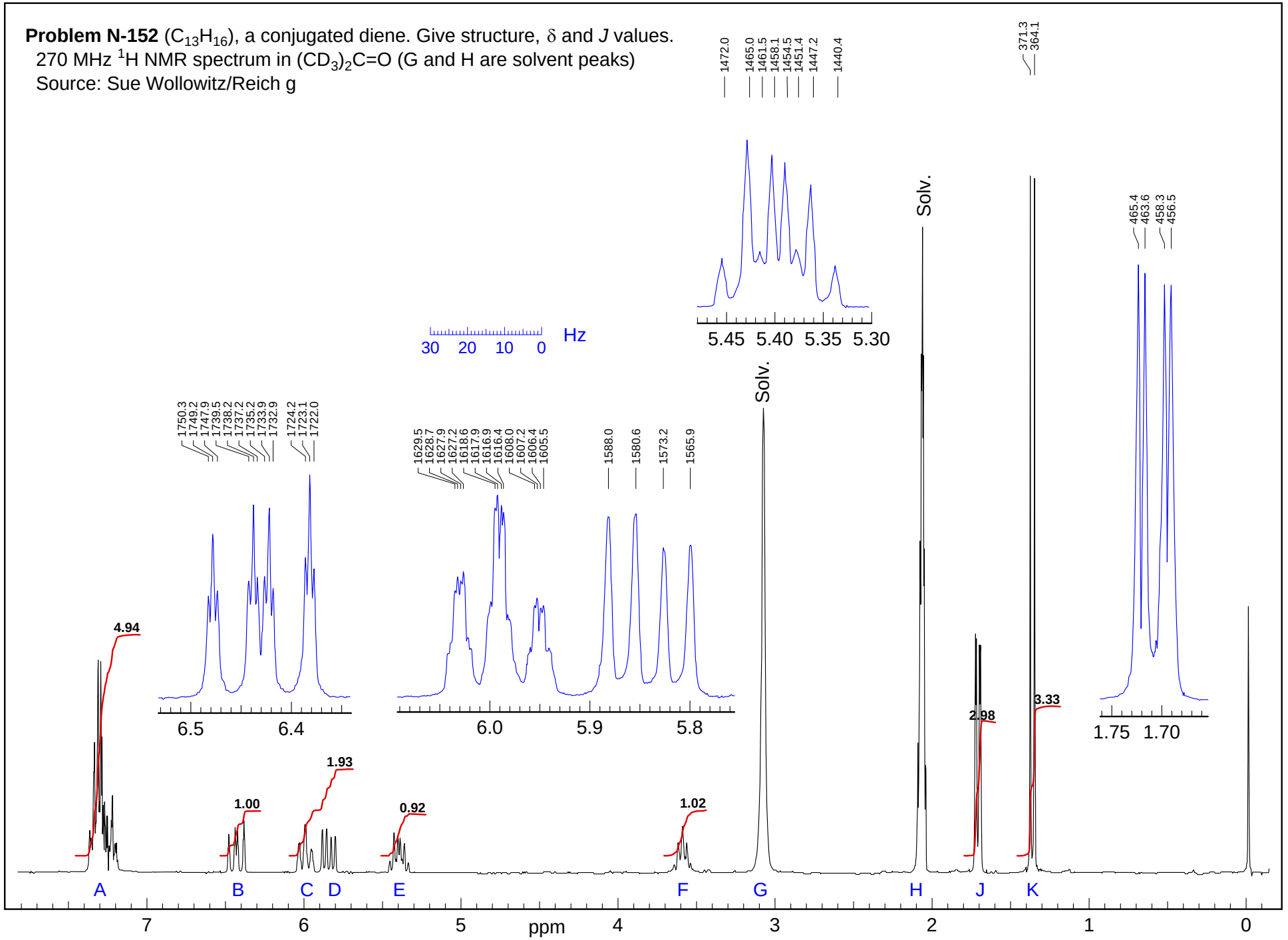
270 MHz ^{1}H NMR spectrum in $(CD_3)_2C=O$

Source: Sue Wollowitz/Reich (digitized hard copy) g



PLT pn-080-to-373.plt

Exercise: Determine the structure of N-152 from the ^{1}H NMR spectrum.

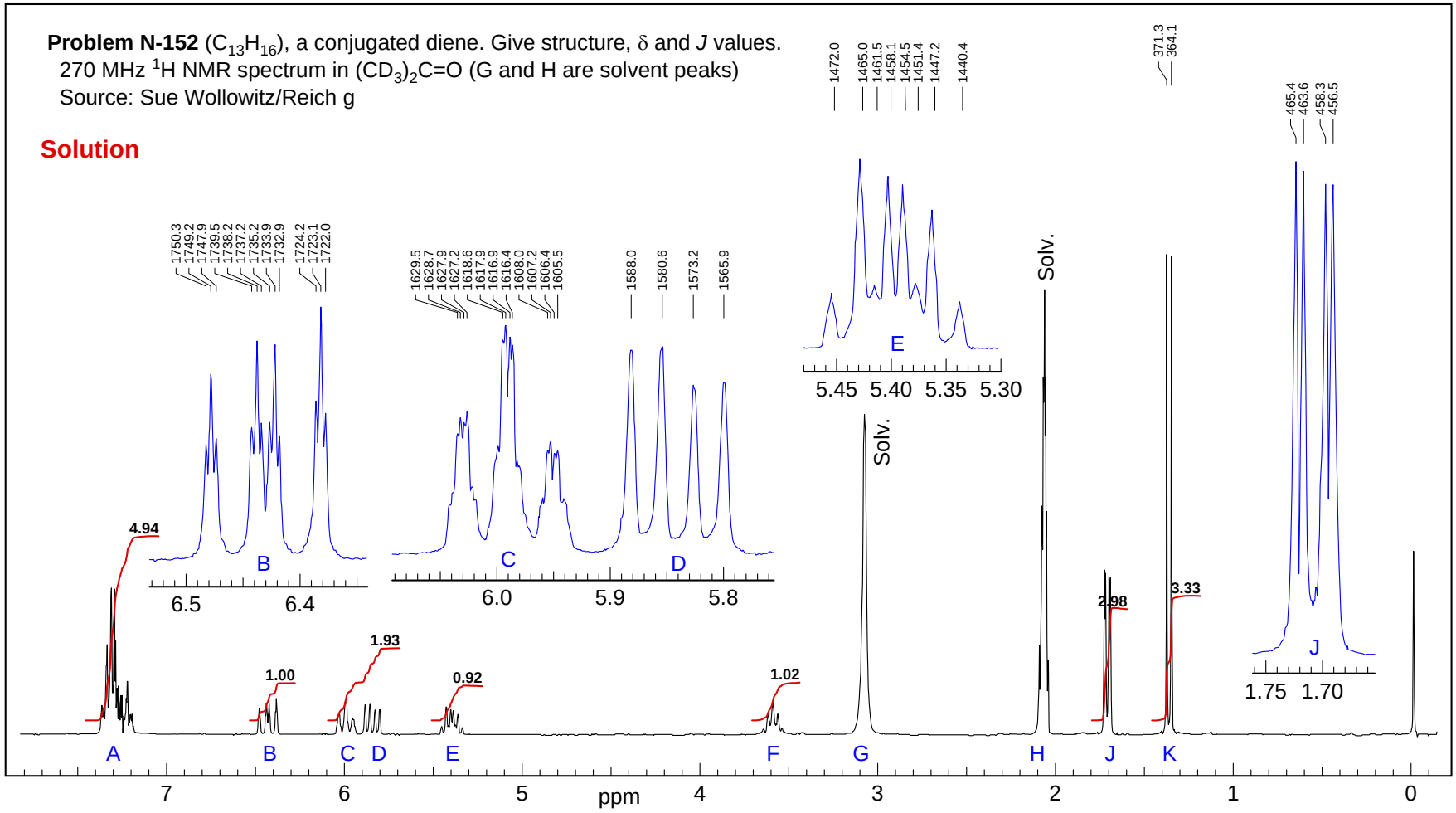


PLT pn-080-to-373.plt

Exercise: Determine the structure of N-152 from the ^{1}H NMR spectrum.

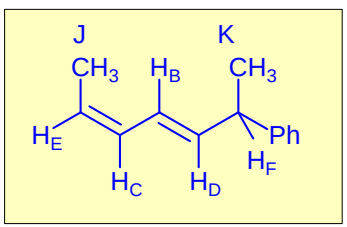
Problem N-152 ($C_{13}H_{16}$), a conjugated diene. Give structure, δ and *J* values.
270 MHz ^{1}H NMR spectrum in $(CD_3)_2C=O$ (G and H are solvent peaks)
Source: Sue Wollowitz/Reich g

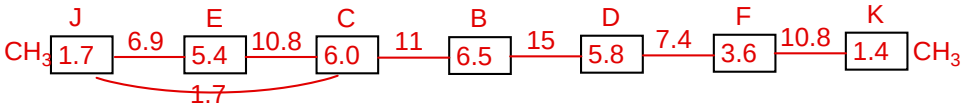
Solution



Coupling constant summary:

						CH_3	CH_3
A	B	C	D	E	F	J	K
m	ddt	tqd	dd	dq	pentet	dd	d
	15.2	11	15.2	10.8	7(pent)	7.1	7.2
	10.9	11	7.4	6.9(q)		1.8	
	1.1	1.7(q)	(0.5)				
	1.1	0.5					





Start the structure with **J**. The methyl dd at δ 1.7 suggests a CH_3-CH=CH unit

The only vinyl proton with a 7 Hz quartet coupling is E, so the end vinyl proton is E (CH_3-CH_E=CH)

H_C also ahows a small quartet (long range) splitting, so it can be assigned to the next proton in the chain. Since the H_C-H_E coupling is only 11 Hz, the double bond must be cis. One can rule out H_B and H_D for the one coupled to H_E because each shows a 15 Hz coupling, which is not possible for the coupling partner of H_E.

The next proton must be B, since it has couplings of 10 and 15, whereas D has 10 and 7 Hz.
H_F is a pentet from nearly equal coupling to the methyl K and H_D

PLT pn-080-to-373.plt