Problem R-11U ($C_2H_3AsF_7NXe$). This problem requires you to interpret the ^{129}Xe and ^{14}N spectra of $[CH_3C{\equiv}N\text{-}Xe\text{-}F]^+ AsF_6^-$ (Emara, A. A. A; Schrobilgen, G. J. *Chem. Commun.* **1987**, 1644)
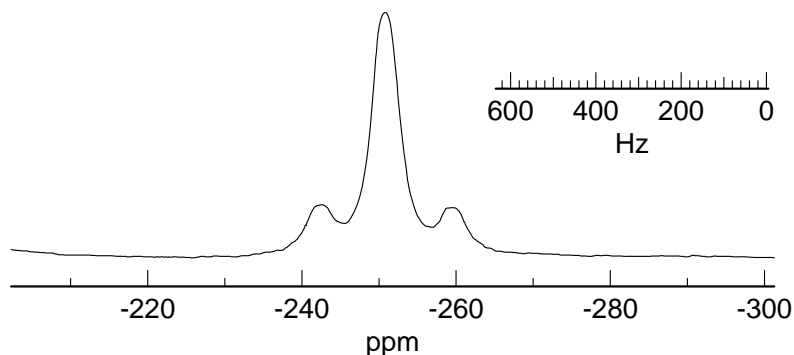
Spectrum 1. 69.56 MHz ^{129}Xe NMR spectrum of $[CH_3C{\equiv}N\text{-}Xe\text{-}F]^+ AsF_6^-$ in HF at -10 °C

Spectrum 2. 69.56 MHz ^{129}Xe NMR spectrum of $[CH_3{}^{13}C{\equiv}N\text{-}Xe\text{-}F]^+$ AsF_6^- in HF at -10 °C
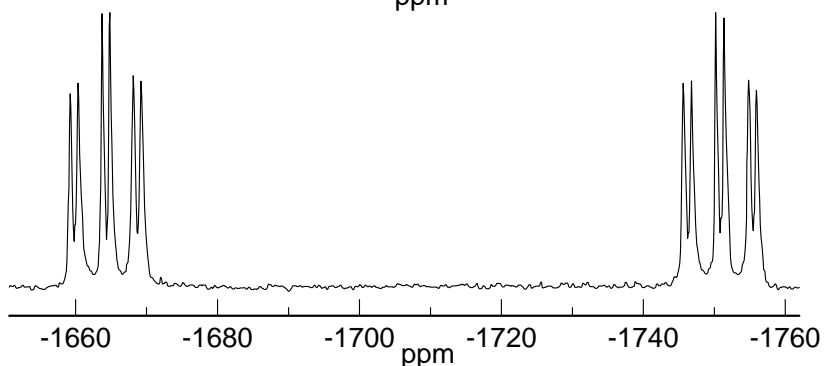
Spectrum 3. 18.075 MHz ^{14}N NMR spectrum of $[CH_3C{\equiv}N\text{-}Xe\text{-}F]^+ AsF_6^-$ in HF at -10 °C
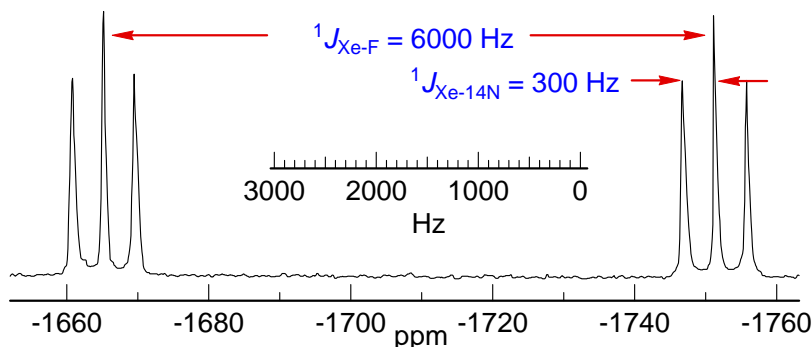

(a) Analyze Spectrum **1** and **2**. Spectrum **2** is of a compound labeled >99% with ^{13}C at the CN carbon. Report coupling constants. Use the form $^nJ_{X\text{-}Y}$ = 00.0 Hz.

(b)   Analyze Spectrum **3**. Make sure you understand and explain the origin of all peaks. Why are the signals somewhat broadened?
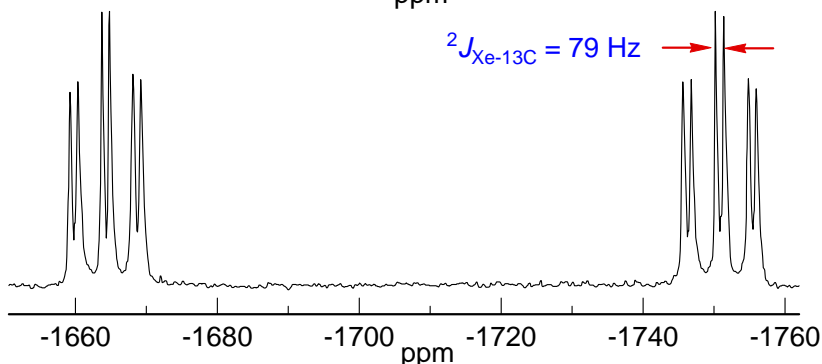
Problem R-11U ($C_2H_3AsF_7NXe$). This problem requires you to interpret the ^{129}Xe and ^{14}N spectra of $[CH_3C{\equiv}N\text{-}Xe\text{-}F]^+ AsF_6^-$ (Emara, A. A. A; Schrobilgen, G. J. *Chem. Commun.* **1987**, 1644)

Spectrum 1. 69.56 MHz ^{129}Xe NMR spectrum of $[CH_3C{\equiv}N\text{-}Xe\text{-}F]^+ AsF_6^-$ in HF at -10 °C

^{129}Xe, I = 1/2, 26.3% abundant

$^1J_{Xe\text{-}F}$ = 6000 Hz

$^1J_{Xe\text{-}14N}$ = 300 Hz

Spectrum 2. 69.56 MHz ^{129}Xe NMR spectrum of $[CH_3{}^{13}C{\equiv}N\text{-}Xe\text{-}F]^+$ AsF_6^- in HF at -10 °C

$^2J_{Xe\text{-}13C}$ = 79 Hz

Spectrum 3. 18.075 MHz ^{14}N NMR spectrum of $[CH_3C{\equiv}N\text{-}Xe\text{-}F]^+ AsF_6^-$ in HF at -10 °C

^{14}N, I = 1, 99.6% abundant
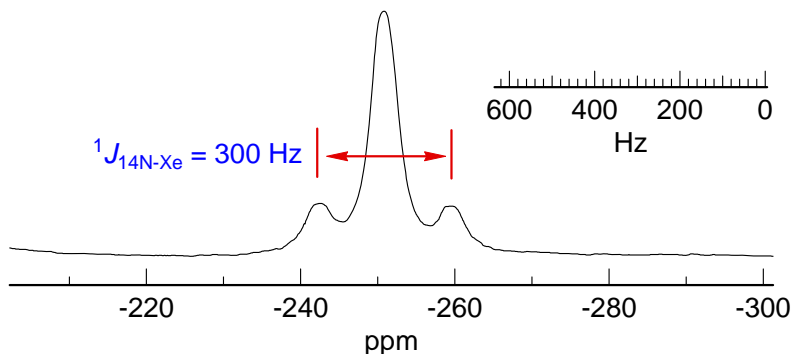
$^1J_{14N\text{-}Xe}$ = 300 Hz

(a) Analyze Spectrum **1** and **2**. Spectrum **2** is of a compound labeled >99% with ^{13}C at the CN carbon. Report coupling constants. Use the form $^nJ_{X\text{-}Y}$ = 00.0 Hz.

δ_{Xe} = 1708 ppm

$^1J_{Xe\text{-}F}$ = 6000 Hz

$^1J_{Xe\text{-}14N}$ = 300 Hz

$^2J_{Xe\text{-}13C}$ = 79 Hz

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Spectrum 1: a doublet (coupling to ^{19}F) of 1:1:1 triplets (from coupling to ^{14}N), J = 6000, 300 Hz

Spectrum 2: a doublet of 1:1:1 triplets of doublets, J = 6000, 300, 79 Hz

(b) Analyze Spectrum **3**. Make sure you understand and explain the origin of all peaks. Why are the signals somewhat broadened?

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Central peak: all of the isotopes of Xe except ^{129}Xe

Outer peaks: ^{129}Xe satelites due to ^{129}Xe - ^{14}N coupling, J ca 300 Hz

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The signals are broadened because ^{14}N T_1 is quite short due to quadrupolar relaxation. There are probably also broadening effects from unresolved coupling to F and CH_3.