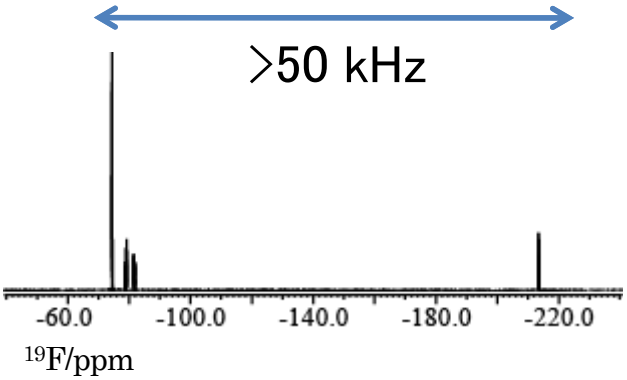
Determine number of fluorines attached to each carbon by ^{13}C NMR spectroscopy!

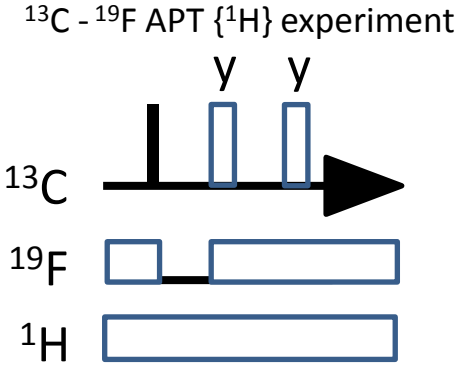
The number of fluorine attached to each carbon is useful in structure analysis of fluorinated compounds. ^{19}F signals are sometimes observed in a very wide chemical shift range. In that case, It is difficult to uniformly excite all ^{19}F signals, and hence APT(Attached Proton Test) experiment is more useful than DEPT.

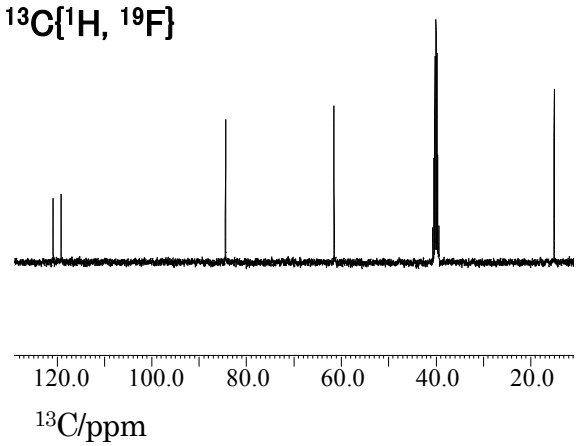
On the other hand, APT is less sensitive than DEPT, so we need to set a higher number of scans. The figures below show ^{19}F, ^{13}C and APT spectra of 5% ethyl 1,1,2,3,3,3-hexafluoropropyl ether in DMSO-d_6 . This sample has ^{19}F signals spread over a frequency range of over 50 kHz, and so uniform excitation is very challenging.

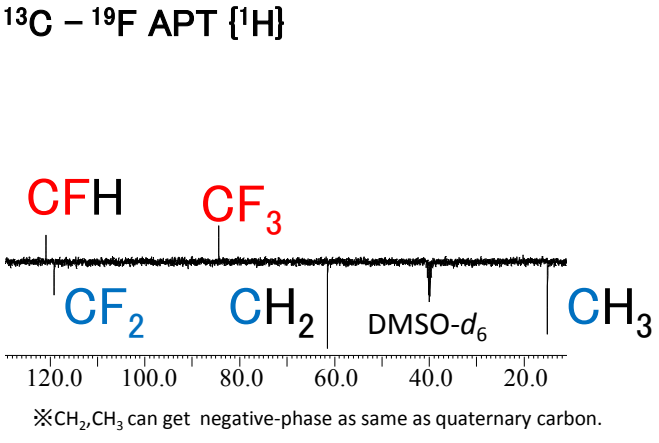
$$CF_3–CHF–CF_2–O–CH_2–CH_3$$

- In the ^{13}C-^{19}F APT spectra, ^{13}C signals of CF_3 and CF have positive signals, while CF_2, C and solvent signals have negative signals.
- By the application of ^{1}H decoupling, we can increase sensitivity!
- ROYALPROBE HFX can perform these ^{1}H,^{19}F,^{13}C triple-resonance measurements even with a standard 2-channel console!









※CH_2,CH_3 can get negative-phase as same as quaternary carbon.

^{13}C {^{1}H, ^{19}F} and ^{13}C-^{19}F APT {^{1}H} spectra, 32 scans

console : JNM-ECZ400S, ROYALPROBE HFX

JEOL Ltd.
3-1-2 Musashino Akishima Tokyo 196-8558 Japan Sales Division Tel. +81-3-6262-3560 Fax. +81-3-6262-3577
www.jeol.com ISO 9001 • ISO 14001 Certified
▼ Local offces
• AUSTRALIA & NEW ZEALAND • BELGIUM • BRAZIL • CANADA • CHINA • EGYPT • FRANCE • GERMANY • GREAT BRITAIN & IRELAND • ITALY • KOREA • MALAYSIA • MEXICO • RUSSIA • SCANDINAVIA • SINGAPORE • TAIWAN • THE NETHERLANDS • USA