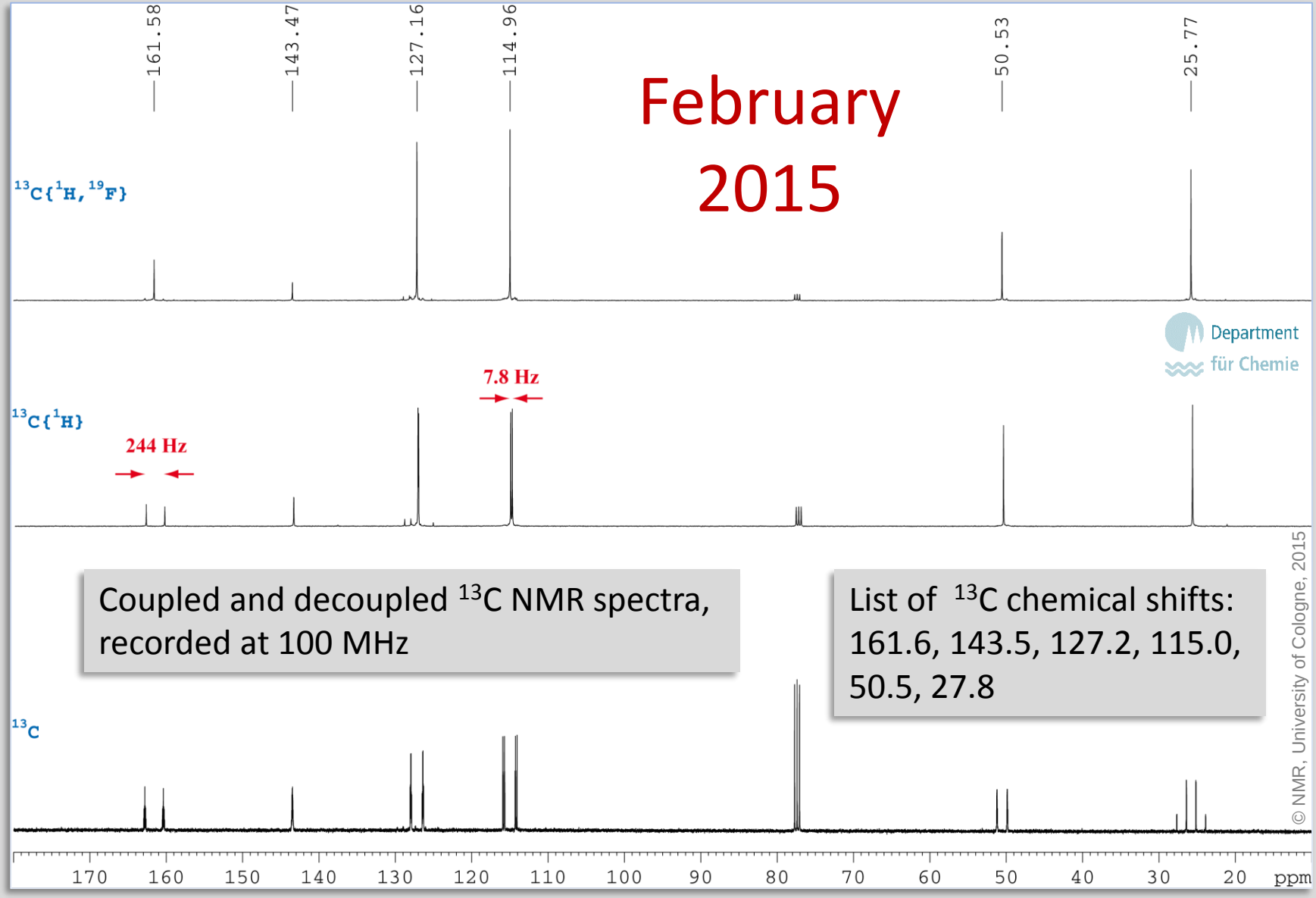
Problem of the Month:



Problem of the Month:
February 2015

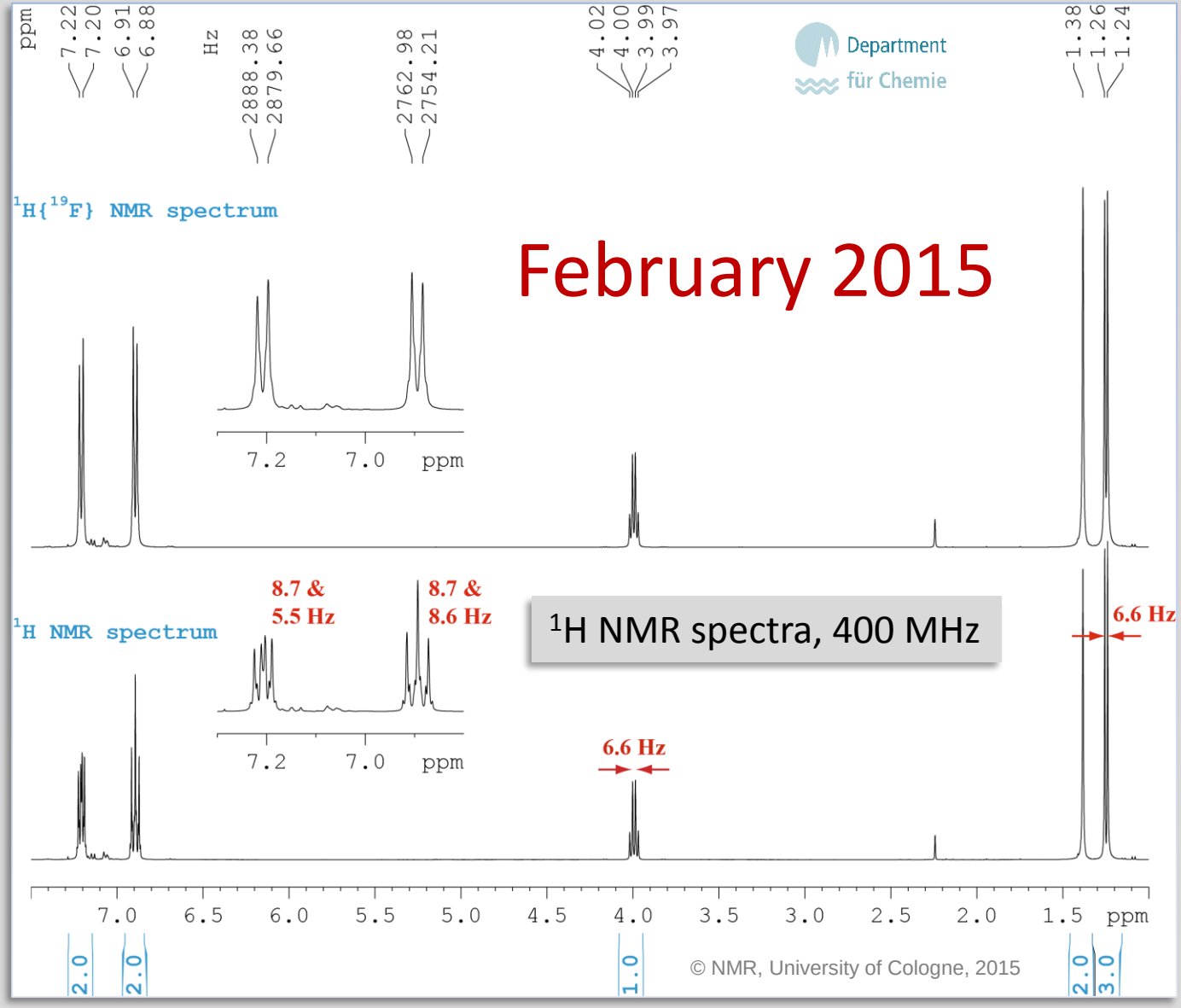
Strategy

(1) First, determine the number of DBE for the molecule. Its molecular formula is $C_8H_{10}FN$.

(2) Various types of ^{13}C NMR spectra are presented on the first page: Without ^{1}H or ^{19}F coupling (top trace), with only ^{19}F coupling visible (middle) and with both, ^{1}H and ^{19}F coupling present (bottom). With this information, you can assign the number of attached hydrogen or fluorine atoms.

(3) Now, assign protons to corresponding carbons from the ^{1}H NMR spectrum on the next page. Try to assign the multiplets and derive the observable spin systems. Note, the upper spectrum is ^{19}F decoupled .

Problem of the Month:



Problem of the Month:
February 2015

Hints

(1) The ^{1}H signal at δ_H 1.38 will cease, once a drop of deuterated water is added to the sample!

(2) This information, together with the number of DBE, should be helpful.

(3) This month‘s problem does not contain any through-bond correlation experiments. The only 2D experiment available as additional information is a heteronuclear Overhauser effect (next page). This type of spectrum gives information about nuclei which are (farely) close in space (maximum 4 Å as a rule of thumb).

(4) Also, you might verify the other part of the aromatic spin system with the ^{19}F NMR spectrum given on the next page.

Problem of the Month:

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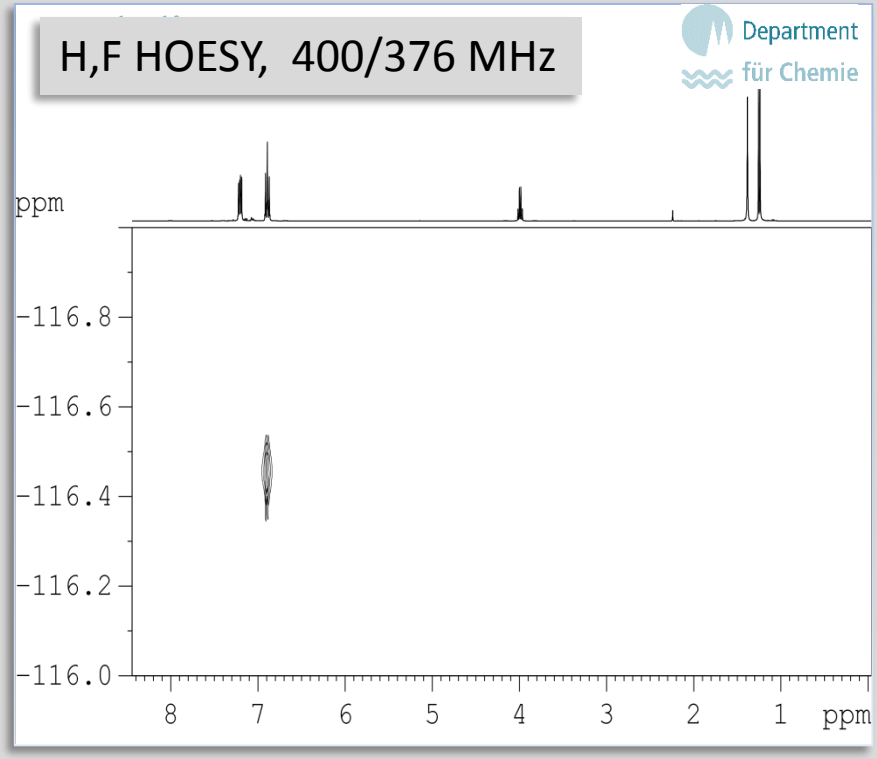

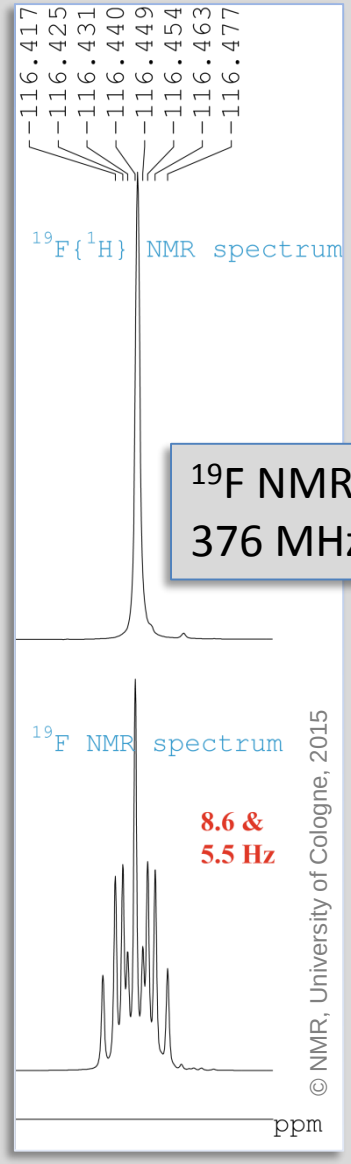

^{19}F NMR spectra, 376 MHz

Problem of the Month:
February 2015

Solution

(1) The target molecule should be, according to DBE and ^{1}H/ ^{13}C chemical shifts in the sp^2 region of the spectra, an aromatic compound. From the sum formula and the hint with the perishing signal at δ_H 1.38 (intensity = 2H), an amine is feasible.

(2) There is an AA'XX' system visible in the ^{1}H NMR spectrum, if ^{19}F is decoupled. In combination with the ^{19}F coupling observed in the $^{13}C\{^{1}H\}$ spectrum, the substitution pattern can be identified. This is affirmed by the NOE spectrum.

(3) To derive the aliphatic amine part, the ^{1}H NMR spectrum is sufficient: Here, a AX_3 spin system is observed.

(4) No solution? Enter the chemical shifts of the ^{13}C signals in nmrsshiftdb2 as a „spectrum search“ (option „complete“) or click here.