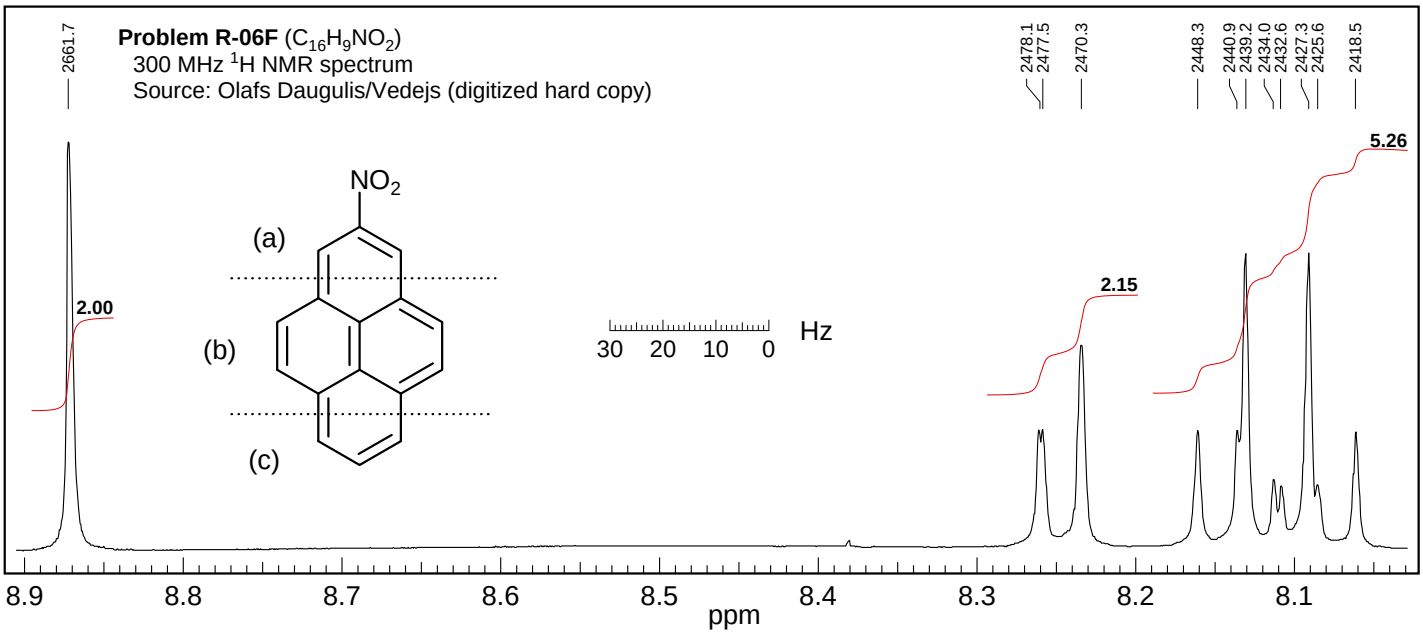
Problem R-06F. You are given the 300 MHz ^{1}H NMR spectrum of a mono-nitro pyrene. Interpret the spectrum, and calculate chemical shifts. **Write the chemical shifts on the structure.**

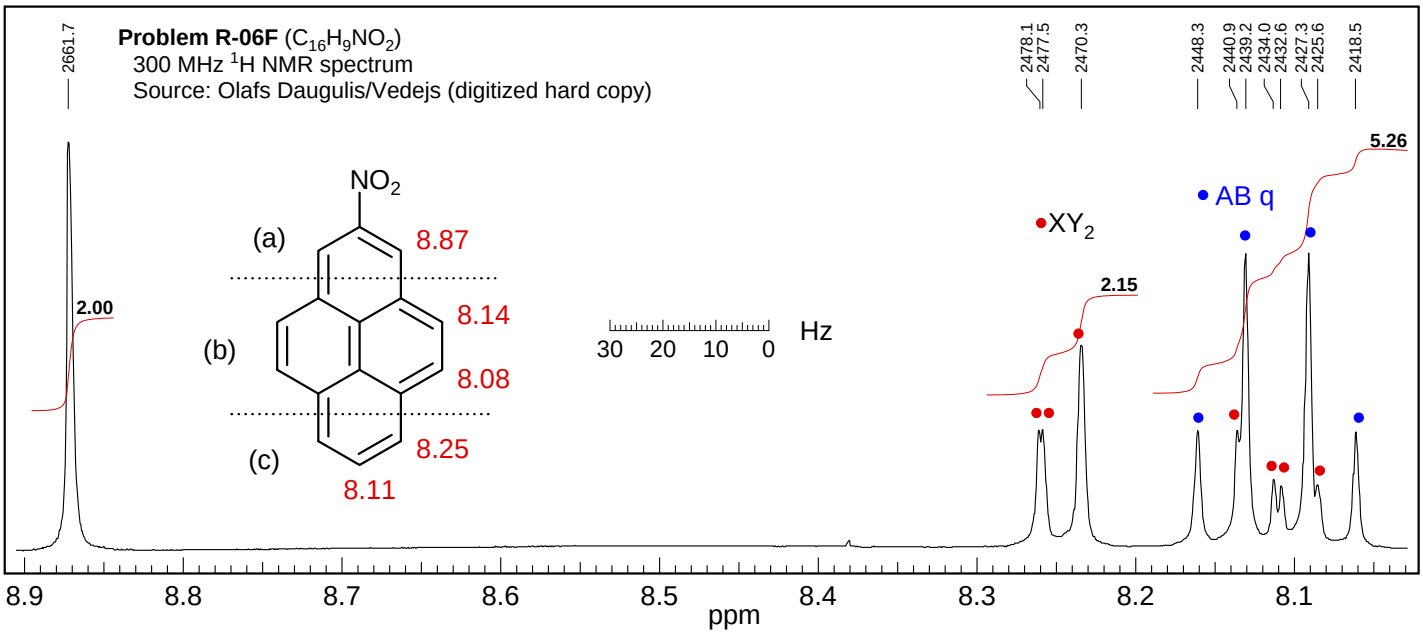


(a) Identify the ^{1}H NMR signals corresponding to protons in the top part of the molecule (marked (a) on the structure).

(b) Identify the ^{1}H NMR signals corresponding to protons in the middle part of the molecule (region (b) on the structure). Mark the peaks with a "b". What kind of pattern is this?_____ Using the frequencies given, calculate accurate shifts and couplings for the protons.

(c) Identify the ^{1}H NMR signals corresponding to protons in the bottom part of the molecule (region (c) on the structure). Mark the peaks with a "c". What kind of pattern is this?_____ Using the frequencies given, calculate accurate shifts and couplings for these protons.

Problem R-06F. You are given the 300 MHz ^{1}H NMR spectrum of a mono-nitro pyrene. Interpret the spectrum, and calculate chemical shifts. **Write the chemical shifts on the structure.**



(a) Identify the ^{1}H NMR signals corresponding to protons in the top part of the molecule (marked (a) on the structure).

These should be the most downfield protons, and a **singlet**

3 δ 8.87, s

(b) Identify the ^{1}H NMR signals corresponding to protons in the middle part of the molecule (region (b) on the structure). Mark the peaks with a "b". What kind of pattern is this? AB Using the frequencies given, calculate accurate shifts and couplings for the protons.

These should be an **AB** pattern

6

ABq 1: 2448.3
2: 2439.2
3: 2427.3
4: 2418.5

J_{AB} = 9.1

J_{AB} = 8.8

ν_c = 2433.3

ν_{AB} = (1-4) (2-3) = (29.8) (11.9) = 18.83

ν_A = 2433.3 + 18.83/2 = 2442.7 Hz; 8.14 δ

ν_A = 2433.3 - 18.83/2 = 2423.88Hz; 8.08 δ

(c) Identify the ^{1}H NMR signals corresponding to protons in the bottom part of the molecule (region (c) on the structure). Mark the peaks with a "c". What kind of pattern is this? AB_2 or XY_2 Using the frequencies given, calculate accurate shifts and couplings for these protons.

These should be an **AB_2** pattern

8

XY_2

X: 1: 2425.6
2: 2432.6
3: 2434.0
4: 2440.9

Y_2: 5: 2470.3
6: 2470.3 (not resolved)
7: 2477.5
8: 2478.1

ν_X = line 3 = 2434.0 Hz; 8.11 δ

ν_Y = (5 + 7)/2 = (2470.3 + 2477.5)/2 = 2473.9 Hz; 8.25 δ

J_{XY} = (1 -4 +6 - 8)/3 = 7.7 Hz

Major problem: not recognizing pattern