Structural analysis of fluorine-containing compounds by NMR using CFH triple resonance probe

A NMR spectrum of fluorine-containing compounds is usually complicated because of the effect derived from strong spin-spin coupling with ^{19}F nucleus, and this makes it difficult to interpret the spectrum in detail. CFH triple resonance probe enables applying new techniques of ^{19}F decoupling and two dimensional NMR of ^{19}F-^{13}C and ^{19}F-^{19}F correlation, and this allows detailed structural analyses.

Features of CFH triple resonance probe

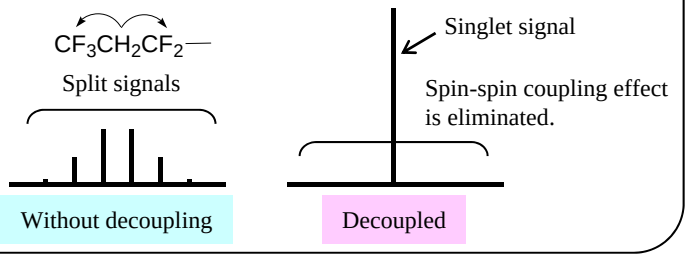
With CFH triple resonance probe, simultaneous ^{1}H and ^{19}F decoupling is available, and various two dimensional correlation spectra concerning ^{19}F nucleus also are applicable.

Applications fluorine-containing compounds, (fluorine) resins, LCM, surfactant, silane coupling agent, electrolytes etc.

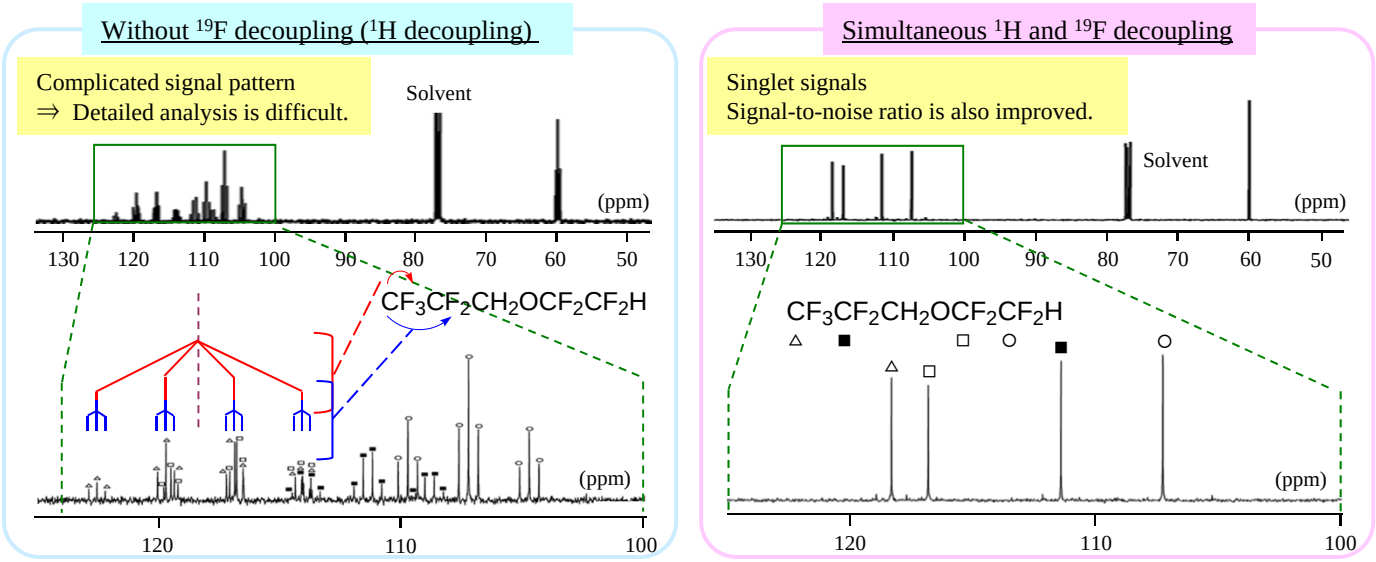
About spin-spin coupling

Spin-spin coupling: Because of the interaction of nuclear spins with bonding electron spins, NMR signals are split.

Decoupling: Eliminate the coupling effect by the irradiation at the resonance frequency of coupled nuclei.

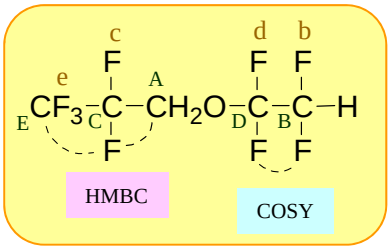


Simultaneous ^{1}H and ^{19}F decoupling on ^{13}C NMR measurement



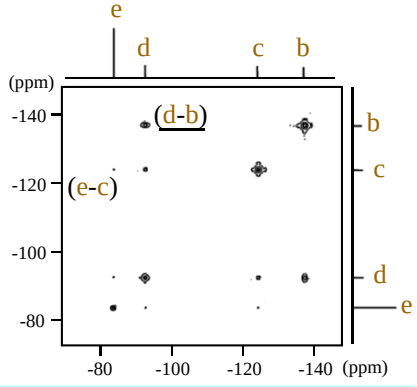
^{13}C NMR spectra of hydrofluoroether ($CF_3CF_2CH_2OCF_2CF_2H$)

Structural analysis by 2D NMR using CFH triple resonance probe



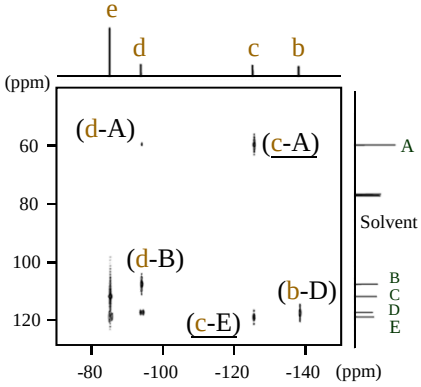
COSY (COrrelation SpectroscopY)
HMBC (Heteronuclear Multiple Bond Connectivity)

^{19}F-^{19}F COSY spectrum



From the correlation signal of d-b, it is found that fluorine atoms of b and d are at the adjacent position.

^{19}F-^{13}C HMBC spectrum



From the correlations of c-A and c-E, connectivity of A-C-E is estimated.