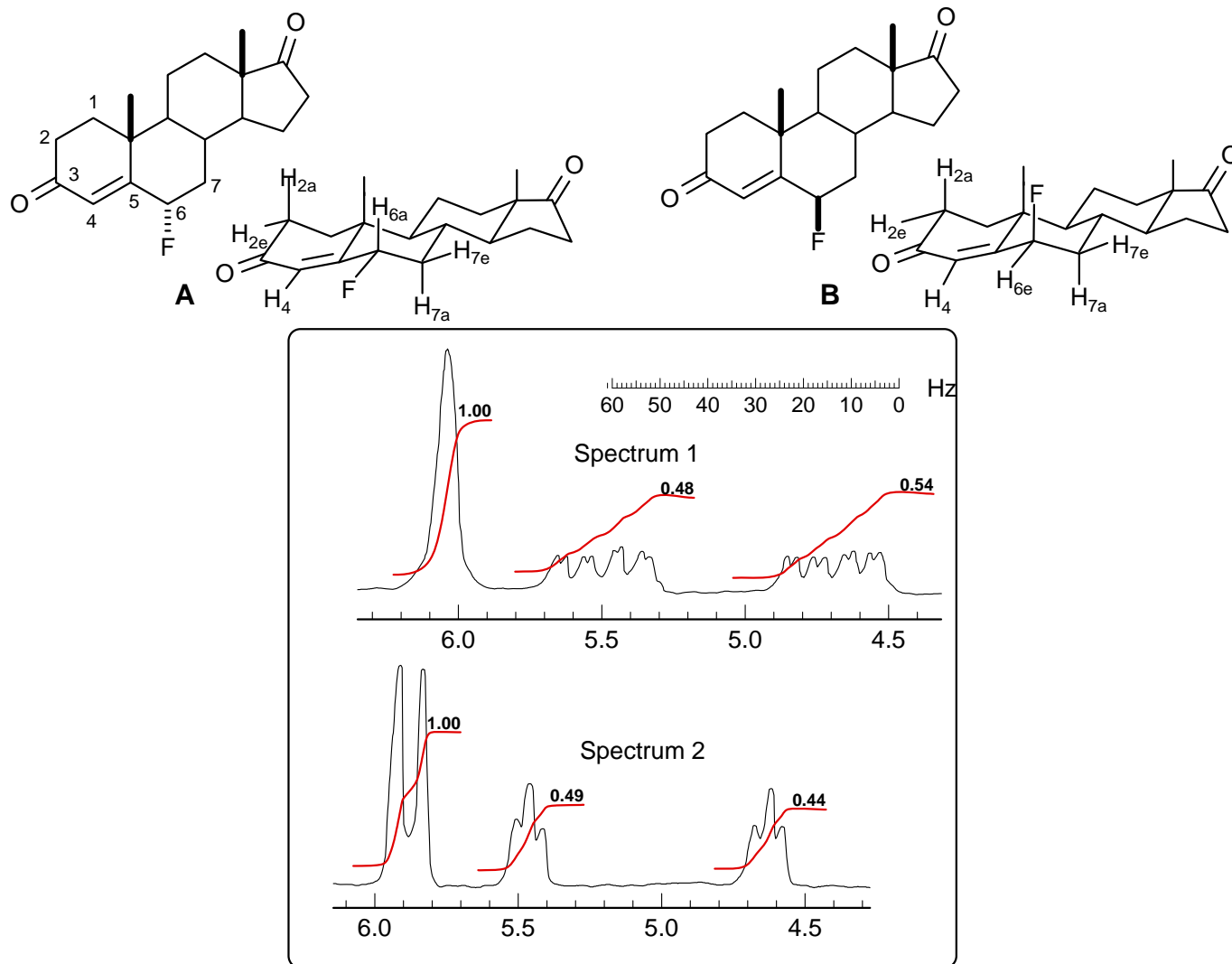


Problem R-11T ($C_{19}H_{25}FO_2$). Below are part of the 60 MHz 1H NMR spectra of two stereoisomers (**A** and **B**) of the fluorinated steroids shown. To aid in your analysis, a conformational drawing is also provided (*J. Am. Chem. Soc.* **1963**, 85, 3038; DOI: 10.1021/ja00902a046).



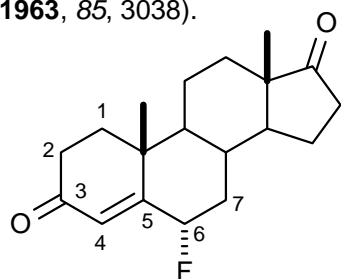
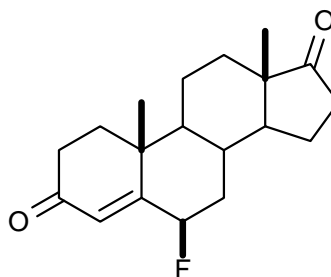
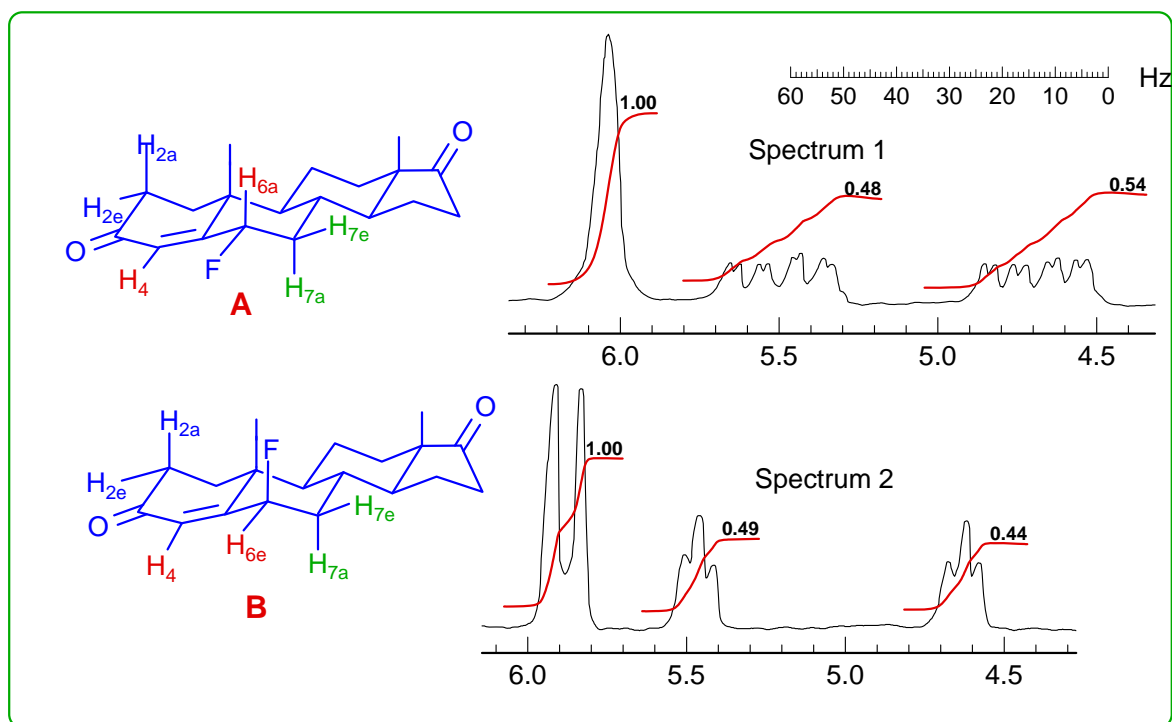
(a) Which protons are being shown here? Analyze the coupling, and report them in the standard format (give δ and identify any couplings you found).

Spectrum 1:

Spectrum 2:

(b) Which isomer corresponds to Spectrum 1 _____, which to Spectrum 2 _____. Explain briefly.

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**A****B**

(a) Which protons are being shown here? Analyze the coupling, and report them in the standard format (give δ and identify any couplings you found).

Spectrum 1:

6

δ 6.05, broad s, H^4

δ 5.1, dddd, $J = 48, 11, 6, 2$ Hz

$$^2J_{H6a-F} = 48 \text{ Hz}$$

$$^3J_{H6a-7a} = 11 \text{ Hz}$$

$$^3J_{H6a-7e} = 6 \text{ Hz}$$

$$^4J_{H6a-4} = 2 \text{ Hz}$$

Spectrum 2:

7

δ 5.89, d, $J = 5$ Hz

δ 5.05, dt, $J = 51, 3$ Hz

$$^2J_{H6e-F} = 51 \text{ Hz}$$

$$^3J_{H6e-7a} = 3 \text{ Hz}$$

$$^3J_{H6e-7e} = 3 \text{ Hz}$$

$$^4J_{H6e-4} < 2 \text{ Hz}$$

(b) Which isomer corresponds to Spectrum 1 **A**, which to Spectrum 2 **B**. Explain briefly.

3

The large H-H coupling in Spectrum 1 ($^3J_{H6a-7a} = 11$ Hz) requires that the proton at H^6 be axial, to get one large ax-ax coupling. The vicinal couplings in Spectrum 2 are all small (3 Hz) so only eq-eq and eq-ax coupling, hence H^6 must be equatorial.