How to Observe ^{19}F on Ares

Note: Ares is the only spectrometer on which you can observe ^{19}F at present.

1. Place your sample in the magnet, lock, and shim. Type 'rpar' [enter] and select F19CPD. Type 'eda' [enter] and select the proper solvent. There is no need to click the little blue test tube. Set the appropriate number of scans (ns) for your concentration bearing in mind that ^{19}F is just as sensitive as ^{1}H.

2. Go over to the magnet and disconnect the ^{1}H channel cable from the probe. Next, disconnect the BB cable from the probe and connect it to the ^{1}H channel. Follow the BB cable over the HPPR (box on floor), and disconnect the two filters in place (ie. Connect the BB cable directly to the HPPR bypassing the filters).

3. Go back to the workstation. Type 'rga' [enter]. When rga is finished. Type 'wobb' [enter]. Click the little button that looks like this ▽   and type in 15. Go back to the spectrometer and use the ^{1}H tune and match screws to tune to the ^{19}F nucleus (as soon as you start to get a response from one screw, you should switch to the other, and go back and forth until you have optimized it to the best of your ability). **NOTE: It is IMPOSSIBLE to get it perfectly tuned and matched.** Contact Russ if you are uncertain about the procedure.

4. When you are tuned and matched to the best of your ability, go back to the workstation and type 'stop' [enter] and 'return' [enter]. Type 'rga' [enter] again and when it is finished you can begin your acquisition with 'zz' [enter]. Process the same way. If you need to reference your 19F nuclei you will either need an internal or external 19F standard. Some people use CFCl3 as an external standard at 0ppm (see below for chart of 19F chemical shifts vs. CFCl3).

5. When you are finished, return the cables to their original positions on the probe and put the filters back in line. Either move to an old ^{1}H data set, or create a new one, type 'rga' [enter]. When rga is finished, type 'wobb' [enter], and once again, click on the ▽ button and change it to 15 and then go over and tune and match the probe back to ^{1}H. **NOTE: It IS POSSIBLE to get 1H perfectly tuned and matched.** When you are finished, type 'stop' [enter] and 'return' [enter]. If you cannot tune and match the probe, contact Russ.

Table of Chemical Shift Ranges

Type of Compound	Chemical Shift Range (ppm) Relative to neat CFCl3

-F-C=O	-70 to -20
-CF3-	+40 to +80
-CF2-	+80 to +140
-CF-	+140 to +250
-ArF-	+80 to +170

Chemical Shift Table For certain compounds, the listed chemical shift pertains to the **F** shown in bold. The primary references for these values are:
1) the 1991 Bruker Almanac, and
2) Compilation of reported F19 NMR chemical shifts, 1951 to mid-1967 by Claude H. Dungan and John R. Van Wazer.
Negative shifts are those that appear upfield of CFCl3 and positive shifts are those that appear downfield.

Compound	Chemical Shift (ppm) Relative to neat CFCl3
CFCl3	0.00
MeF	-271.9
CF3H (in CFCl3)	-78.6
CF3H (in EtO)	-78.6
CF2H2	-143.6
EtF	-213
FCH=CH2	-114
F2C=CH2	-81.3
F2C=CF2	-135
CF3COOH (in CFCl3)	-76.55
CF3COOH (neat)	-78.5
CF3COOH (in CCl4	-76.3
CF3COOC6H6	-73.85
CF3COOCH2C6H6	-75.02
CF3COOCH3	-74.21
CF3COOEt (neat)	-78.7
CF3COO(CH2)n	-74 to -75
C6F6	-164.9
C6H5F	-113.5
p-FC6H4F	-106.0

CFH2Ph	-207
C6H5CF3	-63.72
C4F8	-135.15
C5F10	-132.9
CF3R	-60 to -70
CHF2OR	~-82
(CF3)2CO	-84.6
CH2CN	-251
F2	+422.92
CF3Cl	-28.6
ClF3	+116, -4
ClF5	+247,+412
CF2Cl2	-8
CFCl2CFCl2	-67.8
CFBr3	+7.38
CF2Br2	+7
IF4**F**(equatorial)	+58.9
IF7	+170
AsF3	-40.6
AsF5	-66
[AsF6]-1	-69.5
BF3	-131.3
(CH3)2O.BF3	-158.3
(C2H5)2O.BF3	-153
[BeF4]-1	-163
MoF6	-278
ReF7	+345
SF6	+57.42
SO2F	-78.5
S2O5F2	+47.2
SbF5	-108
[SbF6]-1	-109
SeF6	+55
(C2H5)2SiF2	-143.0

SiF4	-163.3
[SiF6]-2	-127
TeF6	-57
WF6	+166
XeF2	+258
XeF4	+438
XeF6	+550
NF3	147
SOF2	75.68
C6H5SO2F (dilute)	65.464
C6H5SO2F (20% conc)	65.514
SF6 (dilute)	57.617
SF6 (10% conc	57.42
SO2F2	33.17
CBr3F (dilute)	7.388
CBr3F (80% conc)	7.043
CCl2F2	-6.848
CClF3	-28.1
PF3	-34.0
(CF3)3N (dilute)	-55.969
(CF3)3N (30% conc)	-55.969
CF3CF2CF2I	-60.470
CF4	-62.3
C6H5CF3 (dilute)	-63.732
C6H5CF3 (40% conc)	-63.370
PF5	-71.5
CCl2F.CCl2F (dilute)	-67.775
CCl2F.CCl2F (20% conc)	-67.834
(CF3)3CF	-74.625
CF3CO2H (dilute)	-76.530
CF3CO2H (20% conc)	-76.542
CF3(CF2)5CF3	-81.60
CF3(CF2)2CF3	-81.85
[CF3CF2CF2]N	-85.19

POF3	-90.7
CF3CF2C**F**2CF2CN	-107.1
CF3CF2CF2C**F**2CN	-105.764

Homonuclear Couplings

Listed Coupling constant values pertain to **F**s shown in **bold**.

Compound	Coupling Constant (Hz)
(**C**F3**C**F2)2NCF3	10.2
(CF3C**F**2)2NC**F**3	15.18
(CF3CF2)2NC**F**3	6.8
[C**F**3C**F**2]3N	13.6
CF3C**F**2N[CF3]2	<1
CF3CF2N[C**F**3]2	16
CF3C**F**2N[C**F**3]2	6
(**C**F3**C**F2)2O	3.4
(**C**F3]3**C**F	1.4
CF3**C**F2H	2.8
CF3**C**FH2	15.5
CF3C**F**2CH**F**2	4.5
C**F**3CF2CH**F**2	7.3
CF3C**F**2CH2**F**	15.2
C**F**3CF2CH2**F**	7.9
CF2Cl.C**F**2.CH2**F**	15.1
CF2Cl.C**F**2.CH2**F**	7.7
CF2Cl.C**F**2.CH2F	3.9
CF2Br.C**F**2.CH2**F**	15.5
CF2Br.C**F**2.CH2**F**	7.7
CF2Br.C**F**2.CH2F	3.9
C**F**FBr.CHFBr	21
CF**F**Br.CHFBr	24
C**FF**Br.CHFBr	174
C**F**FBr.CHFCl	18
CF**F**Br.CHFCl	18
C**FF**Br.CHFCl	177

CFF Br.**CF**ClBr	13
CFFBr.**CF**ClBr	14
CFFBr.CFClBr	159
CF**F**(SiCl3).**CF**ClBr	16.8
C**FF**(SiCl3).**CF**ClBr	16.8
C**FF**(SiCl3).CFClBr	343
CF3.**CFF**.CFlCl	270.4
CFF=CFCl	76
CFF=C**F**Cl (cis)	56
CFF=C**F**Cl (trans)	116
C**F**Cl=C**F**Cl (cis)	37.5
C**F**Cl=C**F**Cl (trans)	129.57
CFF=CFCF3	57
CFF=CFCF3 (cis)	39
CFF=CFC**F**3 (trans)	116
CFF=CFCF3 (trans)	8
CFF=CFC**F**3 (cis)	22
CFF=C**FCF**3	13
(cyclopropane) CH2.**CFF**.CHCH3	157
(cyclobutane) CH2.**CFF**.CCl2.CCl2	187
(cyclobutene) C**FF**.CH(C2H5).CCl2=CCl	192
(cyclobutane) **CFF**.CFF.CH2.CHCClH2	230
(cyclobutane) CFF.**CFF**.CH2.CHCClH2	240
(cyclohexane) CFH.CFH.CFH.CFH.CFH.C**FF**	284