ELECTRONIC SUPPORTING INFORMATION

The Role of Photocatalysts in Radical Chains of Homolytic Aromatic Substitutions, Radical Addition to Olefins, and Nucleophilic Radical Substitution Mechanisms

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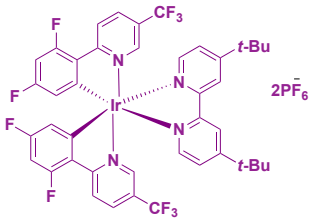
II.-Photocatalytic Reactions. General Procedures

In a 3 mL-reaction vial provided with screw-cap septum and micro stir bar, 0.6 mmol (or 0.2 mmol when noted, as in Table 2) of substrate **1**, 2, or **3** were introduced. 0.5 mol% of PC-1 ($Ir[(dF(CF_3)ppy]_2(dtbbpy)^+$), or 5 mol% of PC-2 (Rose Bengal) or 5 mol% of PC-3 (Zinc phthalocyanine) were introduced. Subsequently, 1.5 equiv of additive (Cs_2CO_3 for PC-1 and PC-2, and ascorbic acid (1.5) collidine (1.5) for PC-3) are placed. Solvent was then introduced (2.5 mL, CH_3CN when using PC-1 and PC-2, and a 1 : 1 mixture of CH_3CN : DMF for PC-3) were added and the mixture is de-oxygenated with a stream of dry Ar for 15 minutes. After deoxygenation, 3 equivalents of R_F-I (*n*-C_4F_9-I) are then introduced through the septum with microliter syringe. A brief deoxygenation with a slight stream of Ar is passed through for 3 additional minutes. The vessel is placed on a stir plate above the heat dissipator, according to Figures S4-S6. and stirred vigorously for 20 hrs. (at 22 °C) under constant irradiation with high power LED for product isolation, or 60-90 s for quantum yield calculation. After the reaction time elapsed, the mixture was extracted thrice with brine/DCM, and the DCM/DMF extracts evaporated in vacuo. TLC analyses were performed employing dichloromethane:*iso*octane (7 : 3) mobile phase (or otherwise noted). The crude residues were analyzed by ^1H NMR, and an ^{19}F NMR integration of the product area is measured. Other runs contain internal standard benzotrifluoride. For isolation purposes, the crude mixture was placed on a silica-gel preparative thin layer glass support and eluted with $CHCl_3$: MeOH or else by column chromatography which was carried out instead of thin layer preparative chromatography. The products reveal intensely under 254 nm-light. The eluants were gathered, evaporated under vacuo, yields calculated by weight and characterized by standard spectroscopic techniques (section VI). NMR integration yields reflect the % of product(s) calculated with the aid of an internal standard (benzotrifluoride for ^{19}F NMR spectra, and 1,3,5-

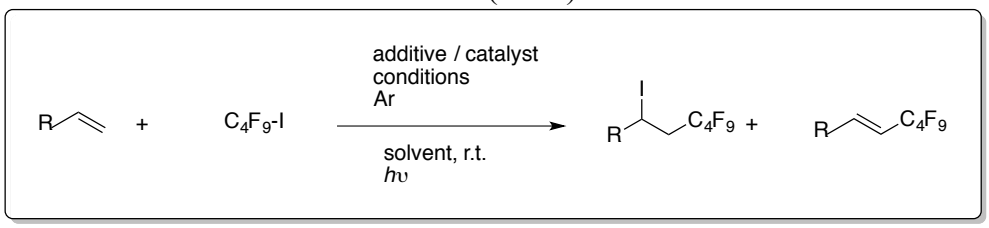
trimethoxybenzene for ^{1}H NMR spectra). For perfluoroalkylthio ether products, a CAM (ceric ammonium molybdate) solution was employed to follow up the reactions by TLC.

III.- Optimization of Reaction Conditions for the Three Photocatalytic Reactions

Table S1. Optimization of reaction conditions for the employment of Ir[(dF(CF$_3$)ppy]$_2$(dtbbpy)$^+$ (PC-1) as photocatalyst in the perfluorobutylation of olefinic systems under blue light irradiation for 20 h



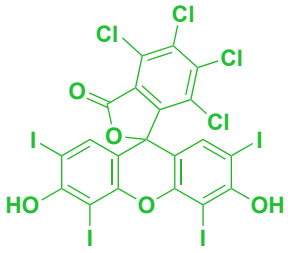
PC-1 (Ir PC)



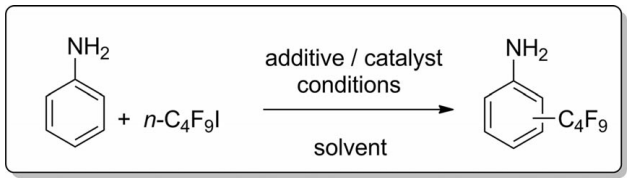
entry	Additive (equiv)/ Catalyst[a]	Irradiation sources	Solvent	Yield (%)[b]
	PC / light source			
1	Cs_2CO_3 (1.5)/ Ir PC	CFL	MeCN	53%[c]
2	Cs_2CO_3 (1.5)/ Ir PC	Blue LED	MeCN	53%[c]
	PC Ir, base, H donor			
3	Li_2CO_3 (1)/ Ir PC	Blue LED	MeCN	0%
4	Na_2CO_3 (1)/ Ir PC	Blue LED	MeCN	6%
5	Cs_2CO_3 (1)/ Ir PC	Blue LED	DMA	0%
6	Cs_2CO_3 (1)/ Ir PC	Blue LED	THF	0%
7	Cs_2CO_3 (1)/ Ir PC	Blue LED	DMF	3%
8	------/ Ir PC	Blue LED	MeCN	0%
9	Cs_2CO_3 (1), THF (1)/ Ir PC	Blue LED	MeCN	9%
10	Cs_2CO_3 (1), TMSS(1)/ Ir PC	Blue LED	MeCN	9%
11	Cs_2CO_3 (1), H_2PO_3 (1.5)/Ir PC	Blue LED	MeCN	3%
	No additive, or PC, or light, or presence of air			
12	----	Blue LED	MeCN	0%
13	Cs_2CO_3 (1)/-----	CFL	MeCN	10%
14	Cs_2CO_3 (1)/ Ir PC	---------	MeCN	0%

[a] Ir PC: (Ir [dF(CF$_3$)PPy]$_2$(dtbPy))PF$_6$ (0.5 mol%).
[b] Total product yield (perfluoroalkylated products) based on NMR integration with internal standard (benzotrifluoride). The substrate used was a glycal: per-acetylated-2-acetoxy galactal. Yields refer to global product yield
[c] 46% isolated

Table S2. Optimization of reaction conditions for the employment of Rose Bengal (PC-2) as photocatalyst in the perfluorobutylation of aniline



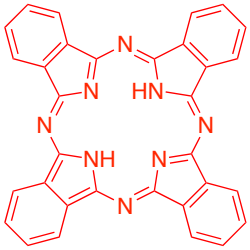
PC-2 (RB)



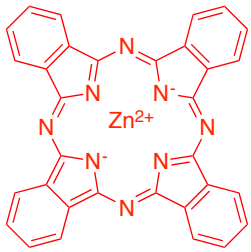
entry	[An]/[R_F-I]/[additive]	additive	conditions	solvent	% 1A[a]
1	1 : 3 : -	-	r.t. / CFL[f]	MeCN	52
2	1 : 3 : 1.5	Cs_2CO_3	r.t. / CFL[f]	MeCN	98
3	1 : 3 : 1.5	Cs_2CO_3	r.t. / CFL[f]	MeCN	81[b]
4	1 : 3 : 1.5	Cs_2CO_3	r.t. / CFL[f]	MeCN	62[c]
5	1 : 3 : 1.5	Cs_2CO_3	r.t. / CFL[f]	H_2O	< 5
6	1 : 3 : 1.5	Cs_2CO_3 /w/o RB	r.t. / CFL	MeCN	50[d]
7	1 : 3 : 1.5	Cs_2CO_3	r.t. / CFL[f]	MeCN	78[e]
8	1 : 3 : 1.5	Cs_2CO_3	r.t. / CFL[f]	MeCN	91
9	1 : 3 : 1.5	Cs_2CO_3	r.t. / dark	MeCN	-

a Yields determined from ^{19}FNMR and ^{1}H NMR spectral integration
b 18 hr reaction
c employing Eosin Y as PC
d without PC RB
e without de-oxygenation
f CFL = compact fluorescent lamp used gave the same results as Green LED for optimization

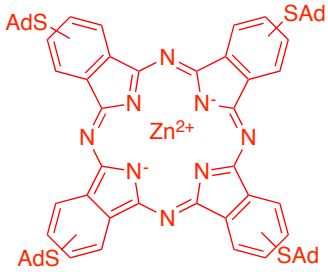
Table S3. Optimization of reaction conditions for photocatalysts (**3-5**) absorbing in the red-region of the electromagnetic spectrum. Reactions of aniline (0.2 mmol) with *n*-C_4F_9I (3 equiv.) in solvent (3 mL, Ar-deoxygenated) under photocatalysis (PC, 0.01 equiv. or otherwise noted), with vigorous constant stirring, under irradiation for 24 h. Substitution product: 2-perfluorobutylaniline and 4-perfluorobutylaniline isomers



PC-4, 29H,31H-Phthalocyanine



PC-3, phthalocyanine Zn salt

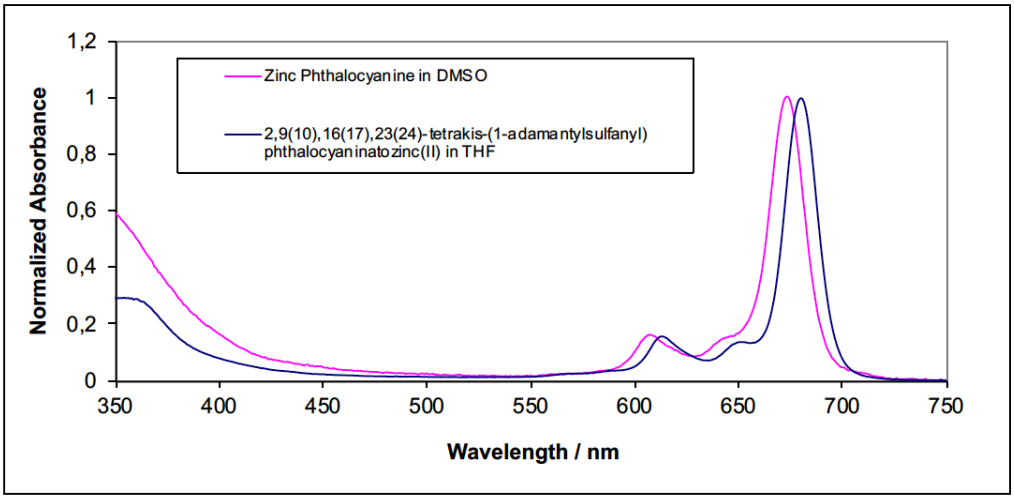


PC-5 SAd = thioadamantyl

entry	PC (equiv.)	Base (equiv.)	Additive (equiv.)	Solvent (mL)	Yield, [a] %
1	**5** (0.018)	TMEDA (1.5)	$Na_2C_2O_4$ (1.5)	MeCN:DMSO (2.1:0.5)	-
2	**5** (0.018)	TMEDA	Ascorbic acid (1.5)	MeCN:DMSO (2.1:0.5)	27
3	**5** (0.018)	2,4,6-collidine (1.5)	Ascorbic acid (1.5)	MeCN:DMF (2.1:0.5)	< 30
4	**5** (0.018)	2,4,6-collidine (1.5)	Ascorbic acid (1.5)	DMF (3)	< 60
5	**5** (0.018)	2,4,6-collidine (1.5)	Ascorbic acid (1.5)	MeCN:DMSO (2.1:0.5)	90
6	**4**, (0.018)	2,4,6-collidine (1.5)	Ascorbic acid (1.5)	THF (3)	30
7	**4**, (0.018)[b]	1.5	1.5	THF (3)	-
8	**3,** (0.018)	2,4,6-collidine 1.5	Ascorbic acid (1.5)	MeCN:DMF (1.5:1.5)[c]	93

a.- ^{19} F NMR and ^{1}H NMR yields (benzotrifluoride as internal standard) of combined *o*-perfluorobutylaniline and *p*-perfluorobutylaniline
b .-Addition of $Zn(OAc)_2$, 2 mg
c.-The necessity of a co-solvent arises from the low solubility of Photocatalyst 3 in MeCN

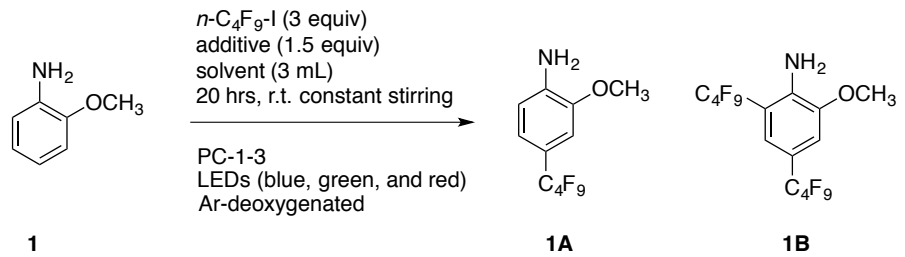
Figure S1. UV-visible spectra of Phthalocyanine Photocatalysts PC-3 and PC-5



The synthesis of **PC-5** i.e.: 2,9(10),16(17),23(24)-tetrakis-1-(adamantyl)sulfanyl)phthalocyaninatozinc (II), has been carried our according to literature procedures.[4]

IV.-Summary of Photocatalytic Reaction Conditions for Substrates 1-3 and Products 1A-3A

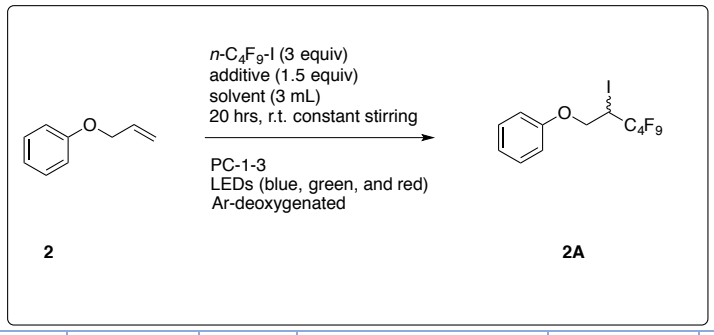
Table S4. Reaction products form the perfluorobutylation of substrate **1** (0.2 mmol) with *n*-C_4F_9-I (3 equiv) employing different PCs (PC-1-3) in indicated Ar-deoxygenated solvent (3 mL), in the presence of additives irradiating at room temperature for 20 h under constant stirring



Entry	System	PC (mol%)	λ_{max}[a] nm	Additive (equiv)	Solvent	Mass balance,[b] %	**1A:1B** Product ratio, %
1	1	PC-1 (0.5)	392[d]	Cs_2CO_3 (1.5)	CH_3CN	94	80:20
2	2	PC-2 (5)	525[e]	Cs_2CO_3 (1.5)	CH_3CN	97	83:17
3	3	PC-3 (5)	657[f]	Ascorbic acid (1.5) 2,4,6-collidine (1.5)	CH_3CN: DMF	98	82:18

a.- λ_{max} of irradiation (LED) employed
b.- ca. 100% mass balance was obtained, indicating that substrate converts only to products shown.
c.-Product **1B** was not isolated, but characterized in the reaction mixture
d.-violet LEDs, 3 Watts
e.-green LEDs, 3 Watts
f.-red LEDs, 3 Watts

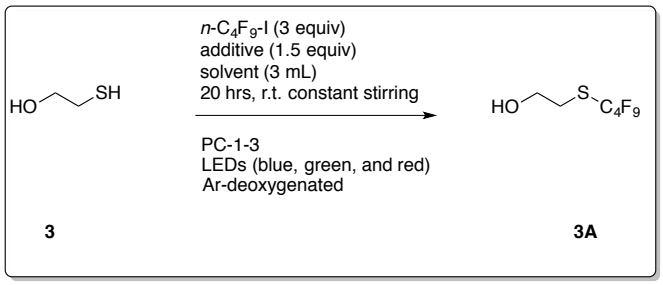
Table S5. Reaction products form the perfluorobutylation of substrate **2** (0.2 mmol) with *n*-C_4F_9-I (3 equiv) employing different photocatalysts PC (PC-1-3) in indicated Ar-deoxygenated solvent (3 mL), with additives at room temperature for 20 h under constant stirring.



Entry	System	PC (mol%)	λ_{max}, nm	Additive	Solvent	Mass balance,[a] %
1	1	PC-1 (0.5)	392[b]	Cs_2CO_3 (1.5 equiv)	CH_3CN	99
2	2	PC-2 (5)	525[c]	Cs_2CO_3 (1.5 equiv)	CH_3CN	98
3	3	PC-3 (5)	657[d]	Ascorbic acid (1.5 equiv) 2,4,6-collidine (1.5 equiv)	CH_3CN: DMF	99

a.- ca. 100% mass balance was obtained, indicating that substrate converts only to product shown.
b.-violet LEDs, 3 Watts
c.-green LEDs, 3 Watts
d.-red LEDs, 3 Watts

Table S6. Reaction products form the perfluorobutylation of substrate **3** (0.2 mmol) with *n*-C_4F_9-I (3 equiv) employing different photocatalysts PC (PC-1-3) in indicated Ar-deoxygenated solvent (3 mL), with additives at room temperature for 20 h under constant stirring.



Entry	System	PC (mol%)	λ_{max}, nm	Additive	Solvent	Mass balance,[a] %
1	1	PC-1 (0.5)	392[b]	Cs_2CO_3 (1.5 equiv)	CH_3CN	100
2	2	PC-2 (5)	525[c]	Cs_2CO_3 (1.5 equiv)	CH_3CN	99.7

3	3	PC-3 (5)	657[d]	Ascorbic acid (1.5 equiv) 2,4,6-collidine (1.5 equiv)	CH_3CN:DMF	100

a.- ca. 100% mass balance was obtained, indicating that substrate converts only to product shown.
b.-violet LEDs, 3 Watts
c.-green LEDs, 3 Watts
d.-red LEDs, 3 Watts

V.-Mechanistic Probes and Luminescence Quenching Experiments

Table S7. Mechanistic Probe Experiments for the Use of PC-1 in the Perfluorobutylation of Substrates

Entry	Additive (equiv)/ Catalyst[a]	Irradiation source	Solvent	Yield (%) 1A
1	Cs_2CO_3 (1), *p*-dinitrobenzene (1) /Ir PC	Blue LED	MeCN	0
2	Cs_2CO_3 (1) /Ir PC/TEMPO	Blue LED	MeCN	0
3	Cs_2CO_3 (1) / 2-phenylpropene	Blue LED	MeCN	0

Table S8. Reactions probing the mechanism for the red-light-(or otherwise noted)-photocatalyzed perfluoroalkylation of aniline (0.2 mmol) with *n*-C_4F_9-I (3 equiv.), in the presence of ascorbic acid (1.5 equiv.), 2,4,6-collidine (1.5 equiv.) in Ar-deoxygenated (or otherwise noted) MeCN : DMF (1 : 1) as solvent, for 24 h. with 15-Watt red LEDs (or otherwise noted). Photocatalyst **2** (0.018 equiv.) employed.

entry	additive	Irradiation source (Watt)	PC (equiv.)	Yield 1A,[a] %
1	TEMPO[b]	Red LED (21)	**2** (0.018)	-
2	*p*-DNB[c]	Red LED (21)	**2** (0.018)	30
3	-	Red LED (21)[d]	**2** (0.018)	70
4	-	-[e]	**2** (0.018)	-
5	-	White light (40)	**2** (0.018)	30
6	-	Red LED (21)	**-**	< 5

a.- ^{19}F NMR and ^{1}H NMR yields (benzotrifluoride as internal standard) of combined *o*-perfluorobutylaniline
b.- 2,2,6,6-Tetramethyl-1-piperidinyloxy, 0.3 equiv.
c.-1,4-dinitrobenzene, 0.3 equiv.
d.-air-saturated MeCN : DMF
e.-24-h reaction conducted in the absence of light, with reaction vial wrapped up in aluminum foil.

Scheme S1. Mechanistic Probe Experiments for the Perfluorobutylation of Anisidine under Three Photocatalytic Systems. **A**.-Use of TEMPO under Three Photocatalytic Systems. **B**.- Use of 2-Phenylpropene as Probe under Three Photocatalytic Systems. **C**.- Use of p-Dinitrobenzene under Photocatalysis with PC-1 and PC-3. **D**.- Use of p-Dinitrobenzene under Photocatalysis with PC-2

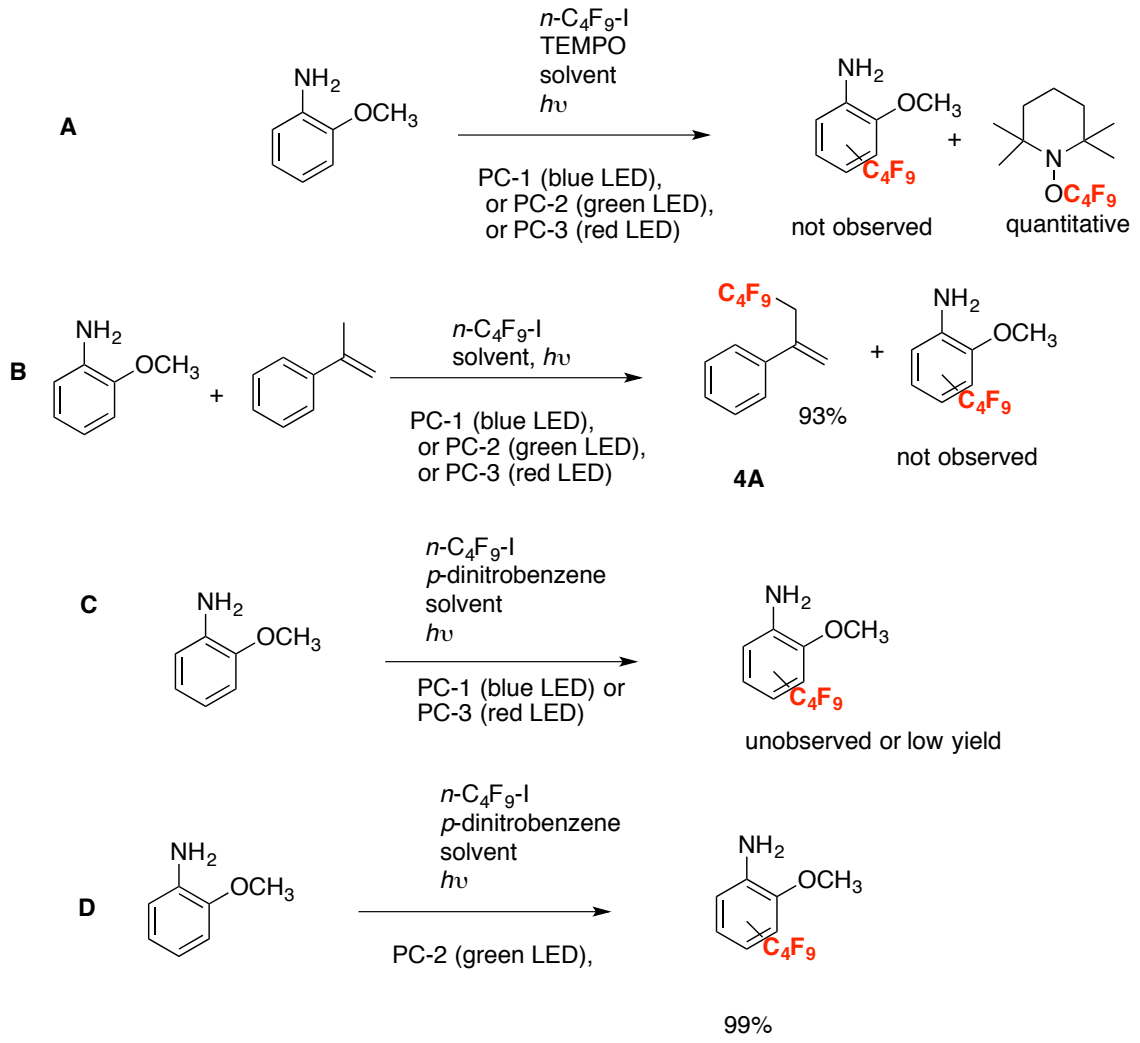
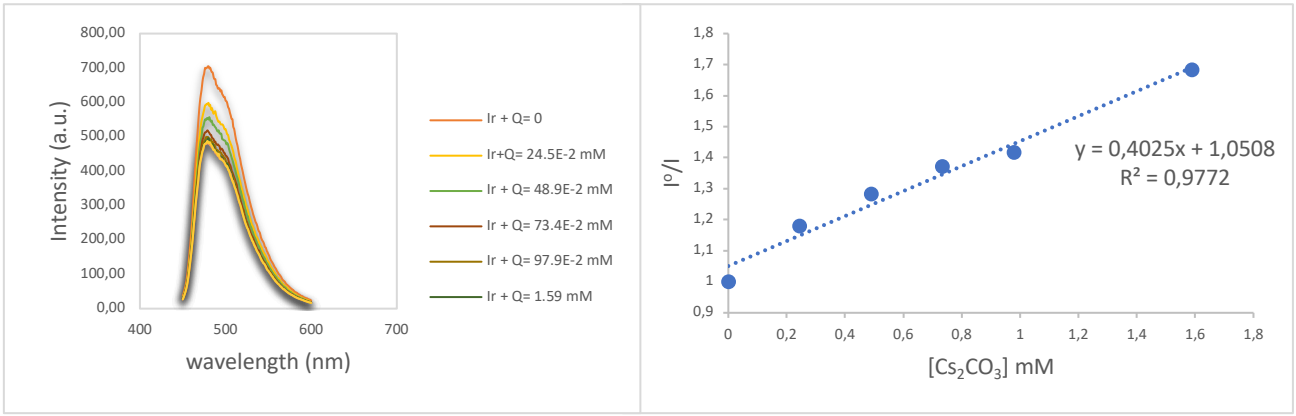
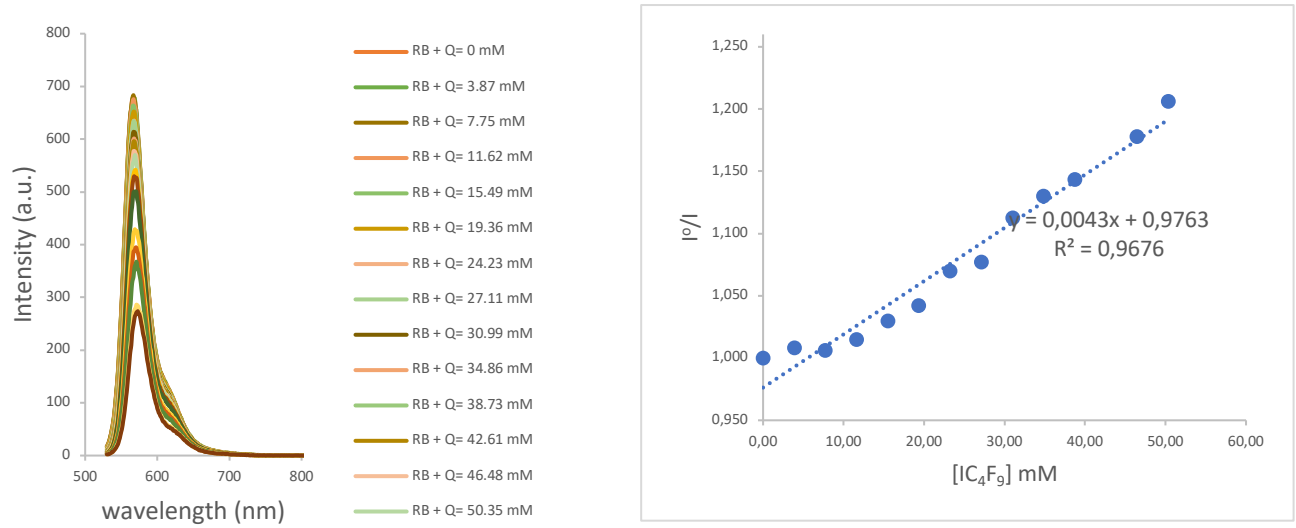


Figure S2. **A.-**Quenching of fluorescence of $Ir[(dF(CF_3)ppy]_2(dtbbpy)^+$ with Cs_2CO_3 DMF solution and Stern Volmer plots. K_{SV} = 402 M^{-1}. **B**.- Quenching of fluorescence of Rose Bengal with *n*-C_4F_9-I and Stern Volmer plots. K_{SV} = 4.3 M^{-1} **C**.- Quenching of fluorescence of Zn-Phthalocyanine with ascorbic acid/collidine and Stern Volmer plots (K_{SV} = 162 M^{-1}).

A



B



C

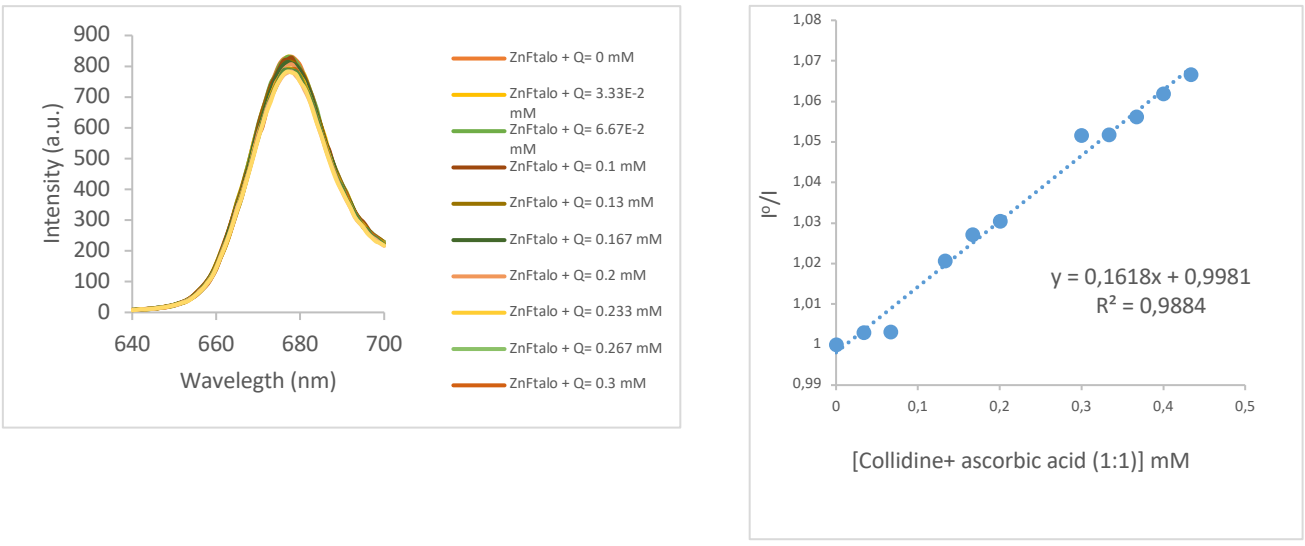
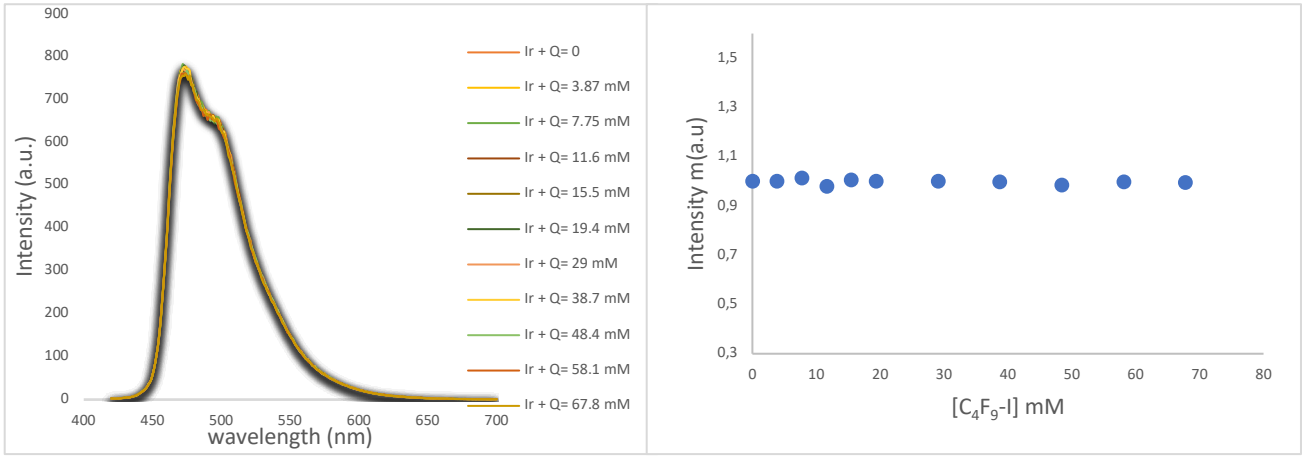


Figure S3. Attempts at quenching the fluorescence spectra of Ir[(dF(CF_3)ppy]$_2$(dtbbpy)$^+$ with *n*-C_4F_9-I. and Stern Volmer plot



VI.- Set-ups for Determination of Quantum Yields

Figure S4. Calibrated violet (392 nm) LEDs arrangement for the measurement of quantum yields of reactions with PC-1

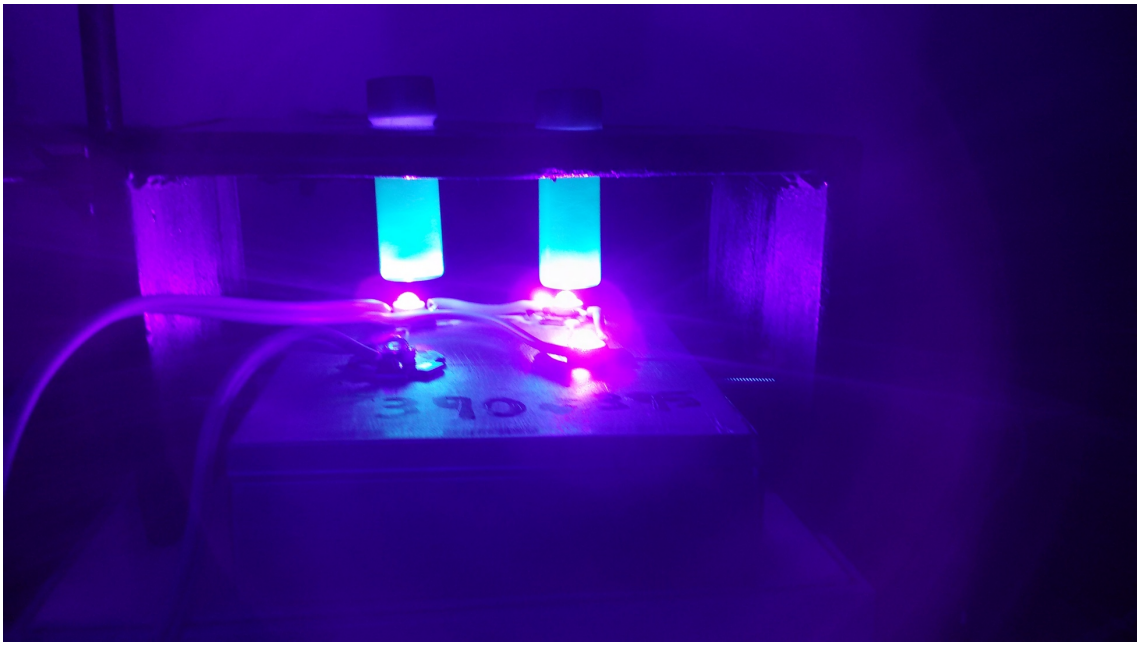


Figure S5. Calibrated green (525 nm) LEDs arrangement for the measurement of quantum yields of reactions with PC-2

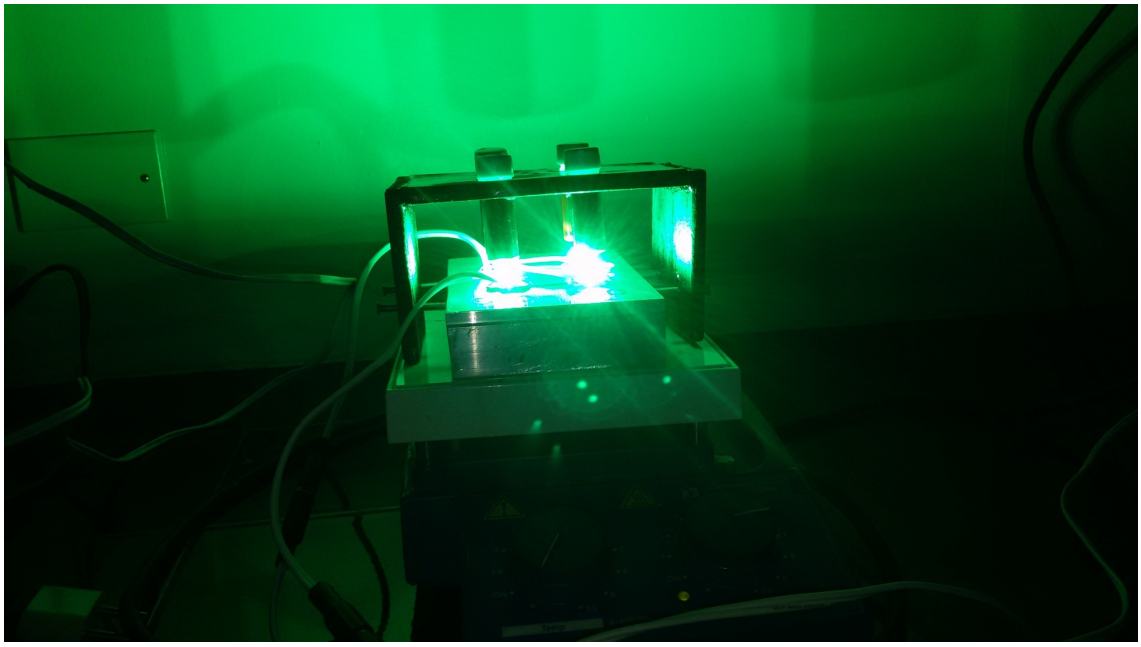
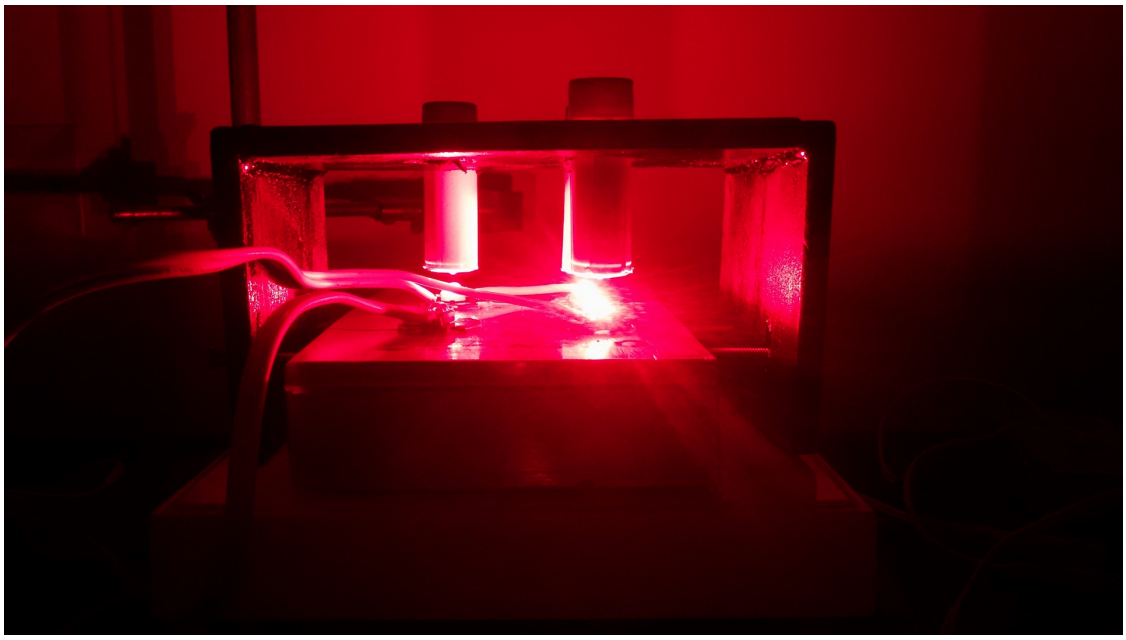


Figure S6. Calibrated red (657 nm) LEDs arrangement for the measurement of quantum yields of reactions with PC-3



VII.a.-Determination of Quantum Yields. From calibrated LEDs

The overall quantum yield for product formation from the perfluoroalkylation of substrates **1-3** can be calculated by dividing the moles of products **1A-3A,** formed by the einsteins of photons consumed (eq 1).

$$\Phi = \frac{\text{moles of product formed}}{\text{flux of moles photons x second}} \qquad (1)$$

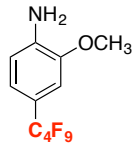
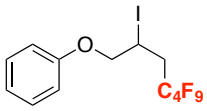
$$\text{flux of moles photons x second} = \frac{\lfloor E_T / hc/\lambda \rfloor}{NA} \text{ x irradiation time (sec)} \qquad (2)$$

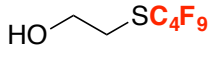
Absolute measurement of incident photon flux was achieved by means of calibrated photodiodes which are widely used for the detection of electromagnetic radiation in the ultraviolet, visible, and infrared range.[1] Silicon photodiodes for light power measurement with resolution of 1 nW were employed. For LEDs with emission maxima at 390 nm a calibrated UV-enhanced silicon sensor for 250-400 nm range (Coherent OP-2 UV) was used; and for LEDs with emission maxima at 525 nm and 657 nm a calibrated silicon sensor for 400-1064 nm (Coherent OP-2 VIS) was employed. In all cases, measurements of the light that passed through the bottom of the vial were performed at the mouth of the vial (vial walls were covered with a bright white optical film to ensure total light reflection).The incident photon flux measured by photodiodes was corroborated by chemical actinometry (potassium ferrioxalate for λ_{max} = 392 nm for PC-1, and λ_{max} = 525 nm for PC-2, and Reinecke salt, for λ_{max} = 657 nm, for PC-3).[1,2] Then, the expression of the flux of moles of photons can be obtained from equation 2, where E_T is the radiant power, *h* de Planck´s constant, c the light speed, λ the wavelength of the LED in meters, and NA the Avogradro´s number.

For the 392 nm LED (E_T = 8 mWatt), the photon flux (number of photons per second) is calculated to be 1.5786 x 10^{16} photons/sec., whereas for the 525 nm LED (with

an energy E_T of 10 mWatt), the photon flux is calculated to be 2.64291 x 10^{16} photons/sec. For the 657 nm LED (E_T = 16 mWatt), the photon flux is 5.29187 x 10^{16} photons/sec. These numbers should be divided by NA. Substrate **1-3**, and additives are transparent at all PCs maxima absorption wavelengths or diode emissions so we could make the limiting assumption that the incident photon flux is absorbed solely by the photocatalyst. After 2 hour- irradiation, the number of moles of product **1-3A** formed is quantified by ^{1}H and ^{19}F NMR spectroscopy using an internal standard (benzotrifluoride, see ESI).

Table S9. Number of moles products **1A, 2A, 3A** formed under the photocatalytic (PC-1-3) reactions of substrates **1-3** with *n*-C_4F_9-I

	entry	λ (nm)	PC	N° of moles x 10^3	Irradiation time
 **1A**[a]	1	392	PC-1	0.090	900 sec
	2	525	PC-2	0.04	1800 sec
	3	657	PC-3	0.112	7380 sec
 **2A**[c]	1	392	PC-1	0.02[b,c]	600 sec
	2	525	PC-2	0.157[b,c]	1200 sec
	3	657	PC-3	0.04[b,c]	5400 sec
	1	392	PC-1	0.160	150 sec
	2	525	PC-2	0.150	150 sec
	3	657	PC-3	0.0360[d]	1200 sec

 **3A**[d]					

a.-Product **1A** was quantified after work-up of the photoreaction, which was extracted into diethyl ether/water, the organic extracts dried and evaporated followed by NMR analysis in $CDCl_3$

b-1.5 equiv of n-C_4F_9-I used

c.-Due to the volatility of substrate **2**, the photoreaction was extracted into $CDCl_3$/water, the deuterated chloroform phase dried with anhydrous sodium sulfate, and subjected directly to NMR analyses without concentration

d.-The photoreaction is carried out in DMSO-d_6, in order to avoid extraction of **3** into the aqueous phase, with concomitant loss of substrate. Quantitative analysis was carried out directly by NMR techniques

The numerator of eq. 1 is calculated from the number of moles produced (column 5 x 10^{-3}) x NA. The number of photons emitted are calculated from the photon flux (*vide infra*) times the irradiation time in sec.

According to the procedure of Yoon and colleagues,[3] the quenching fraction *Q* is calculated according to eq 3:

$$Q = \frac{k_{q\,(\mathbf{PC}\,)}[\mathbf{Q}]}{\tau^{-1} + k_{q(\mathbf{PC})}[\mathbf{Q}]} = \frac{K_{SV}[\mathbf{Q}]}{1 + K_{SV}[\mathbf{Q}]} \qquad (3)$$

Where K_{SV} is the Stern-Volmer coefficient which is determined by Stern Volmer rate quenching experiments (Figure 2). Applying eq. 3, the *Q* values are illustrated in Table 4. The chain length (***L***) is more accurately approximated by dividing the measured quantum yield ϕ by the quenching fraction *Q*.

VII.b.- Determination of Photon Flux by Chemical Actinometry

Determination of the light intensity at 392 nm:

The photon flux of the high-power LED employed (392 nm, 8 mWatt) was also determined by standard ferrioxalate actinometry. A 0.15 M solution of ferrioxalate was prepared by dissolving 2.21 g of potassium ferrioxalate hydrate in 30 mL of 0.05 M H_2SO_4. A buffered solution of phenanthroline was prepared by dissolving 50 mg of phenanthroline and 11.25 g of sodium acetate in 50 mL of 0.5 M H_2SO_4. Both solutions were stored in the dark. To determine the photon flux of the diode, 2.0 mL of the ferrioxalate solution was placed in a cuvette and irradiated for 90.0 seconds at λ = 392 nm. After irradiation, 0.35 mL of the phenanthroline solution was added to the cuvette. The solution was then allowed to rest for 1 h to allow the ferrous ions to completely coordinate to the phenanthroline. The absorbance of the solution was measured at 510 nm. A non-irradiated sample was also prepared and the absorbance at 510 nm measured. Conversion was calculated using eq 1.

$$\text{mol } Fe^{2+} = \frac{V \bullet \Delta A}{l \bullet \varepsilon} \qquad (1)$$

Where V is the total volume (0.00235 L) of the solution after addition of phenanthroline, ΔA is the difference in absorbance at 510 nm between the irradiated and non-irradiated solutions, l is the path length (1.000 cm), and ε is the molar absorptivity at 510 nm (11,100 L mol^{-1} cm^{-1}). The photon flux can be calculated using eq 2.

$$\text{photon flux} = \frac{\text{mol } Fe^{2+}}{\Phi \bullet t \bullet f} \qquad (2)$$

Where Φ is the quantum yield for the ferrioxalate actinometer (1.15 for a 0.15 M solution at λ = 392 nm) t is the time (30.0 s), and f is the fraction of light absorbed at λ = 392 nm (0.99833, *vide infra*). The photon flux was calculated (average of three experiments) to

be 1.783 x 10^{-8} einstein s^{-1}. The ratio between the value obtained from diode calibration and that from chemical actinometry is 1.47.

VIII. Summary of Products 1A, 2A, 3A Quantum Yields, Quenching Fractions, and Chain Lengths with Photocatalysts PC-1-3.

Table S10. Quantum yield values and radical chain lengths for the perfluorobutylation of substrates **1-3** under photocatalysts PCs-1-3

entry	substrate	photocatalyst	K_{SV}[d] (M^{-1})	ϕ[e]	*Q*[f]	*L*[g]
1	**1**	Ir[(dF(CF$_3$)ppy]$_2$(dtbbpy)$^+$ [a]	402	3.81 ± 0.16	0.979	3.9
2		Rose Bengal[b]	4.3	0.51 ± 0.03	0.340	1.5
3		Zn-phthalocyanine[c]	162	0.17 ± 0.01	0.951	0.18
4	**2**	Ir[(dF(CF$_3$)ppy]$_2$(dtbbpy)$^+$ [a]	402	1.27 ± 0.1	0.979	1.3
5		Rose Bengal[b]	4.3	2.98± 0.03	0.340	8.76
6		Zn-phthalocyanine[c]	163	0.08± 0.02	0.951	0.09
7	**3**	Ir[(dF(CF$_3$)ppy]$_2$(dtbbpy)$^+$ [a]	402	40.7±0.5	0.979	41.6
8		Rose Bengal[b]	4.3	228±5	0.340	670
9		Zn-phthalocyanine[c]	162	0.34± 0.03	0.951	0.36

a.-violet LEDs, 3 Watts
b.-green LEDs, 3 Watts
c.-red LEDs, 3 Watts
d.-Stern Volmer quenching constant
e.-Quantum yield determined by two parallel methods: electronic actinometry (for PCs-1-3) and potassium ferrioxalate (for PC-1 and PC-2)
f.-using equation (2)
g.-calculated as the ratio between ϕ and *Q*

Table S11. Excited state redox potentials of PCs-1-3

entry	**PC**	**E* (eV)**	**$E_{PC/PC^{\bullet-}}$ (eV)**	**$E_{PC^*/PC^{\bullet+}}$ (eV)**	**$E_{PC^*/PC^{\bullet-}}$ (eV)**
1	1	2.62	+1.69	-0.93	+1.21
2	2	1.77	+0.74[a]	-0.68	-
3	3	1.12	+0.80	-	+1.02

a.- E_{ox} ($RB^{\cdot+}$/RB)

Figure S7. Quantum yields ϕ, chain lengths ***L***, and quenching fraction ***Q*** for the photoinitiated production of 1A under photocatalysts PCs-1-3

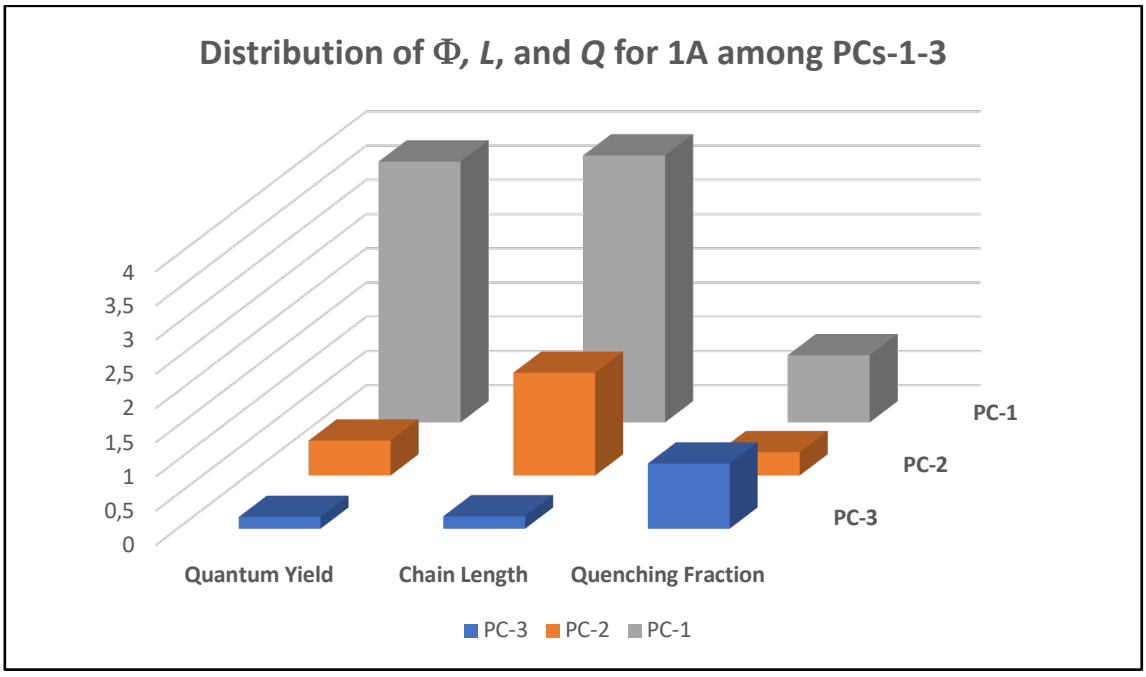


Figure S8. Quantum Yields and Chain Lengths for Product 2A under three photoinitiated Systems, PCs-1-3

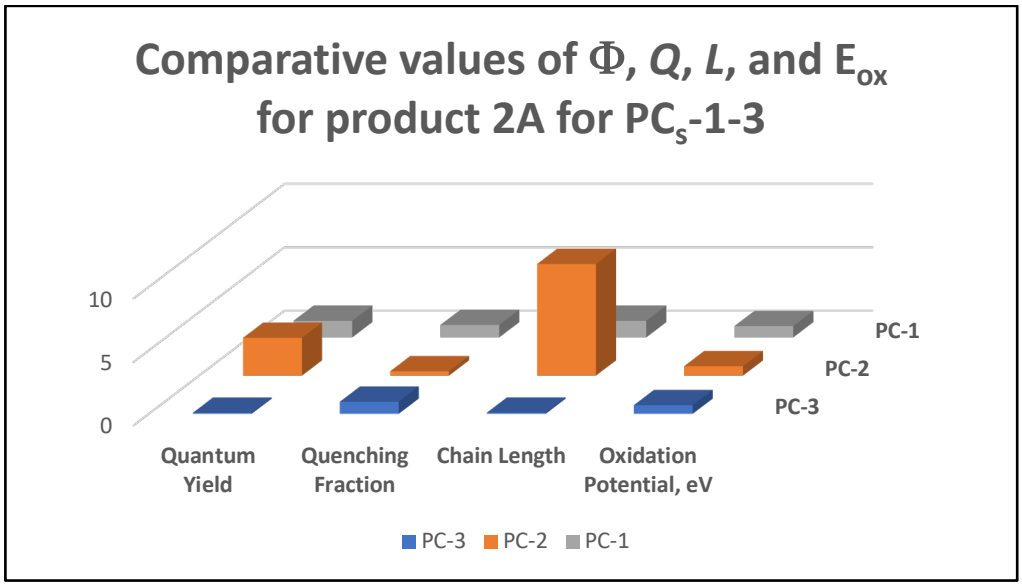
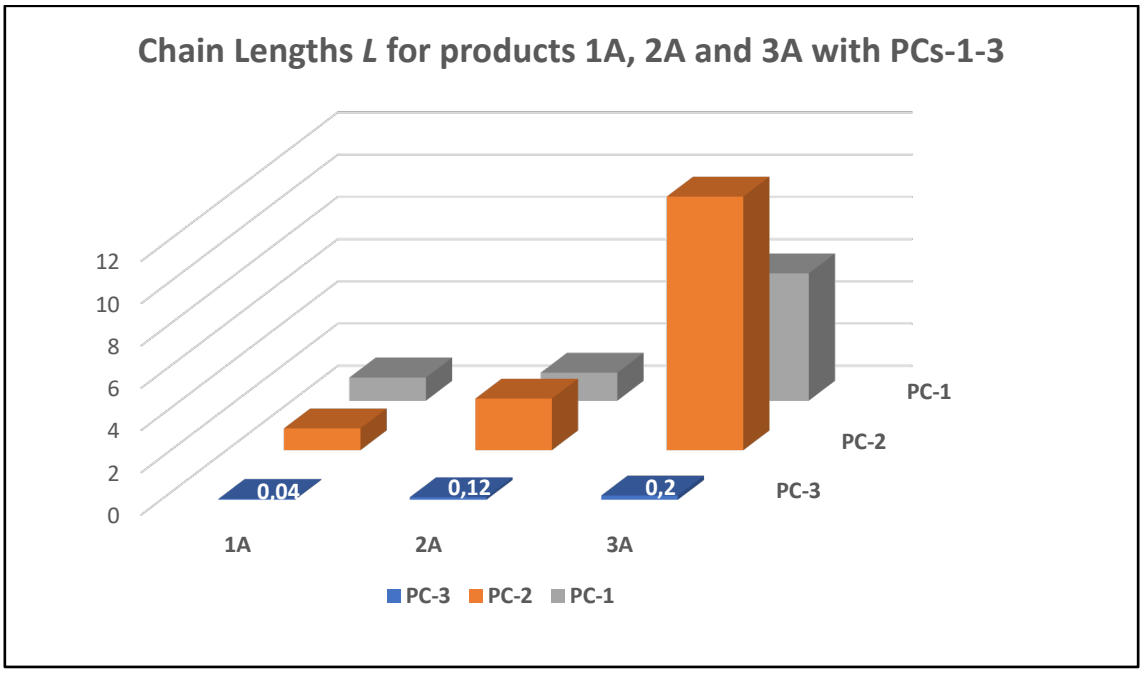
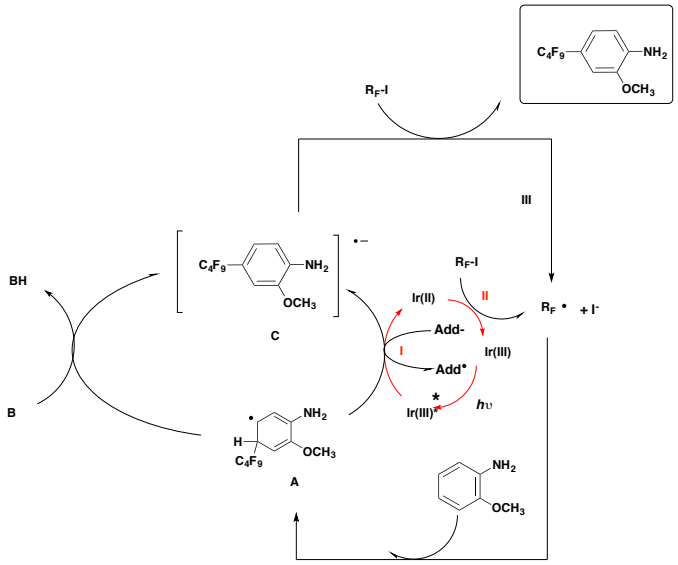


Figure S9. Quantum Yields ϕ and Chain Lengths ***L*** for Products 1A, 2A, and 3A under three Photoinitiated Systems, PC-1-3



Scheme S2. Alternative Photocatalytic Mechanism for the Perfluorobutylation of 2-Anisidine with PC-1 and PC-3

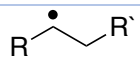


Discussion of Scheme: In Scheme S2 another mechanistic proposal is illustrated employing PC-1 for the perfluorobutylation of 2-anisidine, where the radical anion of the substitution product, intermediate **C,** is formed through base-induced deprotonation of intermediate **A**. In this proposal, the open catalytic cycle is controlled by the ET reduction

from **C** to C_4F_9-I, which produces more C_4F_9 radicals that propagate the chain (step III, Scheme 2S). However, in previous publications we have demonstrated through Linear Free Energy Relationships (Hammet plots) that the actual nature of the intermediate in the radical reactions of perfluoroalkylation of aniline derivatives is the Wheland intermediate **B** (Scheme 2, *vide infra*) rather the radical anion of the substitution product (intermediate **C,** Scheme 2S, ESI).[22] Therefore, Scheme 2**A** is more representative of the actual mechanism for the photocatalytic perfluoroalkylation of aniline derivatives with PC-1.

IX.1.-Table for Redox Potentials and Gibbs Energies

Table S12. Redox Potentials and Rehm Weller Parameters

entry	substrate	E_{red} (V)	E_{ox} (V)	E^*_{ox} (V)	E^*_{red} (V)	E_T (eV)	λ_{max} (nm)	ΔG_{ET}[a] (eV)	ΔG_{ET}[a] (Kcal/mol)
1	**PC-1**	-1.37[b]	+1.69[b]	-0.89[b]	+1.21[b]	2.62[b]	392	-0.1[c]	+2.30
2	**PC-2**	-0.99[b]	+0.74[b]	-0.68[b]	-	1.77[b]	559	+0.18[d]	+4.15
3	**PC-3**	-0.89[e]	-	-	+1.02[e]	1.12[f]	668	+0.38[g]	+ 8.76
4	**Collidinium ascorbate**	-	+0.295[h]	-	-	-	-	-0.725[i]	-16.72
5	**Cs_2CO_3**		+1.23[j]						
6	**n-C_4F_9I**	-1.27[k]							
7		0.47							

a.- From the Rehm Weller equation

$$\Delta G^{o} = E_{(D/D+)} - E_{(A/A-)} - E^{*} + \frac{Z_1 Z_2}{\varepsilon r_{12}} \qquad (1)$$

Coulombic term taken as -0.05 eV

b.- Q.-Q. Zhou, Y.-Q. Zou, L.-Q. Lu, W.-J. Xiao, Visible-Light-Induced Organic Photochemical Reactions through Energy-Transfer Pathways, *Angew. Chemie Int. Ed.,* 2019, *58*, 1586-1604.

c.- $\Delta G_{ET} = E_{Ir(III)/Ir(II)} - E_{C4F9-I} = -1.37\ V - (-1.27\ V) = -0.1\ eV$

d.- $\Delta G_{ET} = E_{RB^{\cdot+}/RB^{*}} - E_{C4F9-I} - E_T - 0.06\ eV = +0.18\ eV$

e.- D. W. Clack, N. S. Hush and I. S. Woolsey, Reduction potentials of some metal phthalocyanines, *Inorganica Chimica Acta*, **1976**, *19,* 129-132.

f.- (a) P. S. Vincett, E. M. Voight and K. E. Rieckhoff, Phosphorescence and Fluorescence of Phthalocyanines, *J. Chem. Phys*.,**1971**, *55*, 4131- (b) A. Harriman, G. Porter and C Richoux, Attempted photoproduction of hydrogen using sulphophthalocyanines as chromophores for three-component systems, *J. Chem. Soc., Faraday Trans. 2*, **1980**, *75*, 1618-1626.

g.- $\Delta G_{ET} = E_{ZnPC/ZnPC^{\bullet-}} - E_{C4F9-I} = - 0.89$ V – (-1.27 V) = + 0.38 V

h.- +0.295 ± 0.05 V was measured in DMF as solvent against SCE using the technique reported by Allen J. Bard, THE ELECTROCHEMISTRY OF ORGANIC COMPOUNDS IN APROTIC SOLVENTS—METHODS AND APPLICATIONS. The literature oxidation potential of E ox = +0.33 V was reported from T. Iyanagi, I. Yamazaki and K. F. Anan, Biochimica et Biophysica Acta 1985, 806, 255-261. The reported value is +0.33 V is also found: E. J. Nanni, Jr., M. D. Stallings, and D. T. Sawyer, J. Am. Chem. Soc. 1980, 102, 4481.

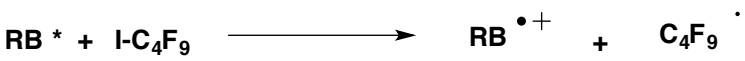
i.- $\Delta G_{ET} = E_{\text{collidinium ascorbate}} - E_{ZnPC^*/ZnPC^{\bullet-}} = +0.295$ V – (+ 1.02 V) = -0.725 eV

j.- Armstrong, D. A.; Waltz, W. L.; Rauk, A. Canadian Journal of Chemistry Volume84 Issue12 Pages1614-1619.

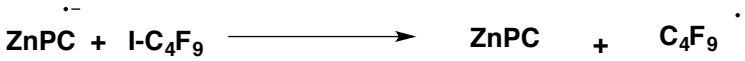
k.- measured in DMF: C.P. Andrieux, L.G. Clis, M. Medebielle, P. Pinson, J.M. Saveant, J. Am. Chem. Soc. 1990, 112, 3509-3520.

IX.2.-Determination of Gibbs Energies and ΔE from Measured Redox Potentials

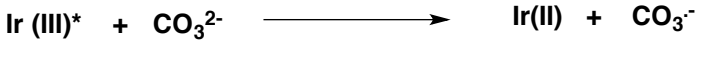
$\Delta G_{ET} = E_{Ir(III)/Ir(II)} - E_{C4F9-I} = -1.37\ V - (-1.27\ V) = -0.1\ eV$



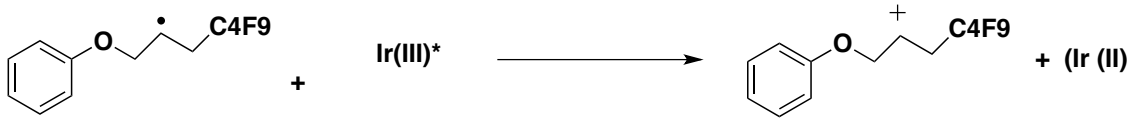
$\Delta G_{ET} = E_{RB^{\cdot+}/RB} - E_{C4F9-I} - E_T - 0.06\ eV = +0.74 - (-1.27\ V) - 1.77\ V - 0.06\ V =$ **+0.18** eV



$\Delta G_{ET} = E_{(ZnPC/ZnPC.-)} - E_{(IC4F9/C4F9)} = -0.89\ V - (-1.27\ V) = +\ 0.38\ V$

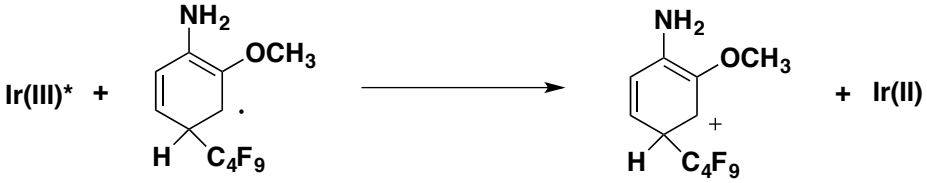


$\Delta G_{ET} = E_{CO_3^{2-}/CO_3^{\cdot-}}\ E_{Ir(III)/Ir(II)} - E_T - 0.06\ V = +1.23\ V - (-1.37\ V) - 2.62\ V - 0.06\ V =$ **-0.08 V**

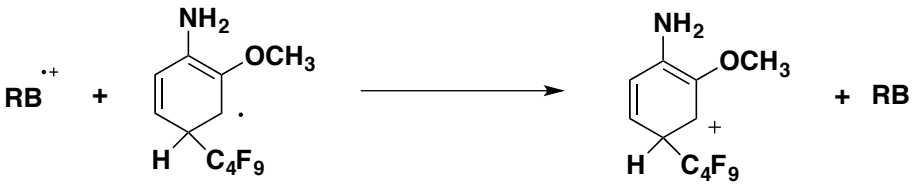


C **D**

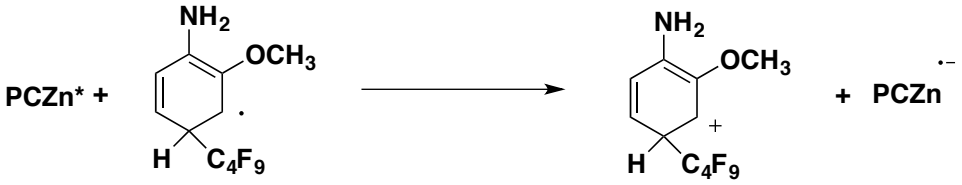
$\Delta G_{ET} = E$ (**D/C**) $- E_{Ir(III)/Ir(II)} - E_T - 0.06\ V = +0.47\ V - (-1.37\ V) - 2.62\ V - 0.06\ V =$ **- 0.84 V**



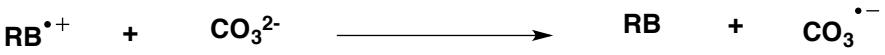
ΔG_{ET} = +0.47 – (-1.37 V) -2.62 V – 0.06 V = **-0.84 V**



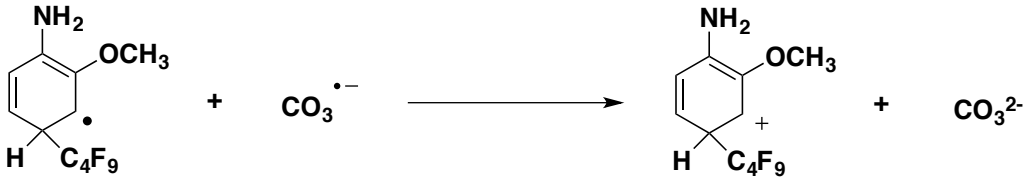
ΔG_{ET} = +0.47 – 0.74 V = **-0.27 V**



ΔG_{ET} = +0.47 – (-0.89 V) – 1.12 V -0.06 V = **+ 0.18 V**



ΔG_{ET} = +1.23 V – 0.74 V = +0.49 V



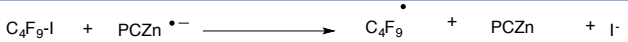
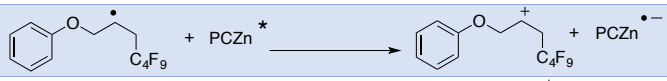
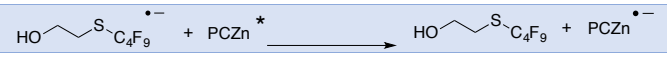
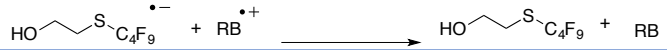
ΔG_{ET} = +0.47V – (+1.23V) = -0.76 V

X.1.-Computational Methods. Table of Calculated Gibbs Energies

Computational methods

All the reactants, products, intermediates and transition states of the proposed mechanism in *N,N*-dimethylformamide (DMF) or acetonitrile (ACN) were optimized at the density functional theory (DFT) level using Gaussian 09 program. The B3LYP[9] method was used in combination with the LanL2DZ basis set. The gradient threshold for geometry optimization was taken as 4,5.10-4 Hartree/Bohr. The polarizable conductor calculation model (CPCM) of solvation was employed in all calculations.[10,11] The excited state properties of Zn-phthalocyanine were obtained with the time-dependent density functional (TD-DFT) formalism.[12,13,14]

Table S13. Simulated ΔG, ΔH, and ΔS at the B3LYP/LANL2DZ theory level at 298 K

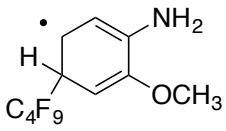
Reaction	ΔG[a]	ΔH [a]	ΔS[a]
	-26.8	-28	-3.8
	-52.3	-53.8	-4.9
	+1.2	+9.6	+28.2
	-12.1	-3.2	+30
	+17.2	+15.9	-4.5
	-8.1	-9.9	-5.9
	+45.4	+53.5	+27.3
	-15.2	-7.0	+27.7
	-43.2	-44.5	-4.5
	-68.67	-70.41	-5.51

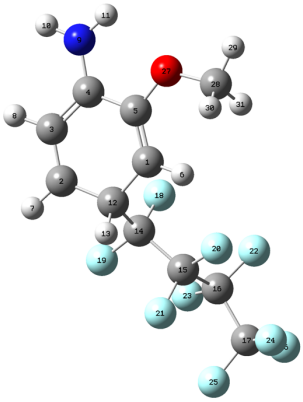
a.- in KCal/mol

Acknowledgments

Thanks are due to the TUPAC Cluster from the Computational Simulation Center of CONICET located in Buenos Aires, Argentina were the computational calculations were conducted. D.Y. and W.E.M.F. acknowledge Doctoral Fellowships from CONICET. M.V.C. acknowledges Postdoctoral Fellowship from CONICET.

X.2.- Supplementary Information on Computational Methods

o-anisidine-C_4F_9 radical: 



ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.063640	0.547110	-0.700930
2	6	0	2.271128	-1.976143	-0.659482
3	6	0	3.519085	-1.835487	-0.089427
4	6	0	4.070679	-0.560023	0.235221
5	6	0	3.310106	0.617510	-0.130298
6	1	0	1.549306	1.445542	-1.017111
7	1	0	1.898051	-2.958988	-0.927403
8	1	0	4.119262	-2.723663	0.100207
9	7	0	5.311109	-0.406965	0.828643
10	1	0	5.873773	-1.206828	1.081642
11	1	0	5.670297	0.522034	0.999973
12	6	0	1.366258	-0.783240	-0.925508
13	1	0	0.981404	-0.839623	-1.957805
14	6	0	0.077008	-0.925523	-0.037042
15	6	0	-1.169750	-0.078785	-0.456038
16	6	0	-2.337323	0.034092	0.588230
17	6	0	-3.732506	0.428951	-0.013724
18	9	0	0.348467	-0.626431	1.324010
19	9	0	-0.374877	-2.276518	-0.050600
20	9	0	-0.779393	1.236628	-0.769190
21	9	0	-1.692761	-0.633543	-1.643842
22	9	0	-1.995709	1.002675	1.542011
23	9	0	-2.511167	-1.183115	1.261302
24	9	0	-3.614453	1.504689	-0.885102
25	9	0	-4.303006	-0.633080	-0.698167
26	9	0	-4.596277	0.792739	1.009638
27	8	0	4.000926	1.805988	0.132699

28	6	0	3.354419	3.081681	-0.179048
29	1	0	4.058990	3.850754	0.141403
30	1	0	3.168908	3.170687	-1.256467
31	1	0	2.410961	3.183703	0.371193

Zero-point correction= 0.196852 (Hartree/Particle)
Thermal correction to Energy= 0.218594
Thermal correction to Enthalpy= 0.219538
Thermal correction to Gibbs Free Energy= 0.144483
Sum of electronic and zero-point Energies= -1452.836920
Sum of electronic and thermal Energies= -1452.815178
Sum of electronic and thermal Enthalpies= -1452.814234
Sum of electronic and thermal Free Energies= -1452.889289

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	137.170	80.388	157.967
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.384
Rotational	0.889	2.981	34.502
Vibrational	135.392	74.426	78.704

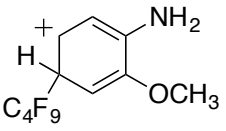
DMF

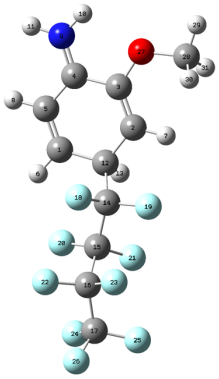
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.063640	0.547110	-0.700930
2	6	0	2.271128	-1.976143	-0.659482
3	6	0	3.519085	-1.835487	-0.089427
4	6	0	4.070679	-0.560023	0.235221
5	6	0	3.310106	0.617510	-0.130298
6	1	0	1.549306	1.445542	-1.017111
7	1	0	1.898051	-2.958988	-0.927403
8	1	0	4.119262	-2.723663	0.100207
9	7	0	5.311109	-0.406965	0.828643
10	1	0	5.873773	-1.206828	1.081642
11	1	0	5.670297	0.522034	0.999973
12	6	0	1.366258	-0.783240	-0.925508
13	1	0	0.981404	-0.839623	-1.957805
14	6	0	0.077008	-0.925523	-0.037042
15	6	0	-1.169750	-0.078785	-0.456038
16	6	0	-2.337323	0.034092	0.588230
17	6	0	-3.732506	0.428951	-0.013724
18	9	0	0.348467	-0.626431	1.324010
19	9	0	-0.374877	-2.276518	-0.050600
20	9	0	-0.779393	1.236628	-0.769190
21	9	0	-1.692761	-0.633543	-1.643842
22	9	0	-1.995709	1.002675	1.542011
23	9	0	-2.511167	-1.183115	1.261302

24	9	0	-3.614453	1.504689	-0.885102
25	9	0	-4.303006	-0.633080	-0.698167
26	9	0	-4.596277	0.792739	1.009638
27	8	0	4.000926	1.805988	0.132699
28	6	0	3.354419	3.081681	-0.179048
29	1	0	4.058990	3.850754	0.141403
30	1	0	3.168908	3.170687	-1.256467
31	1	0	2.410961	3.183703	0.371193

Zero-point correction= 0.196851 (Hartree/Particle)
Thermal correction to Energy= 0.218593
Thermal correction to Enthalpy= 0.219537
Thermal correction to Gibbs Free Energy= 0.144480
Sum of electronic and zero-point Energies= -1452.836936
Sum of electronic and thermal Energies= -1452.815194
Sum of electronic and thermal Enthalpies= -1452.814250
Sum of electronic and thermal Free Energies= -1452.889306

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	137.169	80.388	157.970
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.384
Rotational	0.889	2.981	34.502
Vibrational	135.392	74.427	78.707

o-anisidine-C_4F_9 cation: 



ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.619260	1.656772	-0.443696
2	6	0	2.482484	-0.738094	-0.447957
3	6	0	3.717481	-0.274926	-0.120929

4	6	0	3.951797	1.161214	0.070394
5	6	0	2.859783	2.097226	-0.116580
6	1	0	0.817554	2.372598	-0.584379
7	1	0	2.302390	-1.796589	-0.591366
8	1	0	3.056088	3.156426	0.012832
9	7	0	5.166519	1.558407	0.409469
10	1	0	5.905772	0.867059	0.528408
11	1	0	5.395164	2.537517	0.558939
12	6	0	1.316949	0.193854	-0.681682
13	1	0	1.036661	0.094869	-1.746510
14	6	0	0.081244	-0.284016	0.134421
15	6	0	-1.320599	0.145113	-0.421883
16	6	0	-2.536464	-0.020354	0.558144
17	6	0	-3.941608	-0.087824	-0.139767
18	9	0	0.168093	0.159974	1.477105
19	9	0	0.053546	-1.697085	0.189061
20	9	0	-1.279602	1.495258	-0.812031
21	9	0	-1.569763	-0.605771	-1.585113
22	9	0	-2.546125	1.064074	1.443396
23	9	0	-2.389895	-1.190425	1.313699
24	9	0	-4.074001	0.922246	-1.084242
25	9	0	-4.128772	-1.308981	-0.767221
26	9	0	-4.938910	0.067700	0.809786
27	8	0	4.864332	-1.011125	0.075299
28	6	0	4.816412	-2.475122	-0.083329
29	1	0	5.831494	-2.815072	0.118876
30	1	0	4.117711	-2.910096	0.639373
31	1	0	4.525309	-2.732515	-1.107625

Zero-point correction= 0.201282 (Hartree/Particle)
Thermal correction to Energy= 0.222352
Thermal correction to Enthalpy= 0.223297
Thermal correction to Gibbs Free Energy= 0.150000
Sum of electronic and zero-point Energies= -1452.686161
Sum of electronic and thermal Energies= -1452.665090
Sum of electronic and thermal Enthalpies= -1452.664146
Sum of electronic and thermal Free Energies= -1452.737443

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.528	77.693	154.265
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.384
Rotational	0.889	2.981	34.541
Vibrational	137.751	71.731	76.341

DMF

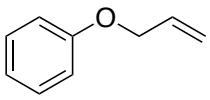
Center	Atomic	Atomic	Coordinates (Angstroms)

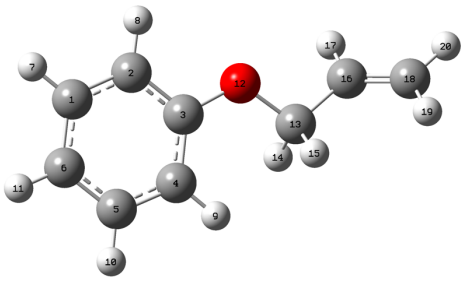
Number	Number	Type	X	Y	Z
1	6	0	-1.619260	-1.656772	-0.443696
2	6	0	-2.482484	0.738094	-0.447957
3	6	0	-3.717481	0.274926	-0.120929
4	6	0	-3.951797	-1.161214	0.070394
5	6	0	-2.859783	-2.097226	-0.116580
6	1	0	-0.817554	-2.372598	-0.584379
7	1	0	-2.302390	1.796589	-0.591366
8	1	0	-3.056088	-3.156426	0.012832
9	7	0	-5.166519	-1.558407	0.409469
10	1	0	-5.905772	-0.867059	0.528408
11	1	0	-5.395164	-2.537517	0.558939
12	6	0	-1.316949	-0.193854	-0.681682
13	1	0	-1.036661	-0.094869	-1.746510
14	6	0	-0.081244	0.284016	0.134421
15	6	0	1.320599	-0.145113	-0.421883
16	6	0	2.536464	0.020354	0.558144
17	6	0	3.941608	0.087824	-0.139767
18	9	0	-0.168093	-0.159974	1.477105
19	9	0	-0.053546	1.697085	0.189061
20	9	0	1.279602	-1.495258	-0.812031
21	9	0	1.569763	0.605771	-1.585113
22	9	0	2.546125	-1.064074	1.443396
23	9	0	2.389895	1.190425	1.313699
24	9	0	4.074001	-0.922246	-1.084242
25	9	0	4.128772	1.308981	-0.767221
26	9	0	4.938910	-0.067700	0.809786
27	8	0	-4.864332	1.011125	0.075299
28	6	0	-4.816412	2.475122	-0.083329
29	1	0	-5.831494	2.815072	0.118876
30	1	0	-4.117711	2.910096	0.639373
31	1	0	-4.525309	2.732515	-1.107625

Zero-point correction= 0.201281 (Hartree/Particle)
Thermal correction to Energy= 0.222352
Thermal correction to Enthalpy= 0.223296
Thermal correction to Gibbs Free Energy= 0.150000
Sum of electronic and zero-point Energies= -1452.686263
Sum of electronic and thermal Energies= -1452.665192
Sum of electronic and thermal Enthalpies= -1452.664248
Sum of electronic and thermal Free Energies= -1452.737544

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.528	77.693	154.265
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.384
Rotational	0.889	2.981	34.541

Vibrational	137.750	71.732	76.340

Allyloxybenzene: 



ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.786312	1.052838	-0.100326
2	6	0	1.407037	1.313822	-0.055021
3	6	0	0.492075	0.240055	0.019539
4	6	0	0.957505	-1.092077	0.047094
5	6	0	2.345808	-1.338014	0.001686
6	6	0	3.265731	-0.275672	-0.071680
7	1	0	3.485640	1.883430	-0.157036
8	1	0	1.025599	2.330919	-0.075199
9	1	0	0.268972	-1.928793	0.099260
10	1	0	2.701587	-2.365272	0.023145
11	1	0	4.333336	-0.474578	-0.106254
12	8	0	-0.861145	0.601713	0.056891
13	6	0	-1.873492	-0.465232	0.198702
14	1	0	-1.636213	-1.055063	1.096773
15	1	0	-1.847047	-1.124262	-0.678957
16	6	0	-3.212381	0.205509	0.340970
17	1	0	-3.288994	0.938727	1.144099
18	6	0	-4.282209	-0.078065	-0.430005
19	1	0	-4.229702	-0.803488	-1.240331
20	1	0	-5.242322	0.405695	-0.266381

Zero-point correction=	0.166842 (Hartree/Particle)
Thermal correction to Energy=	0.175959
Thermal correction to Enthalpy=	0.176903
Thermal correction to Gibbs Free Energy=	0.131754
Sum of electronic and zero-point Energies=	-423.944189
Sum of electronic and thermal Energies=	-423.935071
Sum of electronic and thermal Enthalpies=	-423.934127
Sum of electronic and thermal Free Energies=	-423.979276

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	110.416	34.223	95.023
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.592
Rotational	0.889	2.981	29.760
Vibrational	108.638	28.262	24.671

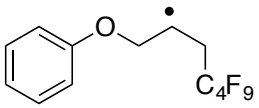
DMF

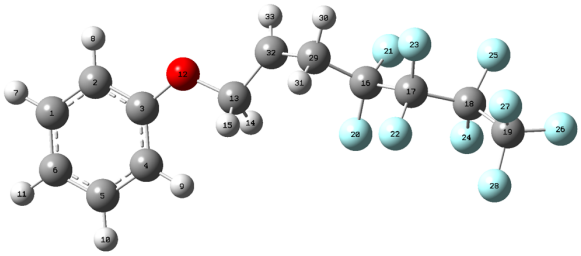
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.786304	1.052858	-0.100355
2	6	0	1.407024	1.313826	-0.054994
3	6	0	0.492073	0.240048	0.019584
4	6	0	0.957514	-1.092078	0.047118
5	6	0	2.345820	-1.338002	0.001666
6	6	0	3.265733	-0.275650	-0.071733
7	1	0	3.485623	1.883457	-0.157078
8	1	0	1.025586	2.330924	-0.075135
9	1	0	0.268991	-1.928802	0.099299
10	1	0	2.701606	-2.365258	0.023108
11	1	0	4.333340	-0.474548	-0.106344
12	8	0	-0.861149	0.601685	0.056963
13	6	0	-1.873509	-0.465282	0.198724
14	1	0	-1.636234	-1.055130	1.096783
15	1	0	-1.847051	-1.124279	-0.678956
16	6	0	-3.212399	0.205461	0.340993
17	1	0	-3.289084	0.938550	1.144235
18	6	0	-4.282173	-0.077989	-0.430104
19	1	0	-4.229615	-0.803297	-1.240532
20	1	0	-5.242296	0.405751	-0.266475

Zero-point correction= 0.166842 (Hartree/Particle)
Thermal correction to Energy= 0.175959
Thermal correction to Enthalpy= 0.176903
Thermal correction to Gibbs Free Energy= 0.131755
Sum of electronic and zero-point Energies= -423.944199
Sum of electronic and thermal Energies= -423.935082
Sum of electronic and thermal Enthalpies= -423.934138
Sum of electronic and thermal Free Energies= -423.979286

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	110.416	34.223	95.022
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.592

Rotational	0.889	2.981	29.760
Vibrational	108.638	28.262	24.671

allyloxybenzene-C_4F_9 radical: 



ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.438978	0.169199	-0.071915
2	6	0	-6.235613	0.890002	-0.003728
3	6	0	-5.006839	0.197101	0.059014
4	6	0	-4.980975	-1.213539	0.054623
5	6	0	-6.198116	-1.923315	-0.015425
6	6	0	-7.428392	-1.243328	-0.079082
7	1	0	-8.382286	0.707528	-0.120653
8	1	0	-6.229310	1.976336	0.001012
9	1	0	-4.046954	-1.762935	0.107848
10	1	0	-6.176202	-3.010326	-0.018754
11	1	0	-8.360710	-1.798644	-0.132846
12	8	0	-3.863819	1.006913	0.129470
13	6	0	-2.540771	0.359968	0.126596
14	1	0	-2.468503	-0.291059	-0.762705
15	1	0	-2.426539	-0.272996	1.018863
16	6	0	0.844008	0.595904	-0.168713
17	6	0	2.253795	0.362389	0.463171
18	6	0	3.416425	-0.031129	-0.513887
19	6	0	4.640582	-0.744282	0.162890
20	9	0	0.352713	-0.675946	-0.571755
21	9	0	1.049101	1.329827	-1.370661
22	9	0	2.136918	-0.643773	1.443536
23	9	0	2.648774	1.538102	1.129195
24	9	0	2.937106	-0.891960	-1.511020
25	9	0	3.890168	1.127702	-1.142093
26	9	0	5.714608	-0.759291	-0.714529
27	9	0	5.030838	-0.076626	1.317262
28	9	0	4.336484	-2.055896	0.492429
29	6	0	-0.166407	1.302731	0.741275
30	1	0	0.244728	2.286901	0.988666

31	1	0	-0.235933	0.723151	1.670792
32	6	0	-1.517852	1.450157	0.091607
33	1	0	-1.723321	2.326354	-0.517802

Zero-point correction= 0.214373 (Hartree/Particle)
Thermal correction to Energy= 0.236643
Thermal correction to Enthalpy= 0.237588
Thermal correction to Gibbs Free Energy= 0.158448
Sum of electronic and zero-point Energies= -1474.871418
Sum of electronic and thermal Energies= -1474.849147
Sum of electronic and thermal Enthalpies= -1474.848203
Sum of electronic and thermal Free Energies= -1474.927342

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.496	81.174	166.563
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.478
Rotational	0.889	2.981	35.466
Vibrational	146.718	75.213	86.241

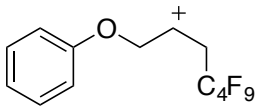
DMF

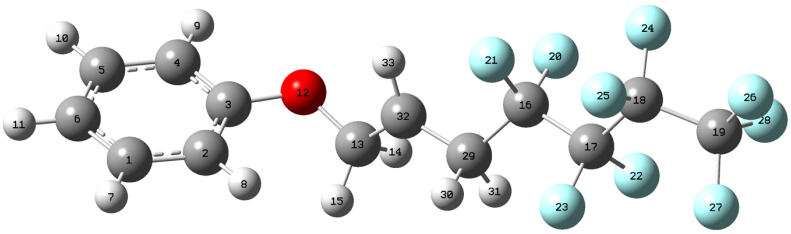
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.439042	0.169161	-0.072284
2	6	0	-6.235718	0.890038	-0.004037
3	6	0	-5.006923	0.197204	0.058986
4	6	0	-4.981000	-1.213454	0.054776
5	6	0	-6.198108	-1.923300	-0.015334
6	6	0	-7.428396	-1.243368	-0.079242
7	1	0	-8.382366	0.707442	-0.121247
8	1	0	-6.229485	1.976373	0.000544
9	1	0	-4.046964	-1.762798	0.108166
10	1	0	-6.176149	-3.010310	-0.018515
11	1	0	-8.360684	-1.798727	-0.133063
12	8	0	-3.863910	1.007026	0.129607
13	6	0	-2.540890	0.359965	0.126835
14	1	0	-2.468647	-0.290981	-0.762528
15	1	0	-2.426822	-0.273086	1.019053
16	6	0	0.843956	0.595870	-0.168648
17	6	0	2.253717	0.362119	0.463231
18	6	0	3.416483	-0.030908	-0.513836
19	6	0	4.640702	-0.744196	0.162717
20	9	0	0.352657	-0.675833	-0.572149
21	9	0	1.049144	1.330160	-1.370343
22	9	0	2.136792	-0.644562	1.443101
23	9	0	2.648622	1.537521	1.129832

24	9	0	2.937317	-0.891457	-1.511295
25	9	0	3.890168	1.128156	-1.141583
26	9	0	5.714663	-0.758926	-0.714794
27	9	0	5.031025	-0.076822	1.317220
28	9	0	4.336737	-2.055900	0.491951
29	6	0	-0.166435	1.302395	0.741579
30	1	0	0.244696	2.286473	0.989364
31	1	0	-0.235963	0.722474	1.670882
32	6	0	-1.517883	1.450063	0.091981
33	1	0	-1.723248	2.326352	-0.517335

Zero-point correction= 0.214372 (Hartree/Particle)
Thermal correction to Energy= 0.236643
Thermal correction to Enthalpy= 0.237587
Thermal correction to Gibbs Free Energy= 0.158445
Sum of electronic and zero-point Energies= -1474.871433
Sum of electronic and thermal Energies= -1474.849162
Sum of electronic and thermal Enthalpies= -1474.848218
Sum of electronic and thermal Free Energies= -1474.927360

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.496	81.175	166.569
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.478
Rotational	0.889	2.981	35.466
Vibrational	146.718	75.213	86.247

allyloxybenzene-C_4F_9 cation: 



ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.176791	-1.754157	-0.212225
2	6	0	-5.008707	-0.985178	-0.388355
3	6	0	-5.042508	0.382281	-0.039360
4	6	0	-6.203531	0.981332	0.490251

5	6	0	-7.353399	0.198948	0.662188
6	6	0	-7.346630	-1.171469	0.307548
7	1	0	-6.161654	-2.807496	-0.476092
8	1	0	-4.111178	-1.466398	-0.761927
9	1	0	-6.188060	2.035102	0.749524
10	1	0	-8.254095	0.651503	1.066636
11	1	0	-8.241606	-1.771816	0.441285
12	8	0	-3.931165	1.246211	-0.158753
13	6	0	-2.827096	0.857939	-0.980676
14	1	0	-2.526468	1.776835	-1.531912
15	1	0	-3.078630	0.152892	-1.796889
16	6	0	0.832617	0.366305	0.125746
17	6	0	2.209444	-0.085960	-0.460654
18	6	0	3.382116	-0.247163	0.570318
19	6	0	4.820969	-0.174015	-0.054460
20	9	0	0.934230	1.729877	0.483048
21	9	0	0.619655	-0.347020	1.330698
22	9	0	2.588877	0.844232	-1.444375
23	9	0	2.029185	-1.321951	-1.105134
24	9	0	3.294268	0.753203	1.547334
25	9	0	3.249453	-1.484561	1.209488
26	9	0	5.750962	-0.630775	0.864795
27	9	0	4.901814	-0.966264	-1.193027
28	9	0	5.151040	1.127661	-0.394701
29	6	0	-0.347422	0.164798	-0.827503
30	1	0	-0.396865	-0.907086	-1.114347
31	1	0	-0.190023	0.703391	-1.768597
32	6	0	-1.657457	0.453867	-0.209284
33	1	0	-1.767096	0.398585	0.878013

Zero-point correction= 0.214284 (Hartree/Particle)
Thermal correction to Energy= 0.236231
Thermal correction to Enthalpy= 0.237175
Thermal correction to Gibbs Free Energy= 0.160238
Sum of electronic and zero-point Energies= -1474.651079
Sum of electronic and thermal Energies= -1474.629133
Sum of electronic and thermal Enthalpies= -1474.628189
Sum of electronic and thermal Free Energies= -1474.705126

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.237	80.727	161.928
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.478
Rotational	0.889	2.981	35.418
Vibrational	146.459	74.766	83.032

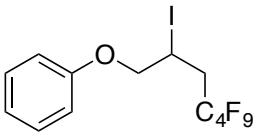
DMF

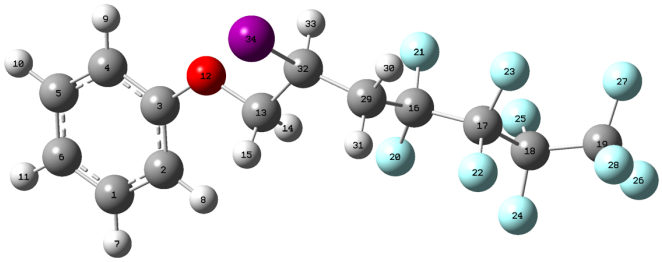
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.208468	-1.746420	-0.152062
2	6	0	-5.030130	-0.999900	-0.354285
3	6	0	-5.045854	0.379195	-0.053428
4	6	0	-6.198899	1.012137	0.453831
5	6	0	-7.359290	0.251880	0.652085
6	6	0	-7.370585	-1.130174	0.346108
7	1	0	-6.207380	-2.808576	-0.378303
8	1	0	-4.138708	-1.505444	-0.710005
9	1	0	-6.169297	2.074131	0.675655
10	1	0	-8.254013	0.730532	1.039362
11	1	0	-8.273439	-1.713520	0.500570
12	8	0	-3.923436	1.223705	-0.202015
13	6	0	-2.822861	0.794791	-1.007686
14	1	0	-2.513679	1.689877	-1.592546
15	1	0	-3.079466	0.062188	-1.797543
16	6	0	0.834813	0.361110	0.111242
17	6	0	2.210396	-0.126306	-0.448036
18	6	0	3.391767	-0.199002	0.583113
19	6	0	4.825564	-0.169446	-0.056942
20	9	0	0.932764	1.743982	0.384489
21	9	0	0.626382	-0.277950	1.357788
22	9	0	2.578373	0.725616	-1.503863
23	9	0	2.030839	-1.409990	-0.991686
24	9	0	3.306145	0.876721	1.476615
25	9	0	3.271272	-1.381663	1.320760
26	9	0	5.764664	-0.549093	0.887783
27	9	0	4.901118	-1.048614	-1.130195
28	9	0	5.146839	1.102788	-0.500842
29	6	0	-0.345916	0.100192	-0.827182
30	1	0	-0.387439	-0.985924	-1.056514
31	1	0	-0.194274	0.591282	-1.794547
32	6	0	-1.656194	0.412487	-0.220947
33	1	0	-1.766436	0.396369	0.867481

Zero-point correction= 0.214255 (Hartree/Particle)
Thermal correction to Energy= 0.236239
Thermal correction to Enthalpy= 0.237183
Thermal correction to Gibbs Free Energy= 0.160098
Sum of electronic and zero-point Energies= -1474.651227
Sum of electronic and thermal Energies= -1474.629244
Sum of electronic and thermal Enthalpies= -1474.628300
Sum of electronic and thermal Free Energies= -1474.705385

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	148.242	80.754	162.240

Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.478
Rotational	0.889	2.981	35.416
Vibrational	146.465	74.792	83.345

allyloxybenzene ATRA product: 



ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.897781	3.354925	-0.963549
2	6	0	-3.891857	2.389827	-0.748799
3	6	0	-4.102211	1.383227	0.216312
4	6	0	-5.301149	1.339247	0.958675
5	6	0	-6.293191	2.307765	0.733399
6	6	0	-6.097984	3.322174	-0.229799
7	1	0	-4.735232	4.130994	-1.707336
8	1	0	-2.975425	2.438235	-1.327487
9	1	0	-5.437807	0.553168	1.695728
10	1	0	-7.215756	2.271287	1.307205
11	1	0	-6.867130	4.069873	-0.402299
12	8	0	-3.173073	0.373473	0.514967
13	6	0	-1.913958	0.342967	-0.219017
14	1	0	-1.358007	1.270173	-0.024855
15	1	0	-2.094866	0.255740	-1.297971
16	6	0	1.272300	0.120595	0.182479
17	6	0	2.765187	-0.152550	-0.194541
18	6	0	3.766756	1.045288	-0.034682
19	6	0	5.275341	0.630811	0.101620
20	9	0	0.951810	1.405516	-0.345020
21	9	0	1.215046	0.259285	1.593682
22	9	0	2.819377	-0.570218	-1.536669
23	9	0	3.228039	-1.227764	0.589967
24	9	0	3.651694	1.883048	-1.150687
25	9	0	3.439971	1.798317	1.101468
26	9	0	6.082018	1.744864	-0.073609

27	9	0	5.538216	0.102091	1.355671
28	9	0	5.619819	-0.312835	-0.858403
29	6	0	0.307885	-0.960164	-0.302760
30	1	0	0.738855	-1.925697	-0.020284
31	1	0	0.267858	-0.924357	-1.395835
32	6	0	-1.108258	-0.844426	0.305287
33	1	0	-1.074846	-0.829594	1.396307
34	53	0	-2.178556	-2.749367	-0.136948

Zero-point correction= 0.218675 (Hartree/Particle)
Thermal correction to Energy= 0.242255
Thermal correction to Enthalpy= 0.243199
Thermal correction to Gibbs Free Energy= 0.160465
Sum of electronic and zero-point Energies= -1486.307604
Sum of electronic and thermal Energies= -1486.284024
Sum of electronic and thermal Enthalpies= -1486.283080
Sum of electronic and thermal Free Energies= -1486.365814

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.017	84.774	174.129
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	44.394
Rotational	0.889	2.981	36.820
Vibrational	150.240	78.812	92.916

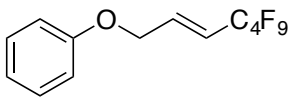
DMF

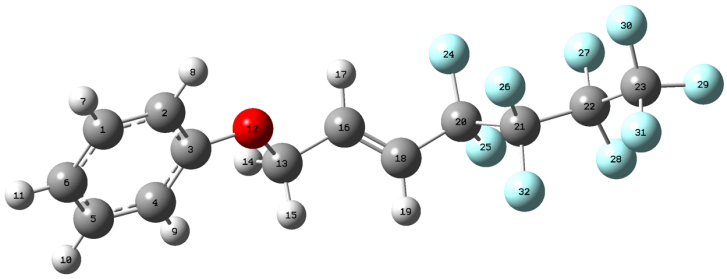
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.896543	3.355655	-0.962877
2	6	0	-3.890709	2.390564	-0.747662
3	6	0	-4.101915	1.383382	0.216659
4	6	0	-5.301586	1.338823	0.957797
5	6	0	-6.293529	2.307350	0.732079
6	6	0	-6.097484	3.322324	-0.230352
7	1	0	-4.733346	4.132175	-1.706051
8	1	0	-2.973678	2.439428	-1.325369
9	1	0	-5.438901	0.552298	1.694248
10	1	0	-7.216670	2.270422	1.304928
11	1	0	-6.866554	4.070015	-0.403209
12	8	0	-3.172869	0.373622	0.515679
13	6	0	-1.913504	0.343237	-0.217905
14	1	0	-1.357409	1.270198	-0.023051
15	1	0	-2.094108	0.256687	-1.296976
16	6	0	1.272354	0.120319	0.182503
17	6	0	2.765077	-0.152675	-0.195174
18	6	0	3.766787	1.045000	-0.034683

19	6	0	5.275354	0.630560	0.101744
20	9	0	0.951596	1.405284	-0.344837
21	9	0	1.215634	0.258951	1.593725
22	9	0	2.818795	-0.569389	-1.537590
23	9	0	3.228046	-1.228528	0.588424
24	9	0	3.651916	1.883251	-1.150338
25	9	0	3.439872	1.797619	1.101732
26	9	0	6.081882	1.744983	-0.071956
27	9	0	5.537860	0.100563	1.355333
28	9	0	5.620393	-0.311959	-0.859160
29	6	0	0.307847	-0.960516	-0.302374
30	1	0	0.738915	-1.925986	-0.019811
31	1	0	0.267533	-0.924860	-1.395440
32	6	0	-1.108160	-0.844615	0.305931
33	1	0	-1.074633	-0.830255	1.396955
34	53	0	-2.178983	-2.749104	-0.137052

Zero-point correction= 0.218676 (Hartree/Particle)
Thermal correction to Energy= 0.242256
Thermal correction to Enthalpy= 0.243200
Thermal correction to Gibbs Free Energy= 0.160465
Sum of electronic and zero-point Energies= -1486.307619
Sum of electronic and thermal Energies= -1486.284039
Sum of electronic and thermal Enthalpies= -1486.283095
Sum of electronic and thermal Free Energies= -1486.365830

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.018	84.773	174.130
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	44.394
Rotational	0.889	2.981	36.819
Vibrational	150.240	78.812	92.917

Allyloxybenzene ATRE product: 



ACN

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	6.870647	-1.633380	-0.404056
2	6	0	5.497991	-1.439391	-0.629598
3	6	0	4.864604	-0.284470	-0.123403
4	6	0	5.596491	0.674264	0.607037
5	6	0	6.974497	0.465255	0.824507
6	6	0	7.618194	-0.681589	0.324238
7	1	0	7.355851	-2.523901	-0.795574
8	1	0	4.910721	-2.162400	-1.188465
9	1	0	5.123176	1.565087	1.006376
10	1	0	7.538708	1.204479	1.387611
11	1	0	8.679921	-0.834188	0.496947
12	8	0	3.491247	-0.182094	-0.400514
13	6	0	2.772348	1.007926	0.065674
14	1	0	3.253004	1.910639	-0.341751
15	1	0	2.786683	1.063334	1.161233
16	6	0	1.373713	0.899079	-0.471046
17	1	0	1.288079	0.585848	-1.509795
18	6	0	0.280279	1.206053	0.251816
19	1	0	0.333073	1.508430	1.293191
20	6	0	-1.095579	1.172333	-0.324893
21	6	0	-2.029176	0.062770	0.272989
22	6	0	-3.569312	0.213323	0.013850
23	6	0	-4.398129	-1.113239	0.143080
24	9	0	-1.088044	0.993074	-1.729150
25	9	0	-1.768084	2.416061	-0.087989
26	9	0	-1.612569	-1.182348	-0.236901
27	9	0	-3.793837	0.716220	-1.275339
28	9	0	-4.095630	1.133366	0.929423
29	9	0	-5.751768	-0.814426	0.192700
30	9	0	-4.182760	-1.948726	-0.941783
31	9	0	-4.060566	-1.797926	1.304159
32	9	0	-1.839920	0.023130	1.666343

Zero-point correction= 0.204711 (Hartree/Particle)
Thermal correction to Energy= 0.226435
Thermal correction to Enthalpy= 0.227379
Thermal correction to Gibbs Free Energy= 0.150603
Sum of electronic and zero-point Energies= -1474.311426
Sum of electronic and thermal Energies= -1474.289702
Sum of electronic and thermal Enthalpies= -1474.288758
Sum of electronic and thermal Free Energies= -1474.365534

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	142.090	79.298	161.590
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.470

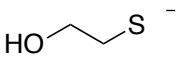
Rotational	0.889	2.981	35.564
Vibrational	140.313	73.337	82.556

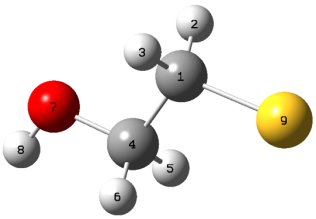
DMF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.870670	-1.633324	-0.404205
2	6	0	5.497981	-1.439392	-0.629622
3	6	0	4.864574	-0.284536	-0.123302
4	6	0	5.596471	0.674187	0.607141
5	6	0	6.974507	0.465244	0.824479
6	6	0	7.618226	-0.681537	0.324082
7	1	0	7.355889	-2.523794	-0.795821
8	1	0	4.910710	-2.162400	-1.188491
9	1	0	5.123135	1.564941	1.006608
10	1	0	7.538722	1.204460	1.387588
11	1	0	8.679976	-0.834089	0.496689
12	8	0	3.491167	-0.182243	-0.400233
13	6	0	2.772323	1.007884	0.065813
14	1	0	3.253067	1.910527	-0.341643
15	1	0	2.786602	1.063362	1.161363
16	6	0	1.373713	0.899104	-0.470980
17	1	0	1.288124	0.585914	-1.509746
18	6	0	0.280282	1.206146	0.251862
19	1	0	0.333102	1.508494	1.293239
20	6	0	-1.095563	1.172467	-0.324883
21	6	0	-2.029121	0.062738	0.272821
22	6	0	-3.569300	0.213289	0.013807
23	6	0	-4.398154	-1.113259	0.143128
24	9	0	-1.087960	0.993366	-1.729176
25	9	0	-1.768167	2.416128	-0.087895
26	9	0	-1.612486	-1.182265	-0.237307
27	9	0	-3.793970	0.716209	-1.275333
28	9	0	-4.095513	1.133322	0.929474
29	9	0	-5.751780	-0.814393	0.192881
30	9	0	-4.182951	-1.948783	-0.941737
31	9	0	-4.060503	-1.797949	1.304179
32	9	0	-1.839817	0.022858	1.666163

Zero-point correction=	0.204710 (Hartree/Particle)
Thermal correction to Energy=	0.226434
Thermal correction to Enthalpy=	0.227379
Thermal correction to Gibbs Free Energy=	0.150603
Sum of electronic and zero-point Energies=	-1474.311442
Sum of electronic and thermal Energies=	-1474.289718
Sum of electronic and thermal Enthalpies=	-1474.288774
Sum of electronic and thermal Free Energies=	-1474.365550

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	142.090	79.299	161.588
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.470
Rotational	0.889	2.981	35.564
Vibrational	140.312	73.337	82.554

2-mercaptoethanol anion: 



ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.062953	0.626130	0.000078
2	1	0	-0.070525	1.258672	-0.887739
3	1	0	-0.070547	1.258464	0.888039
4	6	0	-0.992491	-0.475925	-0.000066
5	1	0	-0.880551	-1.107503	-0.894004
6	1	0	-0.880687	-1.107622	0.893804
7	8	0	-2.338164	0.157522	-0.000158
8	1	0	-3.032786	-0.535348	0.001108
9	16	0	1.826102	-0.120504	-0.000001

Zero-point correction= 0.070074 (Hartree/Particle)
Thermal correction to Energy= 0.075294
Thermal correction to Enthalpy= 0.076239
Thermal correction to Gibbs Free Energy= 0.041712
Sum of electronic and zero-point Energies= -164.580341
Sum of electronic and thermal Energies= -164.575120
Sum of electronic and thermal Enthalpies= -164.574176
Sum of electronic and thermal Free Energies= -164.608703

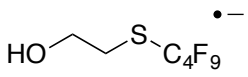
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	47.248	16.608	72.668
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	38.939
Rotational	0.889	2.981	25.198
Vibrational	45.470	10.646	8.530

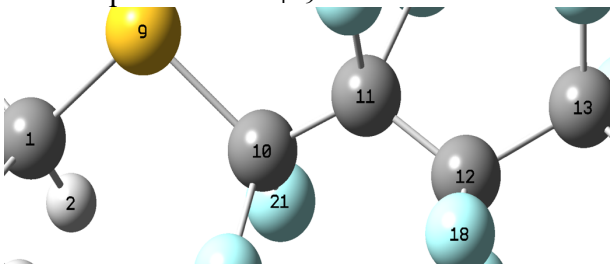
DMF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.062953	0.626130	0.000078
2	1	0	-0.070525	1.258672	-0.887739
3	1	0	-0.070547	1.258464	0.888039
4	6	0	-0.992491	-0.475925	-0.000066
5	1	0	-0.880551	-1.107503	-0.894004
6	1	0	-0.880687	-1.107622	0.893804
7	8	0	-2.338164	0.157522	-0.000158
8	1	0	-3.032786	-0.535348	0.001108
9	16	0	1.826102	-0.120504	-0.000001

Zero-point correction= 0.070074 (Hartree/Particle)
Thermal correction to Energy= 0.075295
Thermal correction to Enthalpy= 0.076239
Thermal correction to Gibbs Free Energy= 0.041713
Sum of electronic and zero-point Energies= -164.580474
Sum of electronic and thermal Energies= -164.575253
Sum of electronic and thermal Enthalpies= -164.574309
Sum of electronic and thermal Free Energies= -164.608836

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	47.248	16.607	72.667
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	38.939
Rotational	0.889	2.981	25.198
Vibrational	45.471	10.646	8.530

2-mercaptoethanol-C_4F_9 radical anion: 



ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.655996	-0.539633	-0.379031
2	1	0	3.378623	-0.103239	-1.340664
3	1	0	4.298538	-1.406887	-0.552918

4	6	0	4.350029	0.477801	0.526597
5	1	0	3.709316	1.352204	0.689262
6	1	0	4.596448	0.024994	1.496818
7	8	0	5.576630	0.857767	-0.188558
8	1	0	6.079031	1.521230	0.329471
9	16	0	2.090719	-1.262184	0.418588
10	6	0	0.839034	-0.030466	-0.210570
11	6	0	-0.528522	-0.314307	0.256778
12	6	0	-1.651361	0.616632	0.087330
13	6	0	-3.099519	0.030219	-0.011704
14	9	0	-4.049275	1.032811	0.251365
15	9	0	-3.395132	-0.437401	-1.284435
16	9	0	-3.333178	-0.988079	0.901920
17	9	0	-1.476084	1.441112	-1.045944
18	9	0	-1.740691	1.563666	1.222837
19	9	0	-1.084789	-1.840071	-0.876207
20	9	0	-0.596868	-1.026912	1.475977
21	9	0	0.905599	0.081998	-1.642924
22	9	0	1.268146	1.339879	0.172155

Zero-point correction= 0.115212 (Hartree/Particle)
Thermal correction to Energy= 0.134621
Thermal correction to Enthalpy= 0.135565
Thermal correction to Gibbs Free Energy= 0.064723
Sum of electronic and zero-point Energies= -1215.511864
Sum of electronic and thermal Energies= -1215.492455
Sum of electronic and thermal Enthalpies= -1215.491511
Sum of electronic and thermal Free Energies= -1215.562353

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	84.476	66.611	149.100
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.953
Rotational	0.889	2.981	33.394
Vibrational	82.698	60.649	71.376

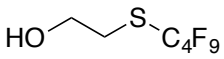
DMF

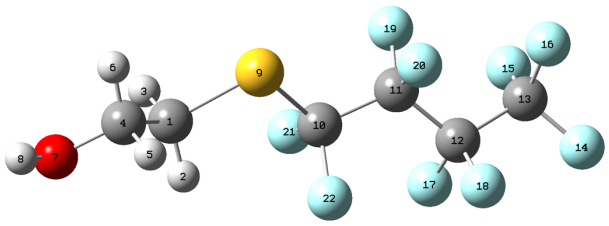
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.655996	0.539633	0.379031
2	1	0	3.378623	0.103239	1.340664
3	1	0	4.298538	1.406887	0.552918
4	6	0	4.350029	-0.477801	-0.526597
5	1	0	3.709316	-1.352204	-0.689262
6	1	0	4.596448	-0.024994	-1.496818
7	8	0	5.576630	-0.857767	0.188558

8	1	0	6.079031	-1.521230	-0.329471
9	16	0	2.090719	1.262184	-0.418588
10	6	0	0.839034	0.030466	0.210570
11	6	0	-0.528522	0.314307	-0.256778
12	6	0	-1.651361	-0.616632	-0.087330
13	6	0	-3.099519	-0.030219	0.011704
14	9	0	-4.049275	-1.032811	-0.251365
15	9	0	-3.395132	0.437401	1.284435
16	9	0	-3.333178	0.988079	-0.901920
17	9	0	-1.476084	-1.441112	1.045944
18	9	0	-1.740691	-1.563666	-1.222837
19	9	0	-1.084789	1.840071	0.876207
20	9	0	-0.596868	1.026912	-1.475977
21	9	0	0.905599	-0.081998	1.642924
22	9	0	1.268146	-1.339879	-0.172155

Zero-point correction= 0.115211 (Hartree/Particle)
Thermal correction to Energy= 0.134621
Thermal correction to Enthalpy= 0.135565
Thermal correction to Gibbs Free Energy= 0.064722
Sum of electronic and zero-point Energies= -1215.511974
Sum of electronic and thermal Energies= -1215.492565
Sum of electronic and thermal Enthalpies= -1215.491621
Sum of electronic and thermal Free Energies= -1215.562463

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	84.476	66.611	149.100
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.953
Rotational	0.889	2.981	33.394
Vibrational	82.698	60.649	71.376

2-mercaptoethanol-C_4F_9: 



CAN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.619473	0.128311	-0.421462

2	1	0	3.331224	1.159742	-0.210988
3	1	0	3.765483	-0.015932	-1.491917
4	6	0	4.866060	-0.260320	0.375604
5	1	0	4.709897	-0.084165	1.447766
6	1	0	5.120880	-1.317996	0.219642
7	8	0	5.924880	0.605545	-0.149032
8	1	0	6.778615	0.403067	0.288551
9	16	0	2.181014	-1.014110	0.123862
10	6	0	0.800329	0.204107	-0.085531
11	6	0	-0.605352	-0.468445	0.008272
12	6	0	-1.817794	0.494585	0.271157
13	6	0	-3.220079	-0.090733	-0.126212
14	9	0	-4.223308	0.689380	0.428410
15	9	0	-3.389325	-0.095017	-1.501640
16	9	0	-3.367036	-1.389803	0.343582
17	9	0	-1.646048	1.685969	-0.446454
18	9	0	-1.856342	0.813007	1.633228
19	9	0	-0.848307	-1.165613	-1.189756
20	9	0	-0.591265	-1.419991	1.042643
21	9	0	0.870873	0.880378	-1.331580
22	9	0	0.844404	1.245205	0.891170

Zero-point correction= 0.118620 (Hartree/Particle)
Thermal correction to Energy= 0.137200
Thermal correction to Enthalpy= 0.138145
Thermal correction to Gibbs Free Energy= 0.069336
Sum of electronic and zero-point Energies= -1215.387475
Sum of electronic and thermal Energies= -1215.368895
Sum of electronic and thermal Enthalpies= -1215.367950
Sum of electronic and thermal Free Energies= -1215.436759

	E (Thermal) Kcal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.095	64.011	144.820
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	42.953
Rotational	0.889	2.981	33.375
Vibrational	84.317	58.050	68.492

DMF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.619569	-0.127176	0.422685
2	1	0	3.330433	-1.158936	0.215081
3	1	0	3.767077	0.019483	1.492612
4	6	0	4.865320	0.258856	-0.376933
5	1	0	4.707650	0.080215	-1.448461

6	1	0	5.120910	1.316761	-0.223833
7	8	0	5.924375	-0.606326	0.148383
8	1	0	6.777673	-0.405219	-0.290683
9	16	0	2.180948	1.014798	-0.123188
10	6	0	0.800387	-0.203550	0.086174
11	6	0	-0.605345	0.468714	-0.008762
12	6	0	-1.817554	-0.494774	-0.271193
13	6	0	-3.219972	0.090325	0.126033
14	9	0	-4.223037	-0.690273	-0.428209
15	9	0	-3.389117	0.095111	1.501474
16	9	0	-3.367314	1.389166	-0.344284
17	9	0	-1.645452	-1.685838	0.446868
18	9	0	-1.856085	-0.813773	-1.633135
19	9	0	-0.848835	1.166916	1.188562
20	9	0	-0.591028	1.419334	-1.043970
21	9	0	0.870340	-0.879078	1.332700
22	9	0	0.845155	-1.245214	-0.889874

Zero-point correction= 0.118621 (Hartree/Particle)
Thermal correction to Energy= 0.137199
Thermal correction to Enthalpy= 0.138144
Thermal correction to Gibbs Free Energy= 0.069365
Sum of electronic and zero-point Energies= -1215.387488
Sum of electronic and thermal Energies= -1215.368910
Sum of electronic and thermal Enthalpies= -1215.367965
Sum of electronic and thermal Free Energies= -1215.436744

	E (Thermal) Kcal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	86.094	64.012	144.756
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	42.953
Rotational	0.889	2.981	33.375
Vibrational	84.316	58.050	68.428

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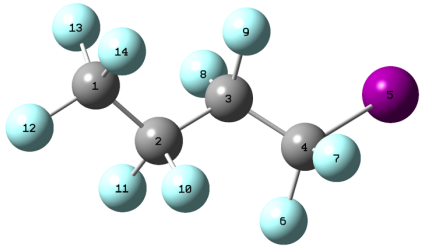

ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.037171	-0.414438	0.102459
2	6	0	1.789608	0.485078	-0.216088
3	6	0	0.400455	-0.231607	-0.043585
4	6	0	-0.838704	0.703746	0.153193
5	53	0	-2.749127	-0.299337	-0.030076
6	9	0	-0.735143	1.745317	-0.794427
7	9	0	-0.732276	1.301008	1.423437
8	9	0	0.200548	-1.027802	-1.181088
9	9	0	0.478570	-1.093735	1.063924
10	9	0	1.858329	1.607571	0.619589
11	9	0	1.905135	0.928086	-1.538386
12	9	0	4.185857	0.201624	-0.369112
13	9	0	2.922619	-1.655005	-0.511477
14	9	0	3.179979	-0.606156	1.467337

Zero-point correction= 0.046177 (Hartree/Particle)
Thermal correction to Energy= 0.060180
Thermal correction to Enthalpy= 0.061124
Thermal correction to Gibbs Free Energy= 0.002895
Sum of electronic and zero-point Energies= -1062.310462
Sum of electronic and thermal Energies= -1062.296459
Sum of electronic and thermal Enthalpies= -1062.295515
Sum of electronic and thermal Free Energies= -1062.353744

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	37.763	48.218	122.554
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.417
Rotational	0.889	2.981	33.028
Vibrational	35.986	42.256	46.109

DMF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.037174	-0.414427	0.102459
2	6	0	1.789602	0.485072	-0.216103
3	6	0	0.400454	-0.231620	-0.043576
4	6	0	-0.838710	0.703725	0.153201
5	53	0	-2.749133	-0.299329	-0.030081
6	9	0	-0.735124	1.745316	-0.794407
7	9	0	-0.732268	1.300987	1.423453
8	9	0	0.200550	-1.027838	-1.181065
9	9	0	0.478592	-1.093732	1.063944
10	9	0	1.858319	1.607589	0.619543
11	9	0	1.905119	0.928054	-1.538412
12	9	0	4.185852	0.201615	-0.369159

13	9	0	2.922614	-1.655022	-0.511418
14	9	0	3.180006	-0.606085	1.467344

Zero-point correction= 0.046176 (Hartree/Particle)
Thermal correction to Energy= 0.060179
Thermal correction to Enthalpy= 0.061123
Thermal correction to Gibbs Free Energy= 0.002893
Sum of electronic and zero-point Energies= -1062.310468
Sum of electronic and thermal Energies= -1062.296465
Sum of electronic and thermal Enthalpies= -1062.295521
Sum of electronic and thermal Free Energies= -1062.353751

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	37.763	48.218	122.555
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.417
Rotational	0.889	2.981	33.028
Vibrational	35.985	42.257	46.110

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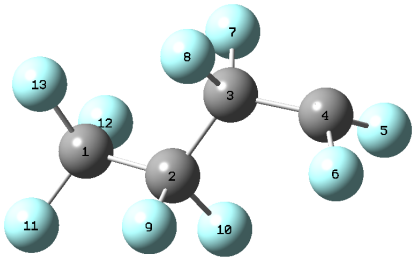


ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.797484	0.048195	-0.087334
2	6	0	-0.325831	-0.492879	-0.125360
3	6	0	0.782286	0.492083	0.398764
4	6	0	2.224257	0.174566	0.024071
5	9	0	2.594007	0.449366	-1.262668
6	9	0	2.700569	-1.033039	0.460232
7	9	0	0.481526	1.778390	-0.085583
8	9	0	0.697042	0.521590	1.802629
9	9	0	-0.265329	-1.668559	0.631180
10	9	0	-0.026500	-0.823464	-1.457458
11	9	0	-2.687937	-0.997801	-0.272167
12	9	0	-2.008863	0.979482	-1.091789
13	9	0	-2.073335	0.646057	1.135530

Zero-point correction= 0.044599 (Hartree/Particle)

Thermal correction to Energy= 0.057114
Thermal correction to Enthalpy= 0.058058
Thermal correction to Gibbs Free Energy= 0.003857
Sum of electronic and zero-point Energies= -1050.874844
Sum of electronic and thermal Energies= -1050.862330
Sum of electronic and thermal Enthalpies= -1050.861385
Sum of electronic and thermal Free Energies= -1050.915587

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	35.839	43.212	114.076
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.055
Rotational	0.889	2.981	31.036
Vibrational	34.062	37.250	39.608

DMF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.797487	0.048190	-0.087321
2	6	0	-0.325832	-0.492886	-0.125369
3	6	0	0.782288	0.492083	0.398743
4	6	0	2.224263	0.174583	0.024060
5	9	0	2.593995	0.449314	-1.262699
6	9	0	2.700621	-1.032976	0.460297
7	9	0	0.481511	1.778383	-0.085616
8	9	0	0.697038	0.521603	1.802609
9	9	0	-0.265315	-1.668566	0.631171
10	9	0	-0.026525	-0.823473	-1.457470
11	9	0	-2.687950	-0.997812	-0.272068
12	9	0	-2.008895	0.979425	-1.091819
13	9	0	-2.073302	0.646122	1.135518

Zero-point correction= 0.044599 (Hartree/Particle)
Thermal correction to Energy= 0.057113
Thermal correction to Enthalpy= 0.058057
Thermal correction to Gibbs Free Energy= 0.003857
Sum of electronic and zero-point Energies= -1050.874848
Sum of electronic and thermal Energies= -1050.862334
Sum of electronic and thermal Enthalpies= -1050.861390
Sum of electronic and thermal Free Energies= -1050.915590

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	35.839	43.212	114.075
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	42.055

Rotational	0.889	2.981	31.036
Vibrational	34.062	37.251	39.607

I anion

ACN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	0.000000	0.000000	0.000000

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.016848
Sum of electronic and zero-point Energies= -11.571193
Sum of electronic and thermal Energies= -11.569776
Sum of electronic and thermal Enthalpies= -11.568832
Sum of electronic and thermal Free Energies= -11.588041

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	0.889	2.981	40.428
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.428
Rotational	0.000	0.000	0.000
Vibrational	0.000	0.000	0.000

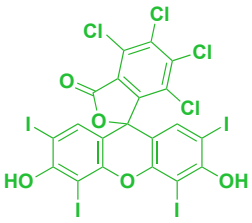
DMF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	0.000000	0.000000	0.000000

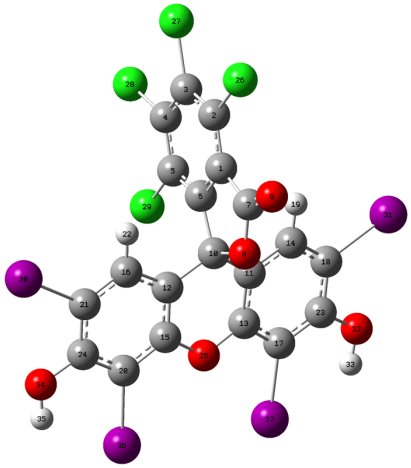
Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.016848
Sum of electronic and zero-point Energies= -11.571310
Sum of electronic and thermal Energies= -11.569894
Sum of electronic and thermal Enthalpies= -11.568950
Sum of electronic and thermal Free Energies= -11.588158

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	0.889	2.981	40.428

Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.428
Rotational	0.000	0.000	0.000
Vibrational	0.000	0.000	0.000



Rose Bengal Ground State:



ACN

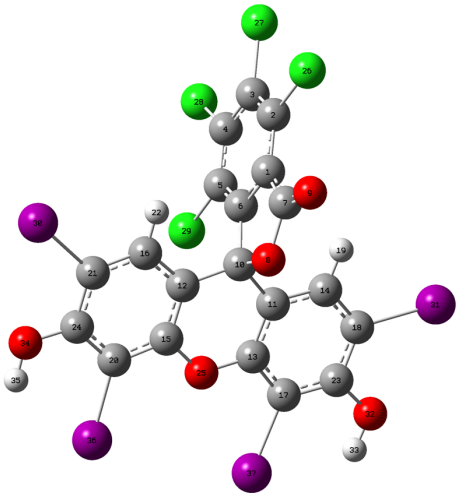
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000134	3.135931	-1.061715
2	6	0	-0.000196	4.496629	-0.729813
3	6	0	-0.000200	4.861570	0.629355
4	6	0	-0.000138	3.865428	1.632198
5	6	0	-0.000080	2.501267	1.281867
6	6	0	-0.000080	2.145551	-0.066796
7	6	0	-0.000114	2.478690	-2.401121
8	8	0	-0.000046	1.099532	-2.192317
9	8	0	-0.000147	2.967176	-3.534902
10	6	0	-0.000027	0.747471	-0.687502
11	6	0	-1.259535	-0.049054	-0.425683
12	6	0	1.259542	-0.048957	-0.425690
13	6	0	-1.207778	-1.441240	-0.235131
14	6	0	-2.522410	0.576777	-0.440892
15	6	0	1.207891	-1.441146	-0.235132
16	6	0	2.522370	0.576970	-0.440905
17	6	0	-2.380646	-2.204036	-0.071945
18	6	0	-3.697556	-0.155722	-0.278113
19	1	0	-2.582599	1.649821	-0.585481
20	6	0	2.380817	-2.203852	-0.071940
21	6	0	3.697571	-0.155440	-0.278124

22	1	0	2.582477	1.650017	-0.585502
23	6	0	-3.638269	-1.560819	-0.093759
24	6	0	3.638390	-1.560540	-0.093756
25	8	0	0.000084	-2.137645	-0.192952
26	17	0	-0.000263	5.752639	-2.009005
27	17	0	-0.000280	6.594136	1.093748
28	17	0	-0.000134	4.340220	3.359304
29	17	0	-0.000012	1.226764	2.549977
30	53	0	5.581286	0.831294	-0.311678
31	53	0	-5.581342	0.830878	-0.311649
32	8	0	-4.834400	-2.229044	0.058808
33	1	0	-4.725573	-3.199092	0.186348
34	8	0	4.834571	-2.228673	0.058819
35	1	0	4.725815	-3.198728	0.186367
36	53	0	2.262907	-4.308352	0.210615
37	53	0	-2.262576	-4.308529	0.210595

Zero-point correction= 0.190737 (Hartree/Particle)
Thermal correction to Energy= 0.221664
Thermal correction to Enthalpy= 0.222608
Thermal correction to Gibbs Free Energy= 0.121355
Sum of electronic and zero-point Energies= -1245.547927
Sum of electronic and thermal Energies= -1245.517000
Sum of electronic and thermal Enthalpies= -1245.516056
Sum of electronic and thermal Free Energies= -1245.617309

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	139.096	109.078	213.106
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	46.495
Rotational	0.889	2.981	40.108
Vibrational	137.319	103.116	126.502

Rose Bengal Excited State



ACN

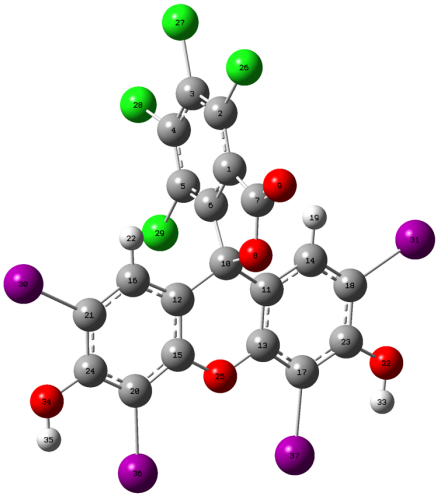
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000414	3.207302	-0.989198
2	6	0	0.000630	4.560598	-0.514837
3	6	0	0.000656	4.822332	0.849765
4	6	0	0.000476	3.765054	1.810978
5	6	0	0.000291	2.425907	1.341837
6	6	0	0.000261	2.153209	-0.009691
7	6	0	0.000337	2.671405	-2.307960
8	8	0	0.000139	1.196587	-2.174015
9	8	0	0.000394	3.142970	-3.478280
10	6	0	0.000088	0.805673	-0.734254
11	6	0	-1.264411	-0.009801	-0.487843
12	6	0	1.264386	-0.010116	-0.487842
13	6	0	-1.210594	-1.401715	-0.232166
14	6	0	-2.519820	0.592446	-0.573894
15	6	0	1.210222	-1.402021	-0.232155
16	6	0	2.519942	0.591817	-0.573901
17	6	0	-2.374348	-2.189751	-0.065176
18	6	0	-3.699001	-0.158243	-0.413648
19	1	0	-2.583862	1.656806	-0.767961
20	6	0	2.373782	-2.190342	-0.065148
21	6	0	3.698938	-0.159161	-0.413636
22	1	0	2.584250	1.656158	-0.767981
23	6	0	-3.630574	-1.563442	-0.156843
24	6	0	3.630160	-1.564343	-0.156802
25	8	0	-0.000265	-2.056521	-0.129237
26	17	0	0.000915	5.912049	-1.720125
27	17	0	0.000941	6.531934	1.442907
28	17	0	0.000408	4.122356	3.580834
29	17	0	0.000095	1.046223	2.524422
30	53	0	5.563741	0.788960	-0.553757
31	53	0	-5.563576	0.790344	-0.553761
32	8	0	-4.826501	-2.219614	-0.013068
33	1	0	-4.736473	-3.184117	0.162853
34	8	0	4.825924	-2.220797	-0.012997
35	1	0	4.735669	-3.185263	0.163006
36	53	0	2.232694	-4.268978	0.318569
37	53	0	-2.233769	-4.268420	0.318547

Zero-point correction= 0.186698 (Hartree/Particle)
Thermal correction to Energy= 0.218372
Thermal correction to Enthalpy= 0.219316
Thermal correction to Gibbs Free Energy= 0.114636
Sum of electronic and zero-point Energies= -1245.448352
Sum of electronic and thermal Energies= -1245.416677

Sum of electronic and thermal Enthalpies= -1245.415733
Sum of electronic and thermal Free Energies= -1245.520414

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	137.031	111.023	220.319
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	46.495
Rotational	0.889	2.981	40.098
Vibrational	135.253	105.061	133.725

Rose Bengal Radical Cation



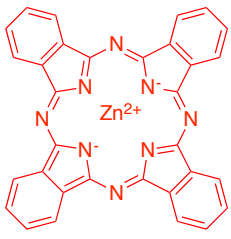
ACN

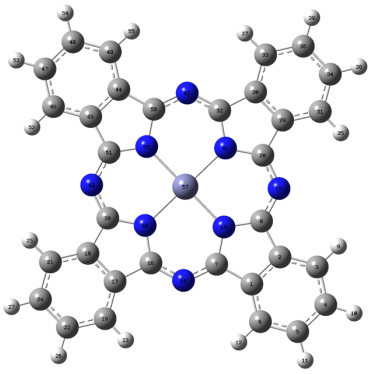
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000311	3.165019	-1.047116
2	6	0	-0.000448	4.525499	-0.714243
3	6	0	-0.000452	4.887436	0.646420
4	6	0	-0.000312	3.890347	1.649097
5	6	0	-0.000182	2.526307	1.297219
6	6	0	-0.000185	2.176110	-0.051547
7	6	0	-0.000265	2.510056	-2.384286
8	8	0	-0.000110	1.117586	-2.167648
9	8	0	-0.000336	2.979533	-3.520881
10	6	0	-0.000066	0.783181	-0.682577
11	6	0	-1.265716	-0.016282	-0.418368
12	6	0	1.265725	-0.016062	-0.418385
13	6	0	-1.208598	-1.418764	-0.216786
14	6	0	-2.521468	0.588862	-0.449682
15	6	0	1.208853	-1.418553	-0.216801
16	6	0	2.521371	0.589301	-0.449707
17	6	0	-2.370228	-2.212644	-0.062882
18	6	0	-3.700733	-0.167691	-0.292264
19	1	0	-2.600443	1.659550	-0.598274
20	6	0	2.370621	-2.212231	-0.062905

21	6	0	3.700768	-0.167047	-0.292290
22	1	0	2.600160	1.660002	-0.598302
23	6	0	-3.628834	-1.580075	-0.100992
24	6	0	3.629116	-1.579444	-0.101020
25	8	0	0.000185	-2.075692	-0.153850
26	17	0	-0.000604	5.778148	-1.993011
27	17	0	-0.000631	6.617419	1.111901
28	17	0	-0.000301	4.360378	3.374908
29	17	0	-0.000022	1.243827	2.555306
30	53	0	5.562032	0.789577	-0.343718
31	53	0	-5.562161	0.788614	-0.343694
32	8	0	-4.820298	-2.240241	0.037912
33	1	0	-4.732798	-3.211961	0.170656
34	8	0	4.820694	-2.239404	0.037881
35	1	0	4.733359	-3.211140	0.170619
36	53	0	2.228341	-4.301608	0.224519
37	53	0	-2.227585	-4.301995	0.224552

Zero-point correction= 0.189843 (Hartree/Particle)
Thermal correction to Energy= 0.220751
Thermal correction to Enthalpy= 0.221695
Thermal correction to Gibbs Free Energy= 0.119858
Sum of electronic and zero-point Energies= -1245.312142
Sum of electronic and thermal Energies= -1245.281235
Sum of electronic and thermal Enthalpies= -1245.280291
Sum of electronic and thermal Free Energies= -1245.382127

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.523	109.154	214.333
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	46.495
Rotational	0.889	2.981	40.098
Vibrational	136.746	103.192	126.362

PCZn Ground State: 



DMF

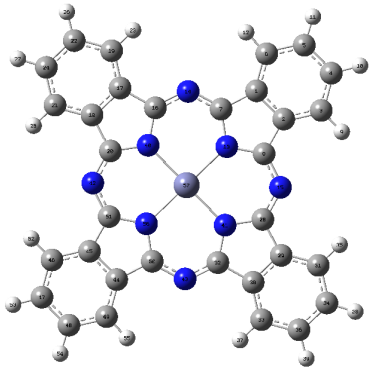
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.608408	3.989113	0.000002
2	6	0	0.216960	4.295227	0.000003
3	6	0	-0.231981	5.625676	0.000004
4	6	0	0.737209	6.648512	0.000004
5	6	0	2.123032	6.343810	0.000004
6	6	0	2.573890	5.008735	0.000003
7	6	0	1.718554	2.521186	0.000001
8	6	0	-0.499327	3.009413	0.000002
9	1	0	-1.292664	5.857916	0.000004
10	1	0	0.422514	7.688769	0.000005
11	1	0	2.845083	7.156094	0.000005
12	1	0	3.634265	4.775176	0.000003
13	7	0	0.438335	1.986417	0.000001
14	7	0	2.880038	1.839797	0.000001
15	7	0	-1.839797	2.880038	0.000002
16	6	0	3.009413	0.499327	0.000001
17	6	0	4.295227	-0.216960	0.000001
18	6	0	3.989113	-1.608408	0.000000
19	6	0	5.625676	0.231981	0.000002
20	6	0	2.521186	-1.718554	-0.000001
21	6	0	5.008735	-2.573890	0.000001
22	6	0	6.648512	-0.737209	0.000003
23	1	0	5.857916	1.292664	0.000003
24	6	0	6.343810	-2.123032	0.000002
25	1	0	4.775176	-3.634265	-0.000000
26	1	0	7.688769	-0.422514	0.000004
27	1	0	7.156094	-2.845083	0.000002
28	6	0	-2.521186	1.718554	0.000001
29	6	0	-3.989113	1.608408	0.000002
30	6	0	-4.295227	0.216960	0.000001
31	6	0	-5.008735	2.573890	0.000003
32	6	0	-3.009413	-0.499327	-0.000001
33	6	0	-5.625676	-0.231981	0.000001
34	6	0	-6.343810	2.123032	0.000003
35	1	0	-4.775176	3.634265	0.000004

36	6	0	-6.648512	0.737209	0.000002
37	1	0	-5.857916	-1.292664	0.000000
38	1	0	-7.156094	2.845083	0.000004
39	1	0	-7.688769	0.422514	0.000003
40	7	0	1.986417	-0.438335	-0.000001
41	7	0	-1.986417	0.438335	-0.000000
42	7	0	1.839797	-2.880038	-0.000002
43	7	0	-2.880038	-1.839797	-0.000002
44	6	0	-1.608408	-3.989113	-0.000004
45	6	0	-0.216960	-4.295227	-0.000004
46	6	0	0.231981	-5.625676	-0.000005
47	6	0	-0.737209	-6.648512	-0.000007
48	6	0	-2.123032	-6.343810	-0.000007
49	6	0	-2.573890	-5.008735	-0.000005
50	6	0	-1.718554	-2.521186	-0.000002
51	6	0	0.499327	-3.009413	-0.000002
52	1	0	1.292664	-5.857916	-0.000005
53	1	0	-0.422514	-7.688769	-0.000008
54	1	0	-2.845083	-7.156094	-0.000008
55	1	0	-3.634265	-4.775176	-0.000005
56	7	0	-0.438335	-1.986417	-0.000001
57	30	0	0.000000	0.000000	-0.000001

Zero-point correction= 0.414781 (Hartree/Particle)
Thermal correction to Energy= 0.442551
Thermal correction to Enthalpy= 0.443495
Thermal correction to Gibbs Free Energy= 0.357637
Sum of electronic and zero-point Energies= -1732.129019
Sum of electronic and thermal Energies= -1732.101249
Sum of electronic and thermal Enthalpies= -1732.100305
Sum of electronic and thermal Free Energies= -1732.186163

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	277.705	115.450	180.703
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	44.938
Rotational	0.889	2.981	38.133
Vibrational	275.928	109.488	97.633

PCZn Excited State



DMF

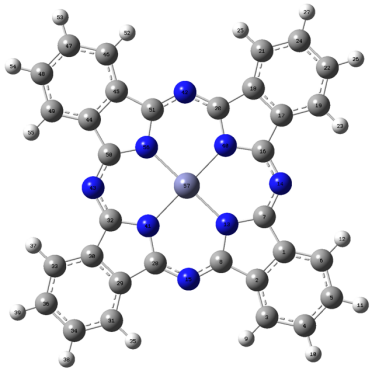
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.787343	4.222436	-0.000209
2	6	0	-0.645318	4.246332	-0.000231
3	6	0	-1.346127	5.465588	-0.000339
4	6	0	-0.598851	6.661842	-0.000428
5	6	0	0.821161	6.638225	-0.000406
6	6	0	1.528271	5.417775	-0.000295
7	6	0	1.183111	2.817462	-0.000080
8	6	0	-1.087882	2.855480	-0.000097
9	1	0	-2.432152	5.484969	-0.000352
10	1	0	-1.114319	7.618741	-0.000514
11	1	0	1.368162	7.577450	-0.000472
12	1	0	2.614347	5.401342	-0.000269
13	7	0	0.034293	2.035628	-0.000013
14	7	0	2.474194	2.376194	-0.000002
15	7	0	-2.393192	2.458117	-0.000018
16	6	0	2.851407	1.092715	0.000041
17	6	0	4.259073	0.639331	0.000240
18	6	0	4.235614	-0.781717	0.000129
19	6	0	5.468362	1.343812	0.000489
20	6	0	2.813530	-1.188161	-0.000045
21	6	0	5.421307	-1.525326	0.000251
22	6	0	6.670307	0.595695	0.000622
23	1	0	5.484548	2.429424	0.000591
24	6	0	6.647117	-0.816920	0.000496
25	1	0	5.402437	-2.610876	0.000169
26	1	0	7.625468	1.113650	0.000825
27	1	0	7.584769	-1.365933	0.000597
28	6	0	-2.813531	1.188161	0.000011
29	6	0	-4.235615	0.781717	0.000189
30	6	0	-4.259072	-0.639331	0.000179
31	6	0	-5.421309	1.525325	0.000379
32	6	0	-2.851407	-1.092715	-0.000002
33	6	0	-5.468361	-1.343813	0.000373
34	6	0	-6.647117	0.816918	0.000568
35	1	0	-5.402440	2.610875	0.000390

36	6	0	-6.670306	-0.595698	0.000565
37	1	0	-5.484546	-2.429425	0.000386
38	1	0	-7.584770	1.365930	0.000728
39	1	0	-7.625467	-1.113653	0.000722
40	7	0	2.027838	-0.034377	-0.000090
41	7	0	-2.027838	0.034378	-0.000104
42	7	0	2.393192	-2.458116	-0.000095
43	7	0	-2.474193	-2.376193	-0.000046
44	6	0	-0.787343	-4.222435	-0.000219
45	6	0	0.645318	-4.246331	-0.000223
46	6	0	1.346128	-5.465587	-0.000310
47	6	0	0.598852	-6.661841	-0.000396
48	6	0	-0.821161	-6.638225	-0.000397
49	6	0	-1.528270	-5.417775	-0.000306
50	6	0	-1.183111	-2.817462	-0.000124
51	6	0	1.087882	-2.855480	-0.000133
52	1	0	2.432153	-5.484968	-0.000315
53	1	0	1.114319	-7.618740	-0.000465
54	1	0	-1.368162	-7.577450	-0.000466
55	1	0	-2.614346	-5.401341	-0.000302
56	7	0	-0.034293	-2.035627	-0.000075
57	30	0	-0.000001	-0.000000	0.000003

Zero-point correction= 0.411799 (Hartree/Particle)
Thermal correction to Energy= 0.439966
Thermal correction to Enthalpy= 0.440910
Thermal correction to Gibbs Free Energy= 0.354049
Sum of electronic and zero-point Energies= -1732.064580
Sum of electronic and thermal Energies= -1732.036413
Sum of electronic and thermal Enthalpies= -1732.035469
Sum of electronic and thermal Free Energies= -1732.122330

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	276.083	116.911	182.814
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	44.938
Rotational	0.889	2.981	38.135
Vibrational	274.305	110.950	99.741

PCZn Radical Anion



DMF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.189249	0.974778	-0.000002
2	6	0	4.277388	-0.447216	-0.000003
3	6	0	5.522810	-1.095726	-0.000004
4	6	0	6.682723	-0.295647	-0.000004
5	6	0	6.595113	1.120570	-0.000004
6	6	0	5.345415	1.771687	-0.000003
7	6	0	2.755805	1.309712	-0.000001
8	6	0	2.896589	-0.956903	-0.000002
9	1	0	5.588903	-2.179523	-0.000004
10	1	0	7.662094	-0.766816	-0.000005
11	1	0	7.508920	1.708890	-0.000005
12	1	0	5.277971	2.855383	-0.000003
13	7	0	2.030228	0.127140	-0.000001
14	7	0	2.261449	2.562288	-0.000001
15	7	0	2.562288	-2.261449	-0.000002
16	6	0	0.956903	2.896589	-0.000001
17	6	0	0.447216	4.277388	-0.000001
18	6	0	-0.974778	4.189249	0.000000
19	6	0	1.095726	5.522810	-0.000002
20	6	0	-1.309712	2.755805	0.000001
21	6	0	-1.771687	5.345415	-0.000001
22	6	0	0.295647	6.682723	-0.000003
23	1	0	2.179523	5.588903	-0.000003
24	6	0	-1.120570	6.595113	-0.000002
25	1	0	-2.855383	5.277971	0.000000
26	1	0	0.766816	7.662094	-0.000004
27	1	0	-1.708890	7.508920	-0.000002
28	6	0	1.309712	-2.755805	-0.000001
29	6	0	0.974778	-4.189249	-0.000002
30	6	0	-0.447216	-4.277388	-0.000001
31	6	0	1.771687	-5.345415	-0.000003
32	6	0	-0.956903	-2.896589	0.000001
33	6	0	-1.095726	-5.522810	-0.000001
34	6	0	1.120570	-6.595113	-0.000003
35	1	0	2.855383	-5.277971	-0.000004

36	6	0	-0.295647	-6.682723	-0.000002
37	1	0	-2.179523	-5.588903	0.000000
38	1	0	1.708890	-7.508920	-0.000004
39	1	0	-0.766816	-7.662094	-0.000003
40	7	0	-0.127140	2.030228	0.000001
41	7	0	0.127140	-2.030228	0.000000
42	7	0	-2.562288	2.261449	0.000002
43	7	0	-2.261449	-2.562288	0.000002
44	6	0	-4.189249	-0.974778	0.000004
45	6	0	-4.277388	0.447216	0.000004
46	6	0	-5.522810	1.095726	0.000005
47	6	0	-6.682723	0.295647	0.000007
48	6	0	-6.595113	-1.120570	0.000007
49	6	0	-5.345415	-1.771687	0.000005
50	6	0	-2.755805	-1.309712	0.000002
51	6	0	-2.896589	0.956903	0.000002
52	1	0	-5.588903	2.179523	0.000005
53	1	0	-7.662094	0.766816	0.000008
54	1	0	-7.508920	-1.708890	0.000008
55	1	0	-5.277971	-2.855383	0.000005
56	7	0	-2.030228	-0.127140	0.000001
57	30	0	0.000000	0.000000	0.000001

Zero-point correction= 0.415834 (Hartree/Particle)
Thermal correction to Energy= 0.443824
Thermal correction to Enthalpy= 0.444768
Thermal correction to Gibbs Free Energy= 0.357303
Sum of electronic and zero-point Energies= -1732.251391
Sum of electronic and thermal Energies= -1732.223401
Sum of electronic and thermal Enthalpies= -1732.222456
Sum of electronic and thermal Free Energies= -1732.309922

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	278.504	116.005	184.086
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	44.938
Rotational	0.889	2.981	38.133
Vibrational	276.726	110.043	99.638

XI. Spectral Characterization of Compounds

2-methoxy-4-(perfluorobutyl)aniline,[16] **1A**: yellow oil, 80%. Isolated and purified mass obtained: 54 mg. TLC (CH_2Cl_2/iso-octane 1:1 v/v): R_f = 0.5. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.01 (d, 1 H, *J* = 10 Hz), 6.92 (s, 1 H), 6.73 (d, 1 H, *J* = 10 Hz), 4.15 (b s, 2H), 3.90 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ: 146.5, 139.7, 120.4 (t, CF_2), 118.7 (m, CF_2), 118.1 (t, CF_3), 116.7 (m), 113.5, 112.5, 109.7, 108.4, 55.6.

^{19}F NMR (564.603 MHz $CDCl_3$) δ: -81.11 (t, 3 F), -109.32 (t, 2 F), -122.78 (m, 2 F), -125.68 (m, 2 F). HRMS-EI+ (M+H): Calcd. For $C_{11}H_9F_9NO$: 342.0535; found, 342.05388.

2-methoxy-4,6-bis(perfluorobutyl)aniline,[16] **1B**: yellow oil, 10%. Isolated and purified mass obtained: 11.7 mg. TLC (CH_2Cl_2/iso-octane 1:1 v/v): R_f = 0.7; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.16 (s, 1 H), 6.99 (s, 1 H), 3.94 (s, 3 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ: 147.0, 139.8, 136.9, 119.7, 116.1, 109.8, 56.1. ^{19}F NMR (564.603 MHz $CDCl_3$) δ: -80.94 (t, 3 F), -81.04 (t, 3 F), -109.30 (t, 2 F), - 110.15 (t, 2 F), -122.83 (m, 2 F), -122.98 (m, 2 F), -125.64 (m, 2 F), -125.86 (m, 2F). HRMS-EI+ (M+H): Calcd. For $C_{15}H_8F_{18}NO$: 560.03130; found, 560.0292.

((4,4,5,5,6,6,7,7,7-nonafluoro-2-iodoheptyl)oxy)benzene, **2A**. Colorless crystals. Yield: 53%, Isolated and purified mass obtained: 51 mg. TLC (CH_2Cl_2: iso-octane 8:2 v/v): R_f= 0.5. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.32 (dt, 2 H, *J* = 4.9, 0.8 Hz), 7.02 (br t, 1 H, *J* = 4.9 Hz), 6.91 (dd, 2 H, *J* = 5.8, 0.8 Hz), 4.52 (quint, 1 H, *J* = 4.52 Hz), 4.32 (dd, 1 H, *J* = 3.3, 6.9 Hz), 4.18 (dd, 1 H, *J* = 4.5, 6.9 Hz), 3.19 (m, 1 H), 2.82 (m, 1 H). ^{13}C NMR (151 MHz, $CDCl_3$) δ: 157.6, 129.7, 121.9, 114.9, 72.7, 37.7 (t), 12.7 ppm. ^{19}F NMR (564.63MHz, $CDCl_3$) δ: -81.02 (t, 3 F), -113.8 (m, 2 F), -124.5 (m, 2 F), -125.8 (m, 2 F). HRMS-EI+ (M + Na) Calcd. For $C_{13}H_{10}F_9INaO$: 502.9525; found, 502.9502.

2-((perfluorobutyl)thio)ethanol 3A[17]: Yield: 75 %. Yellow oil. Isolated and purified mass obtained: 12 mg. TLC (ethyl acetate: hexane 1:1 v/v): R_f = 0.7. ^{1}H-NMR (600 MHz, Cl_3CD) δ : 3.89 (t, 2 H, *J* = 6.1 Hz), 3.14 (t, 2 H, *J* = 6.1 Hz), 1.97 (bs, 1 H). ^{13}C NMR (150 MHz, Cl_3CD) δ : 61.6, 31.7. ^{19}F NMR (564.603 MHz, Cl_3CD) δ : -81.0 (t, 3 F), -87.0 (m, 2 F), -120.7 (m, 2 F), -125.5 (m, 2 F).

(5,5,6,6,7,7,8,8,8-nonafluorooct-1-en-2-yl)benzene 4A,[18] Yield: 93%. Isolated and purified mass obtained: 62 mg. Yellow oil. TLC (Hexene: ethyl acetate 1:1 v/v): Rf= 0.55. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.30-7.38 (m, 5 H), 5.65 (s, 1 H), 5.38 (s, 1 H), 3.29 (t, 2 H, JH-F= 18.5 Hz). ^{13}C NMR (151 MHz, CDCl3) δ: 36.2 (t, JC-CF = 21.9 Hz), 120.6, 126.1, 128.0, 128.5, 136.1, 140.3 ppm. ^{19}F NMR (564.63MHz, CDCl3) δ: -81.1 (t, 3 F), -112.6 (m, 2 F), -124.03 (m, 2 F), -125.9 (m, 2 F).

XII.-References

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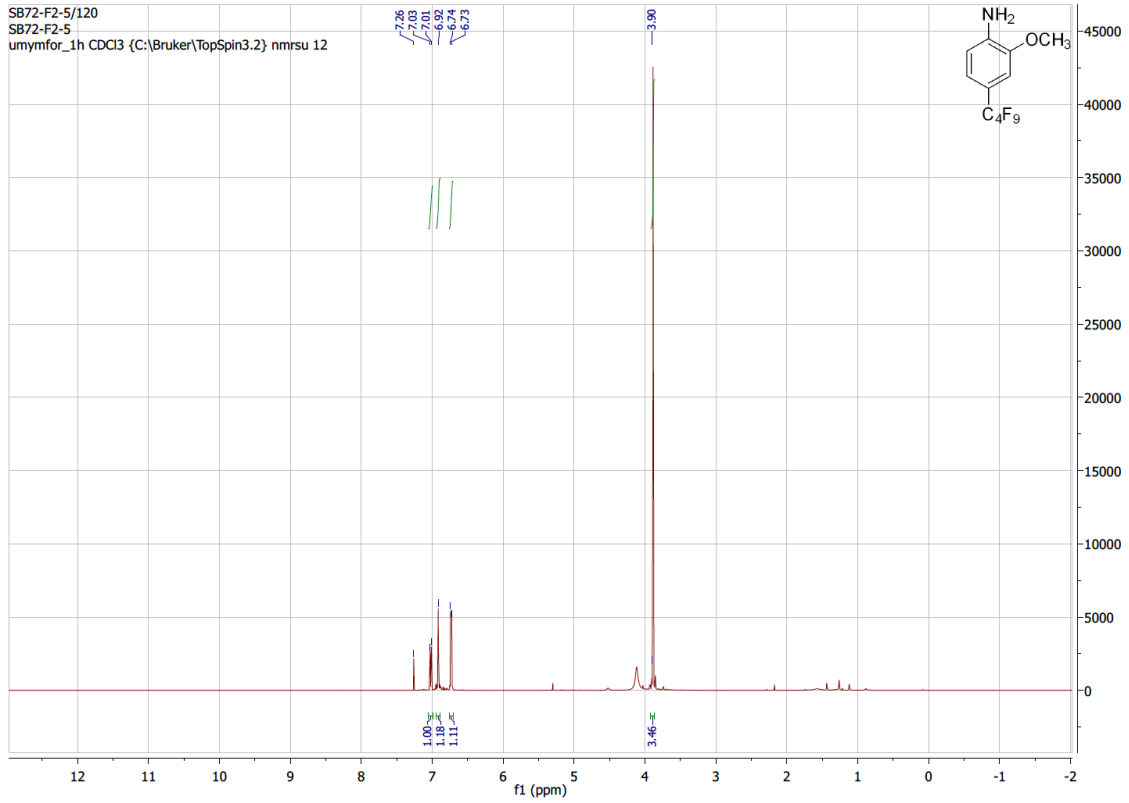
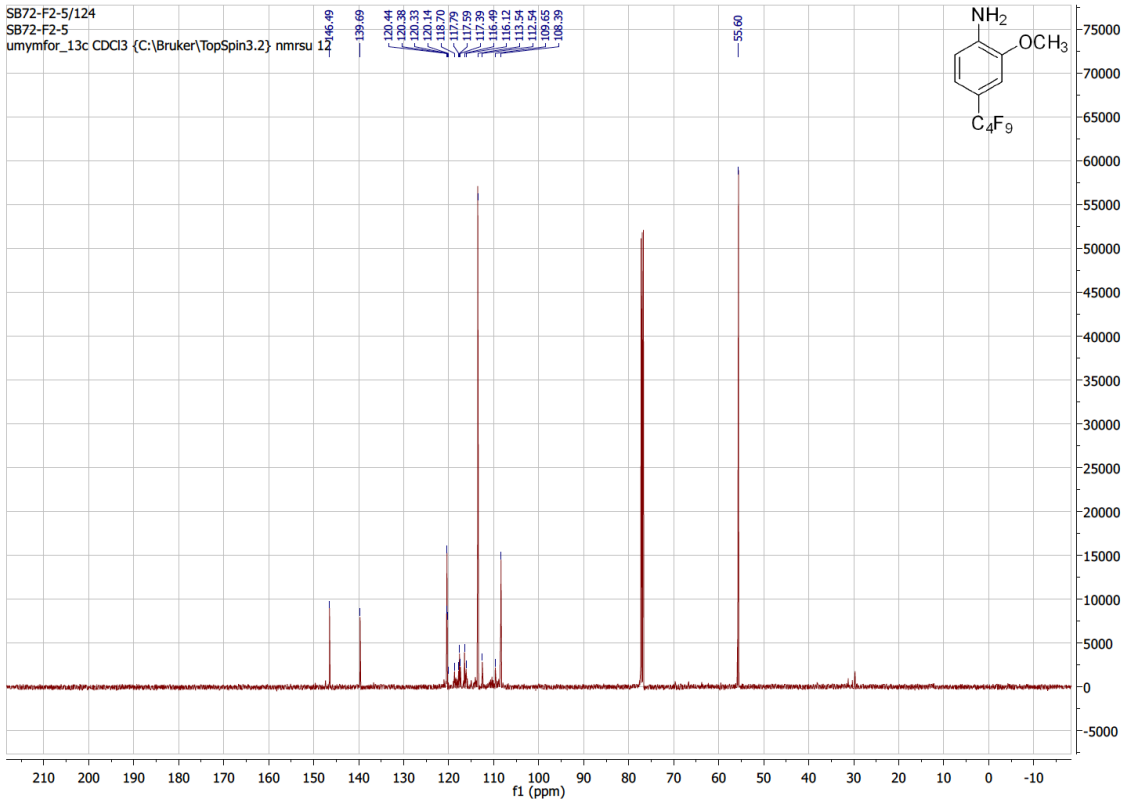
XIII.- Copies of Spectra

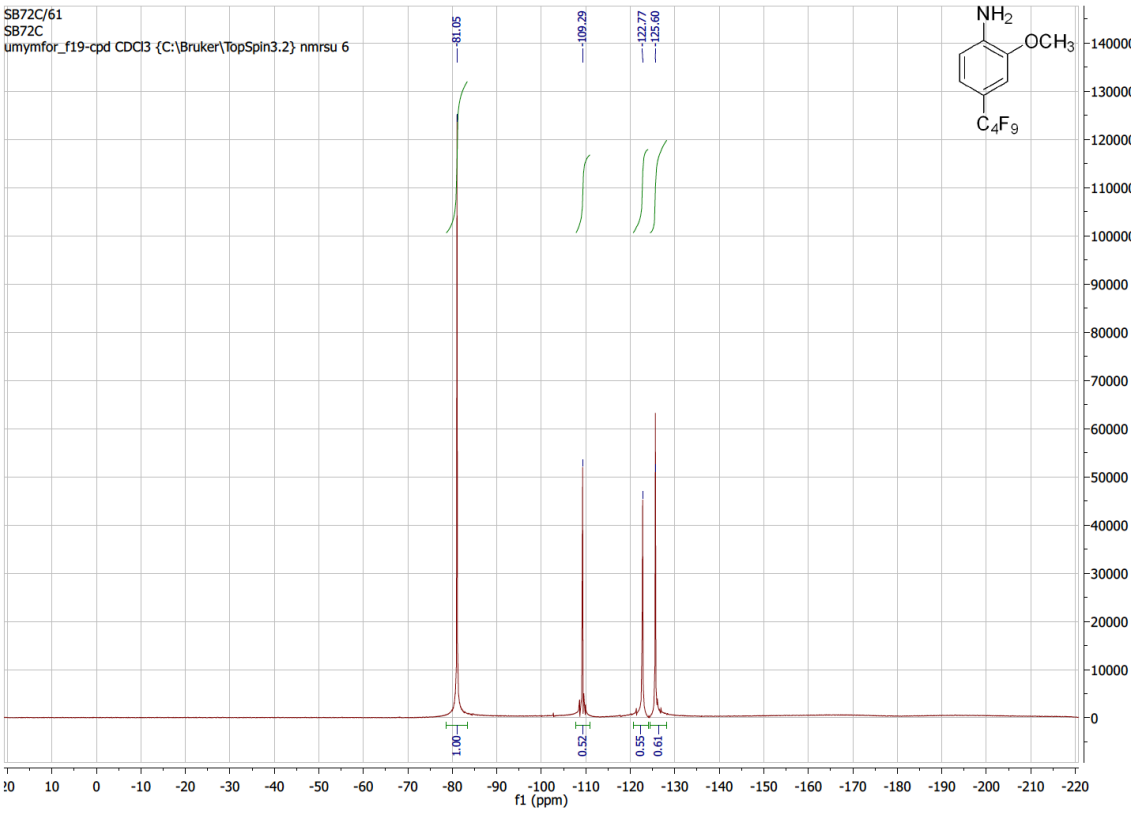
^{1}H NMR (600 MHz) spectrum of **1A** in $CDCl_3$,



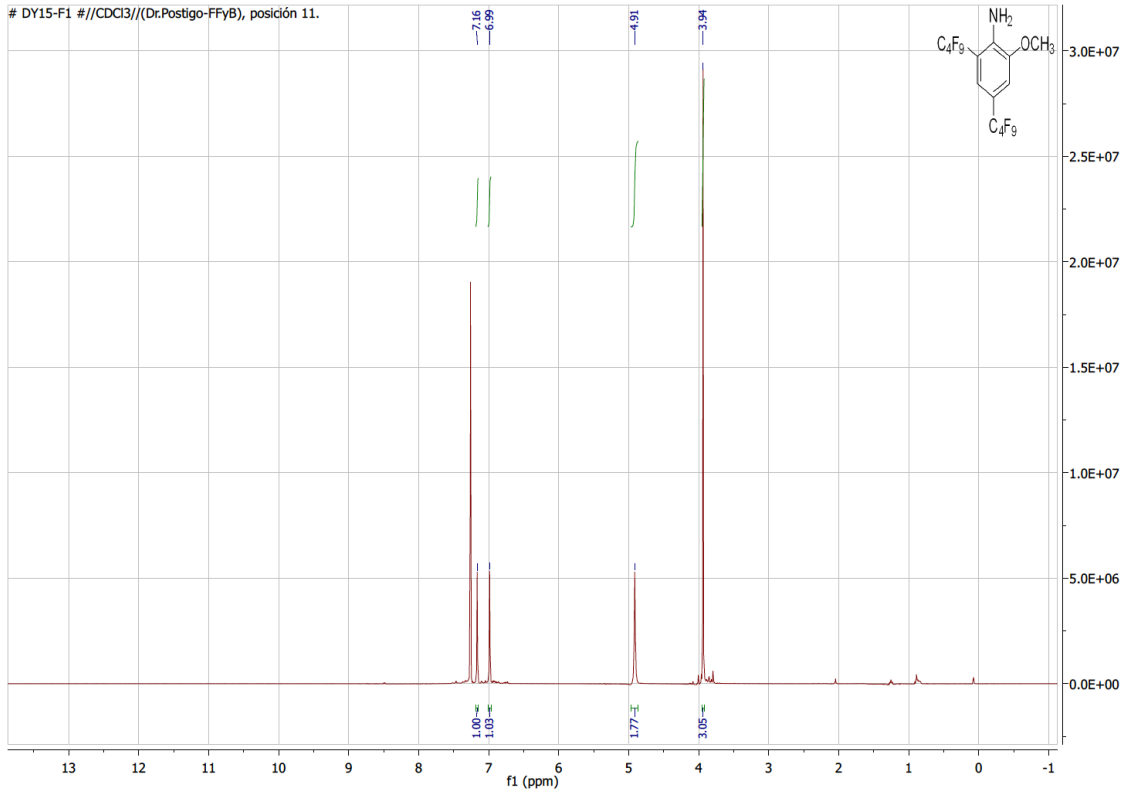
^{13}C NMR (150.903 MHz) spectrum of **1A** in $CDCl_3$



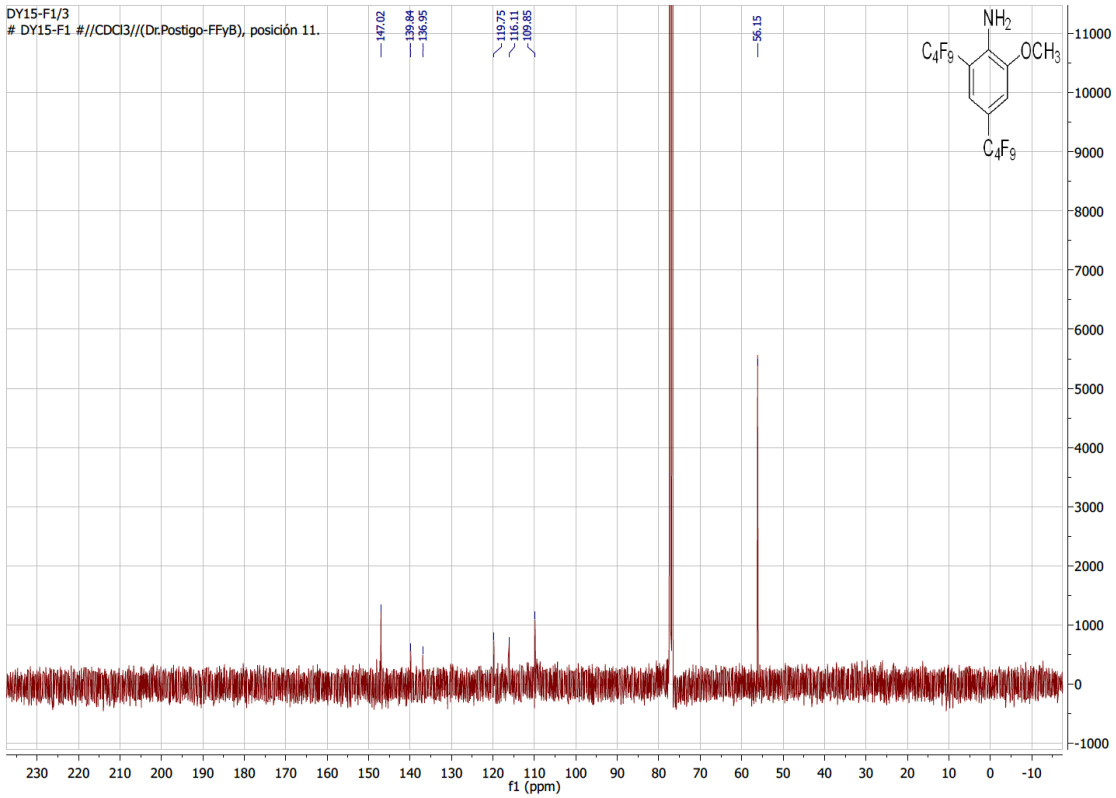
^{19}F NMR (564.686 MHz) spectrum of **1A** in $CDCl_3$



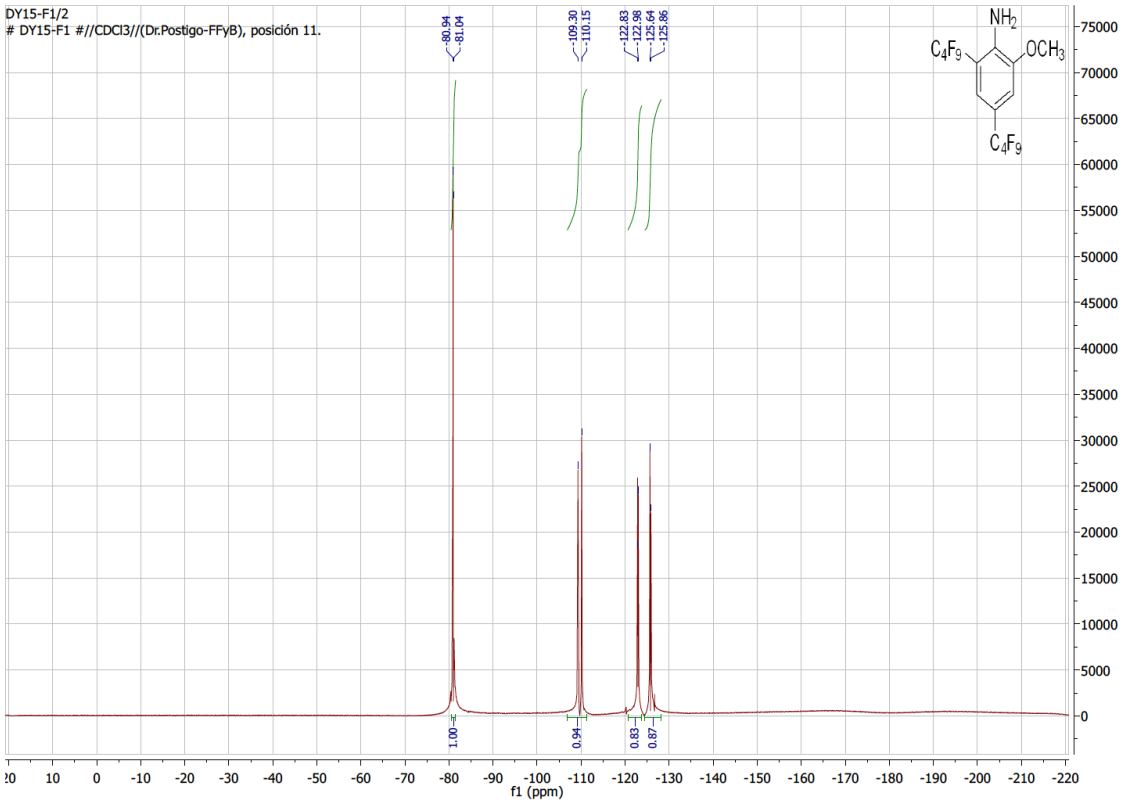
^{1}H NMR (600 MHz) spectrum of **1C** in $CDCl_3$



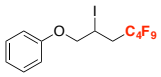
^{13}C NMR (150.903 MHz) spectrum of **1C** in $CDCl_3$

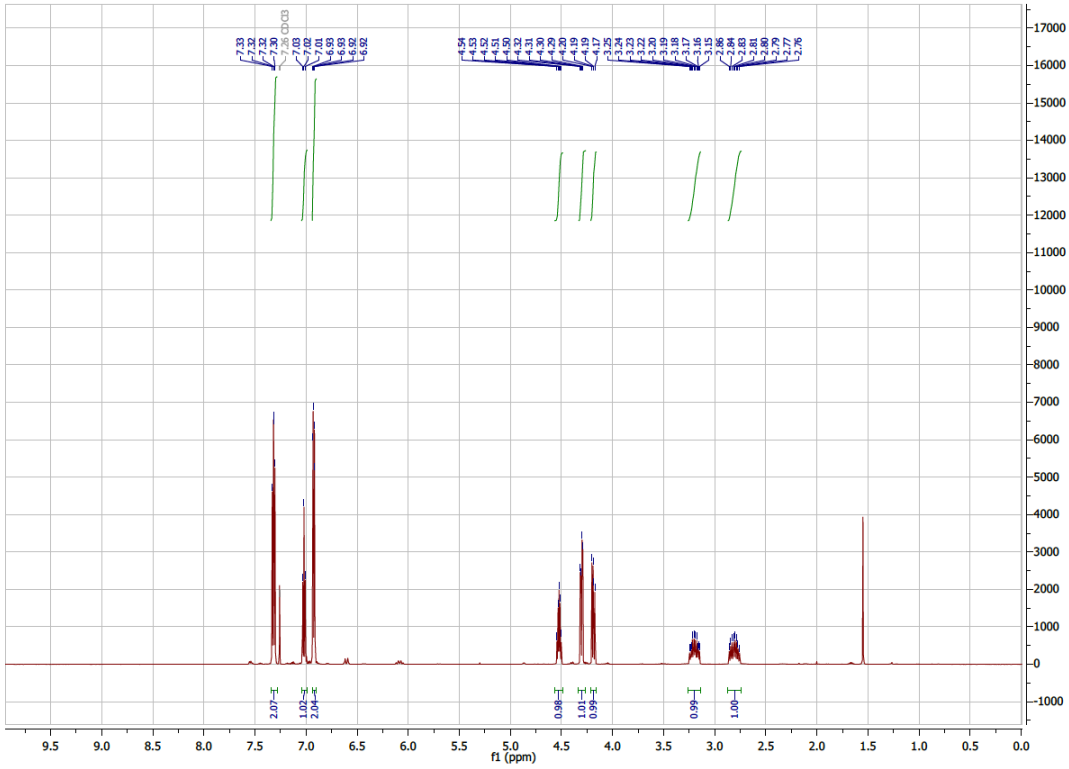


^{19}F NMR (564.686 MHz) spectrum of **1C** in $CDCl_3$

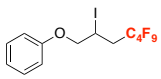


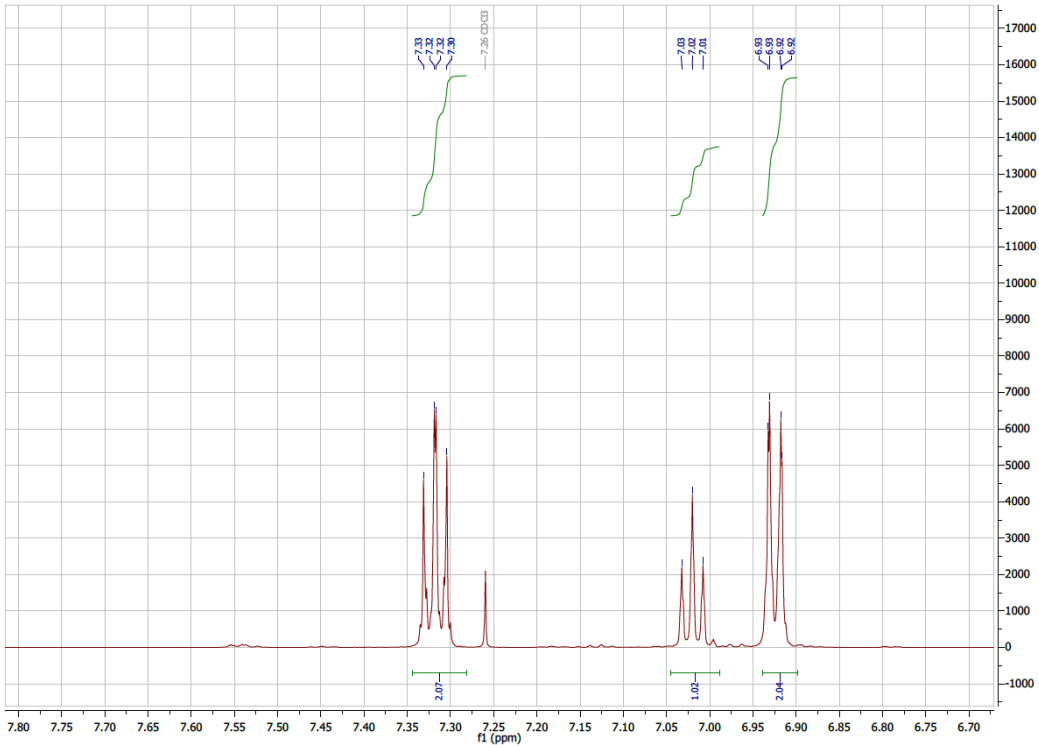
^{1}H NMR (600 MHz) spectrum of **2A** in $CDCl_3$





^{1}H NMR (600 MHz) spectrum of **2A** in $CDCl_3$. Aromatic region





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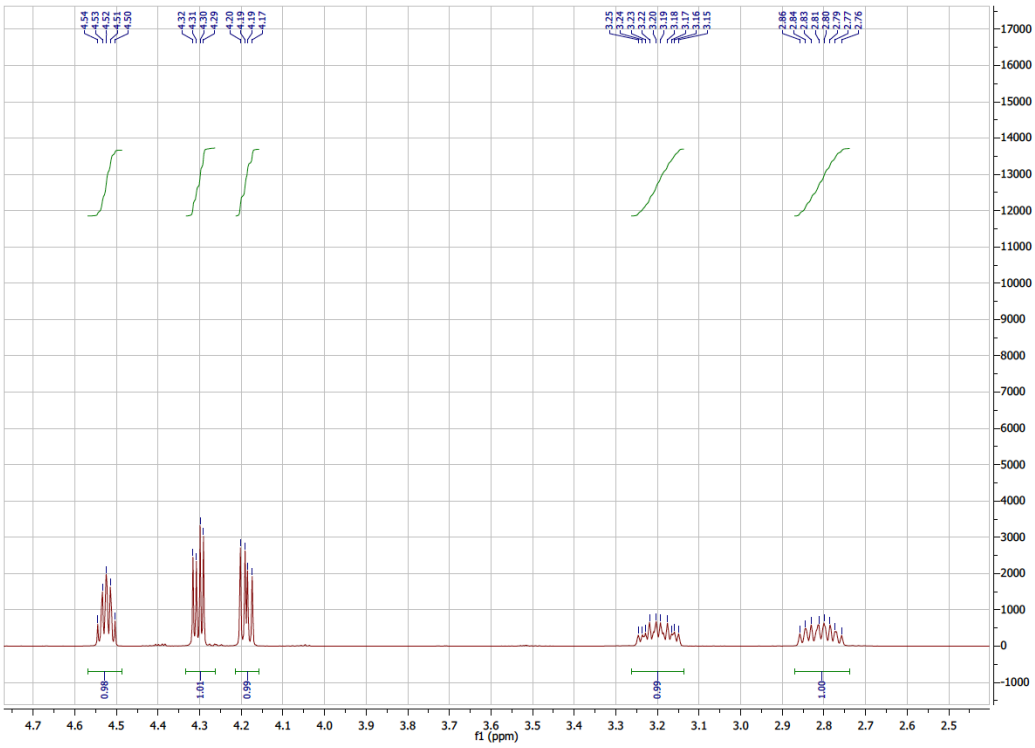
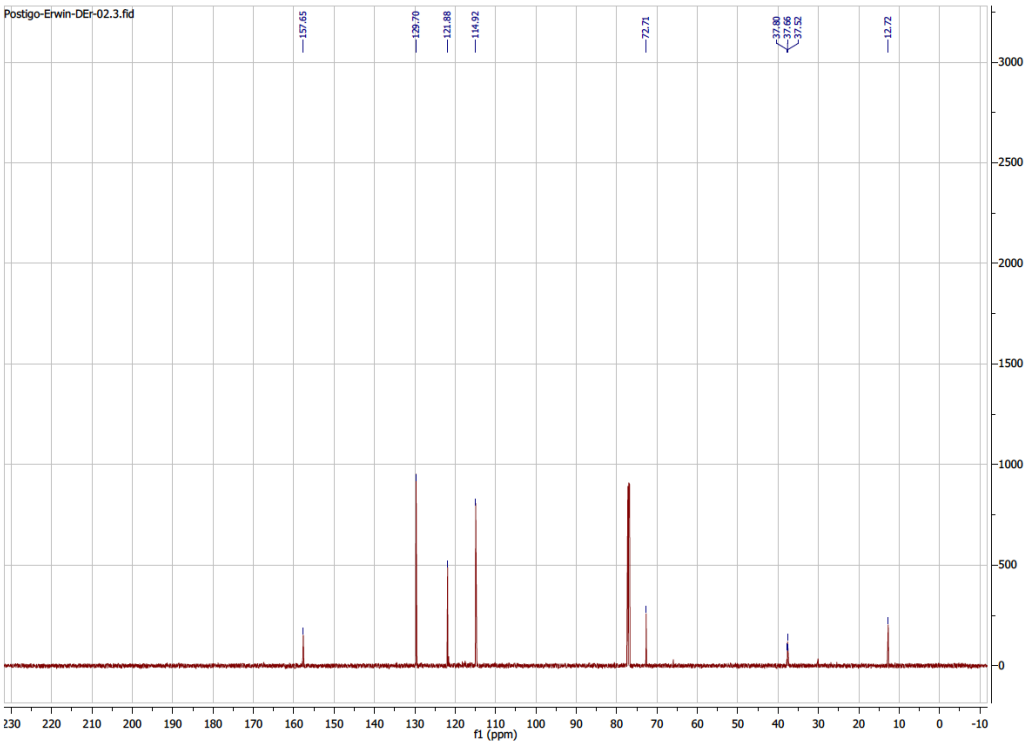
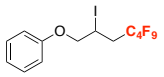
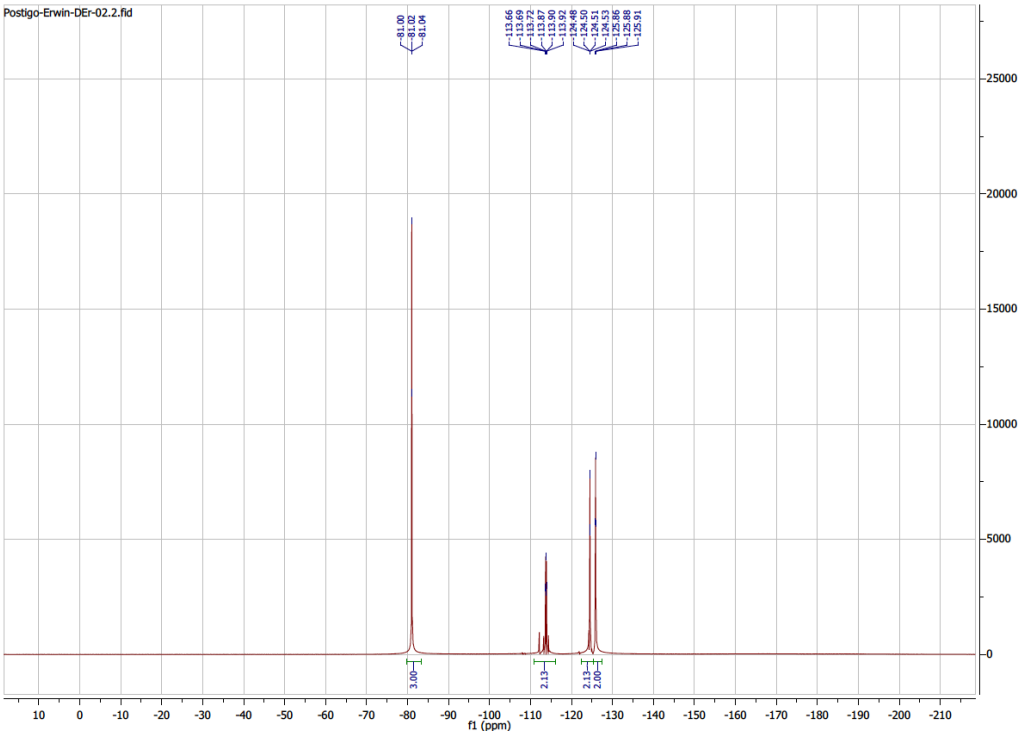


^{13}C NMR (150.903 MHz) spectrum of **2A** in $CDCl_3$



^{19}F NMR (564.686 MHz) spectrum of **2A** in $CDCl_3$





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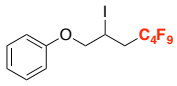
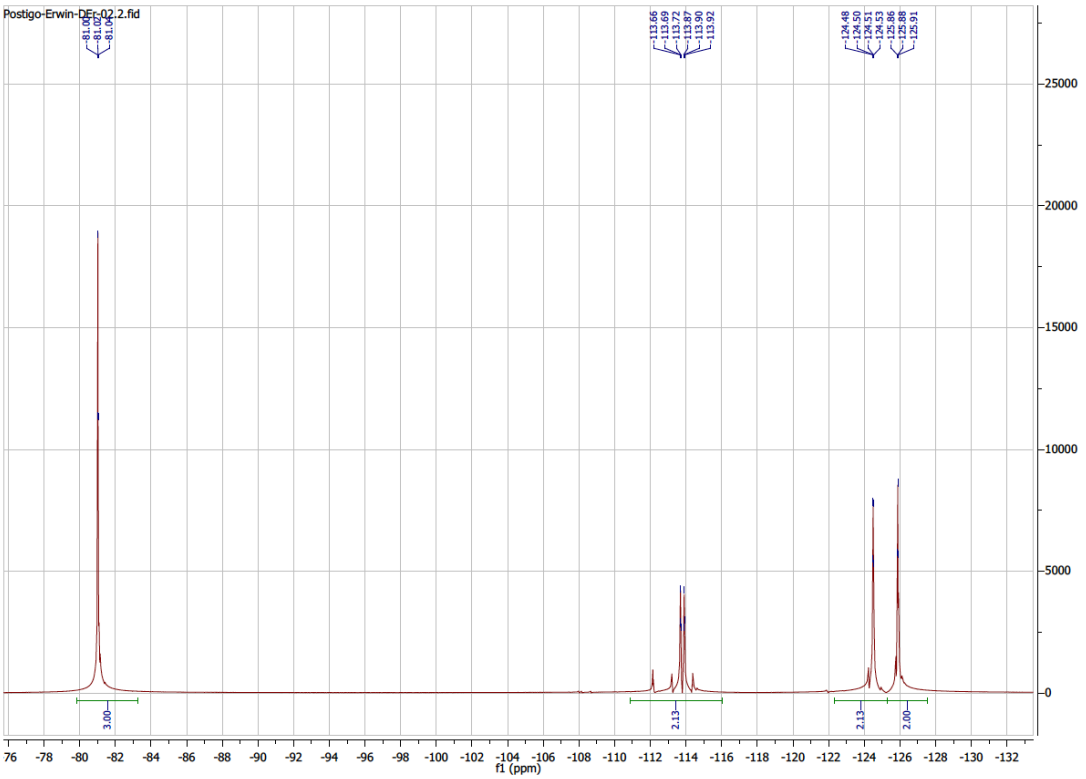
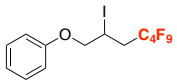
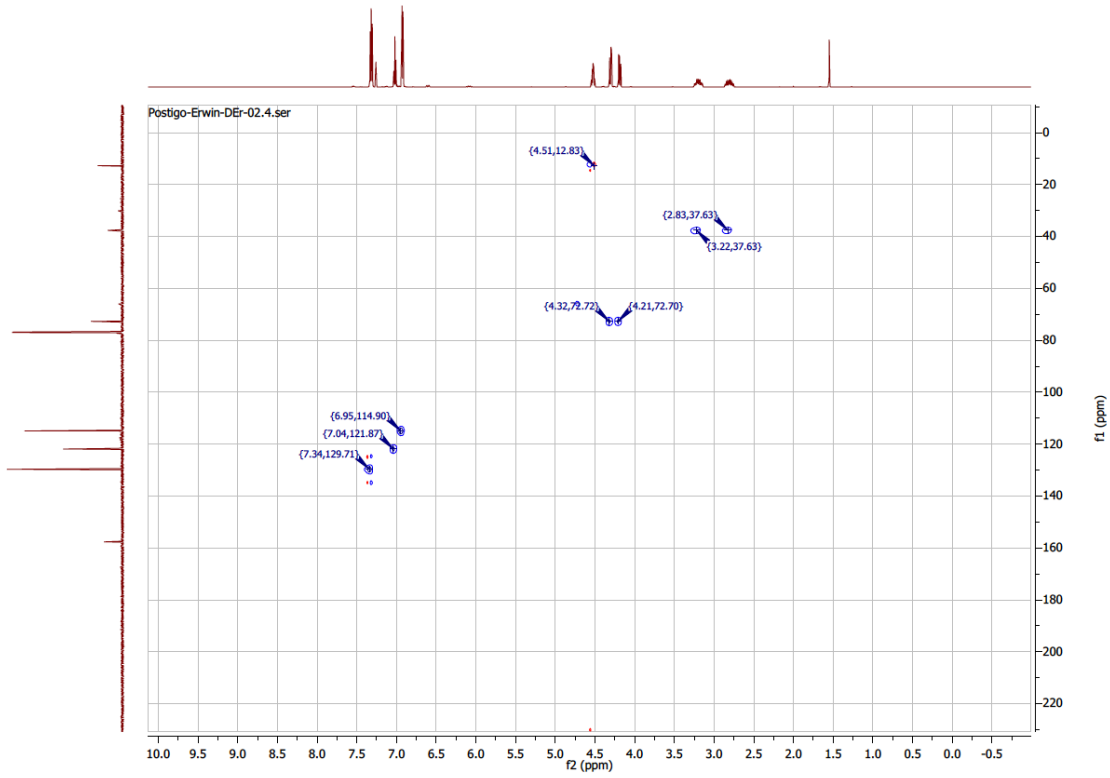


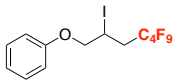


HSQC spectrum of **2A** in $CDCl_3$





HRMS spectrum of **2A**



Analysis Info

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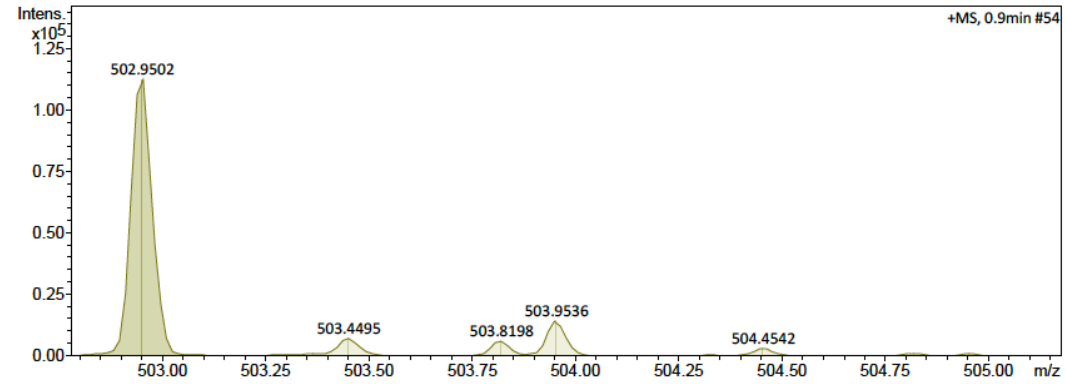
Sample Name	Aliloxi-C4F9 iodo	Instrument	micrOTOF-Q II
Comment	Sv: DCM + MeOH Erwin Mora / Alberto Postigo		

UMYMFOR CONICET FCEN - UBA

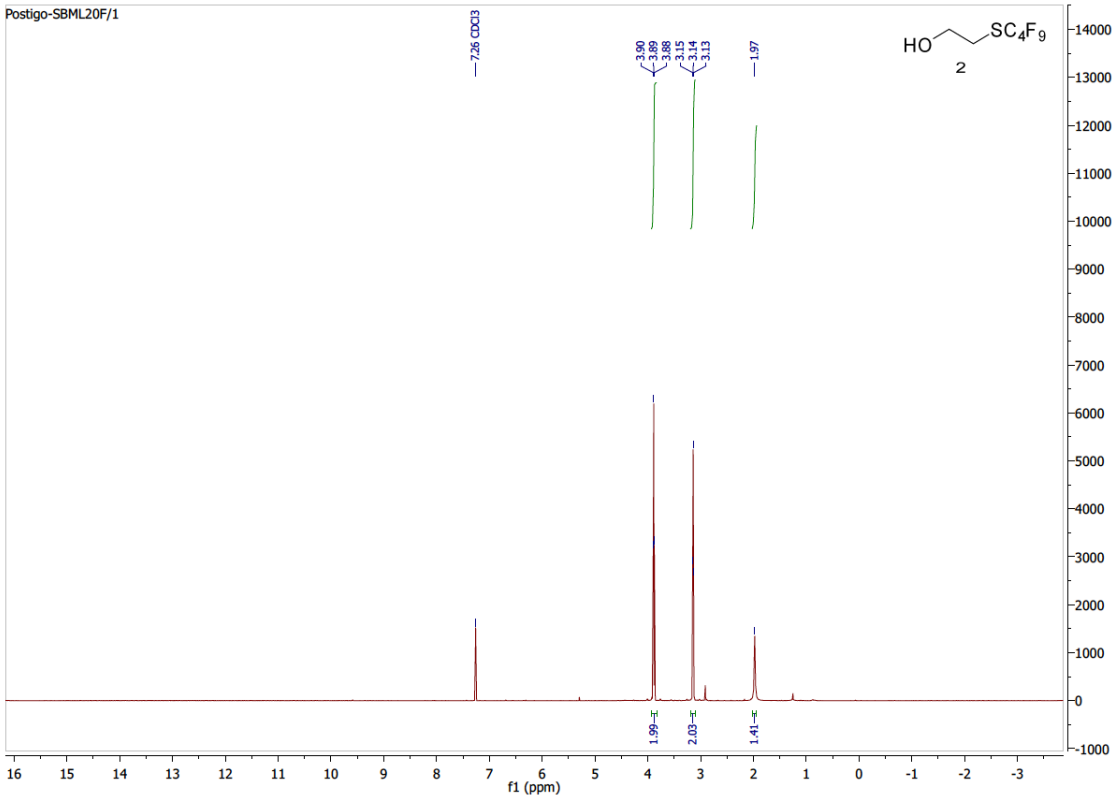
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

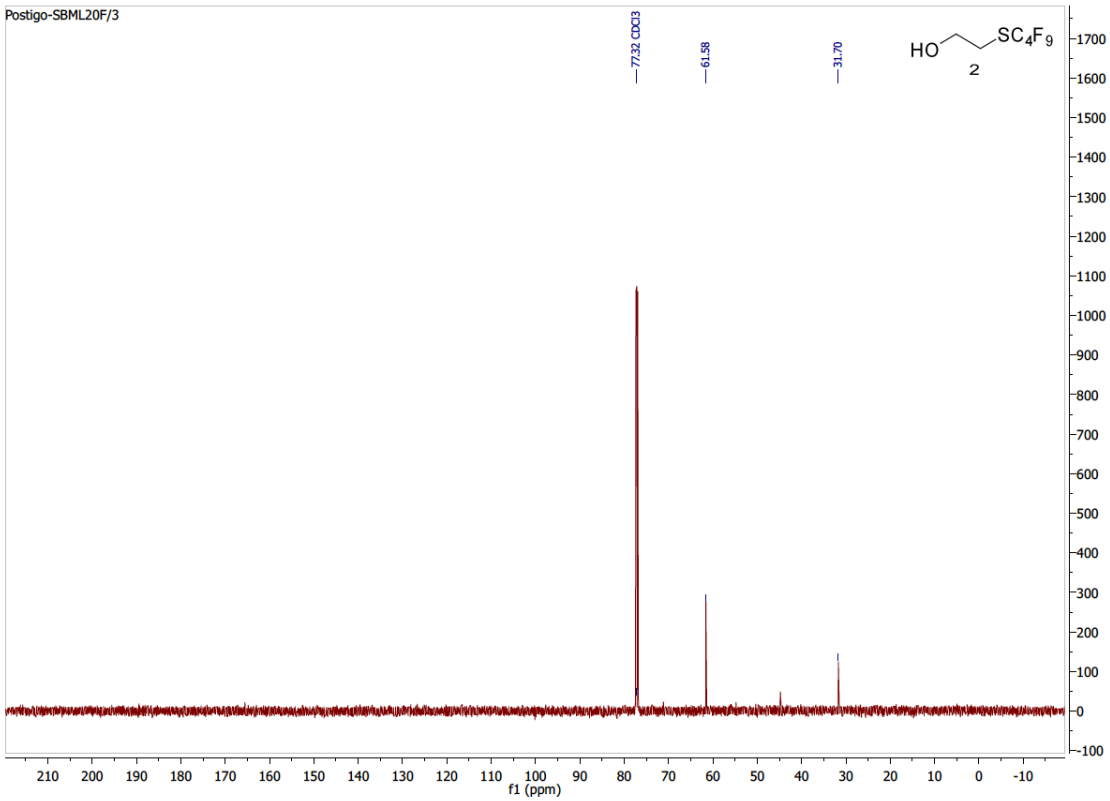


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
502.9502	1	C13H10F9INaO	502.9525	4.6	10.0	1	100.00	3.5	even	ok

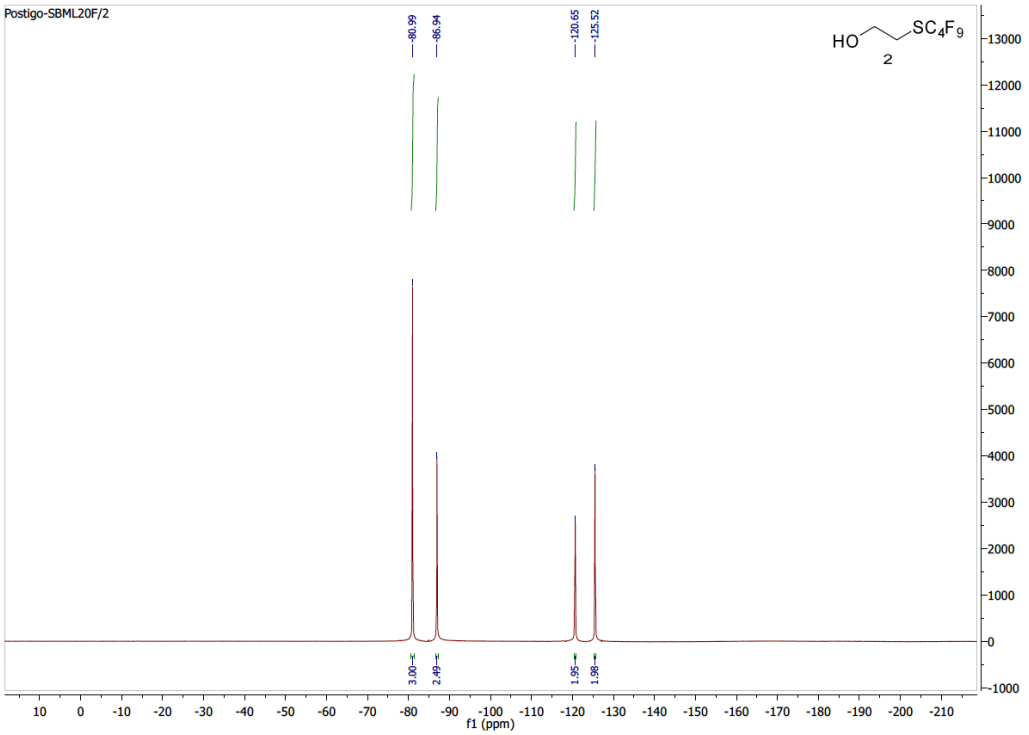
^{1}H NMR (600 MHz) spectrum of 2-((perfluorobutyl)thio)etanol **3A** in $CDCl_3$



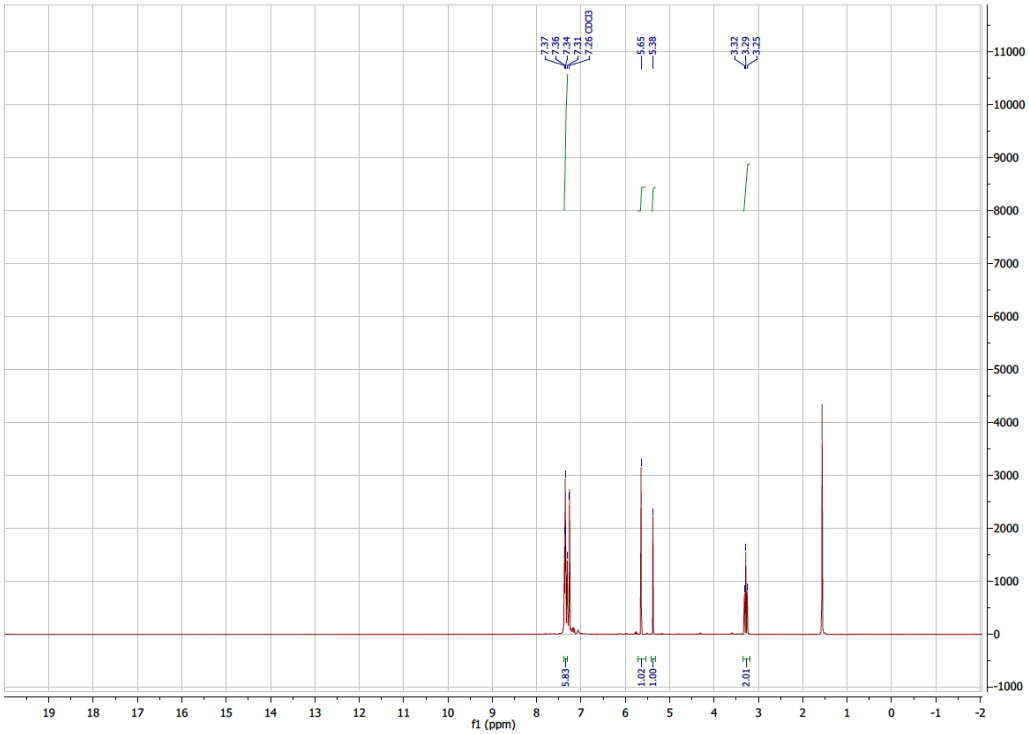
^{13}C NMR (150.903 MHz) spectrum of 2-((perfluorobutyl)thio)etanol **3A** in $CDCl_3$

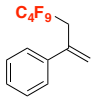


^{19}F NMR (564.686 MHz) spectrum of 2-((perfluorobutyl)thio)ethanol **3A** in $CDCl_3$

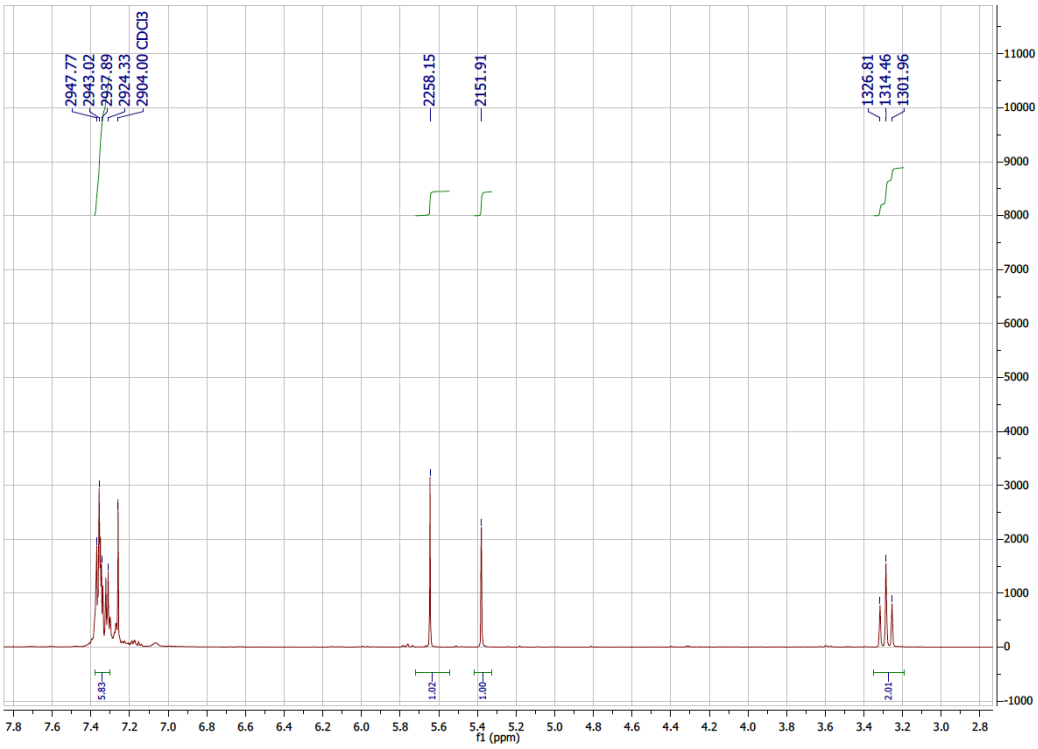


^{1}H NMR (600 MHz) spectrum of **4A** in $CDCl_3$..

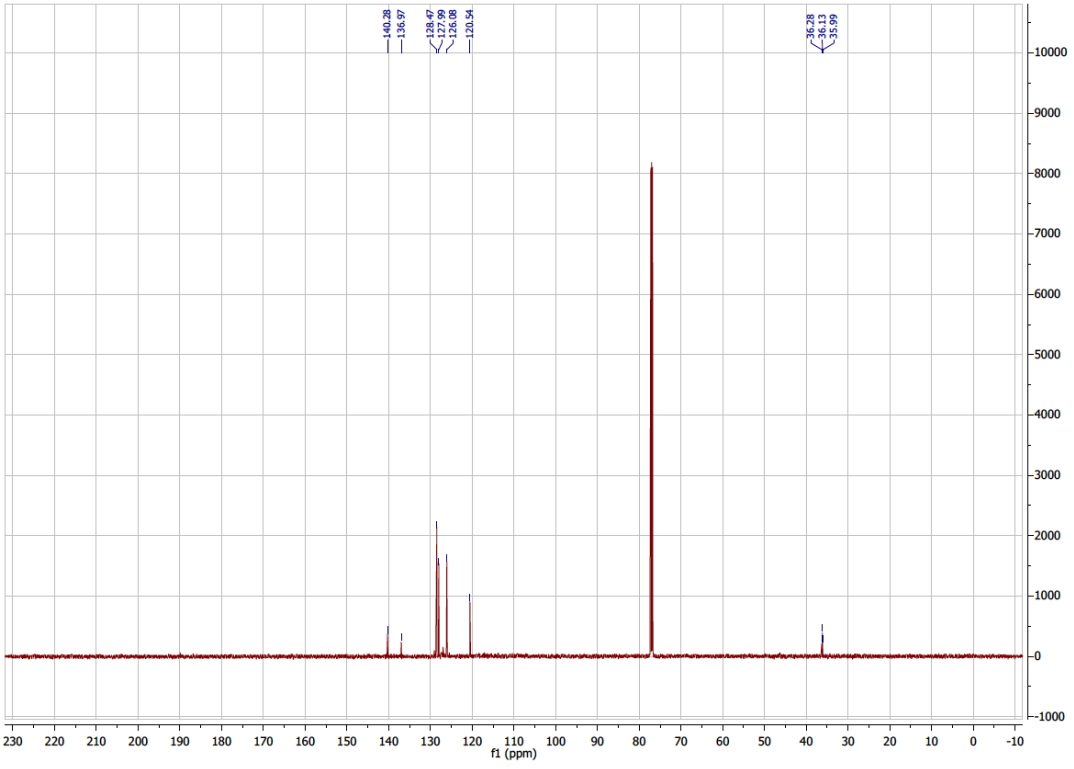


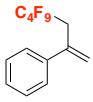


^{1}H NMR (600 MHz) spectrum of **4A**. Enlargement

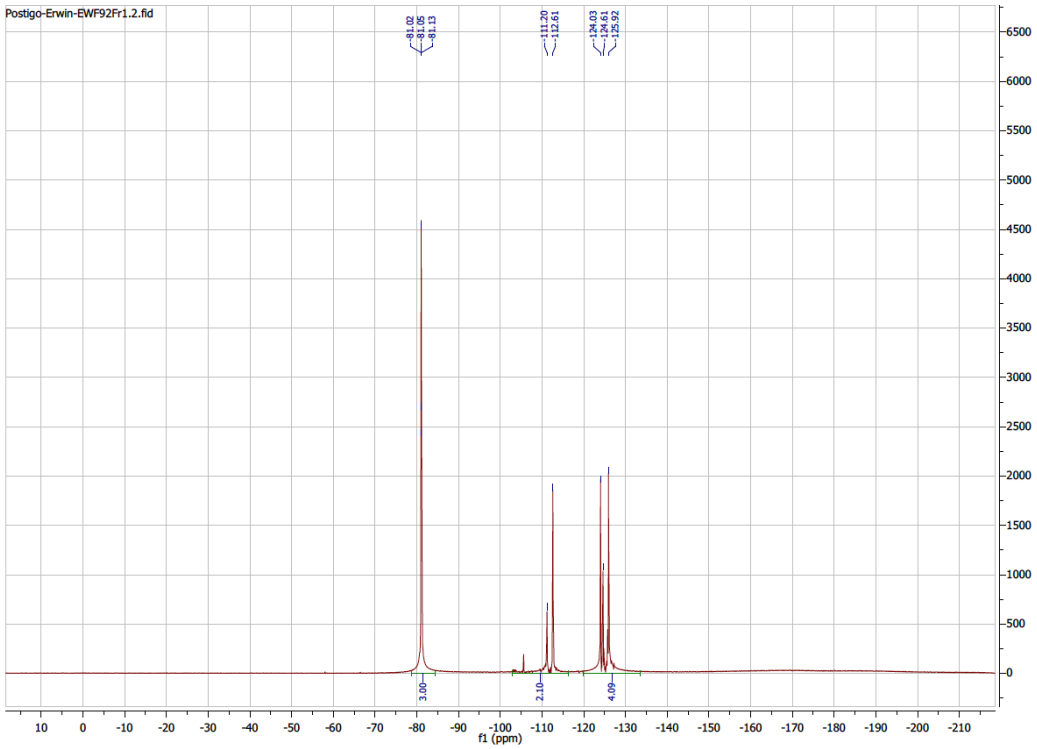


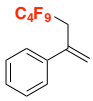
^{13}C NMR (150.903 MHz) spectrum of **4A** in $CDCl_3$.



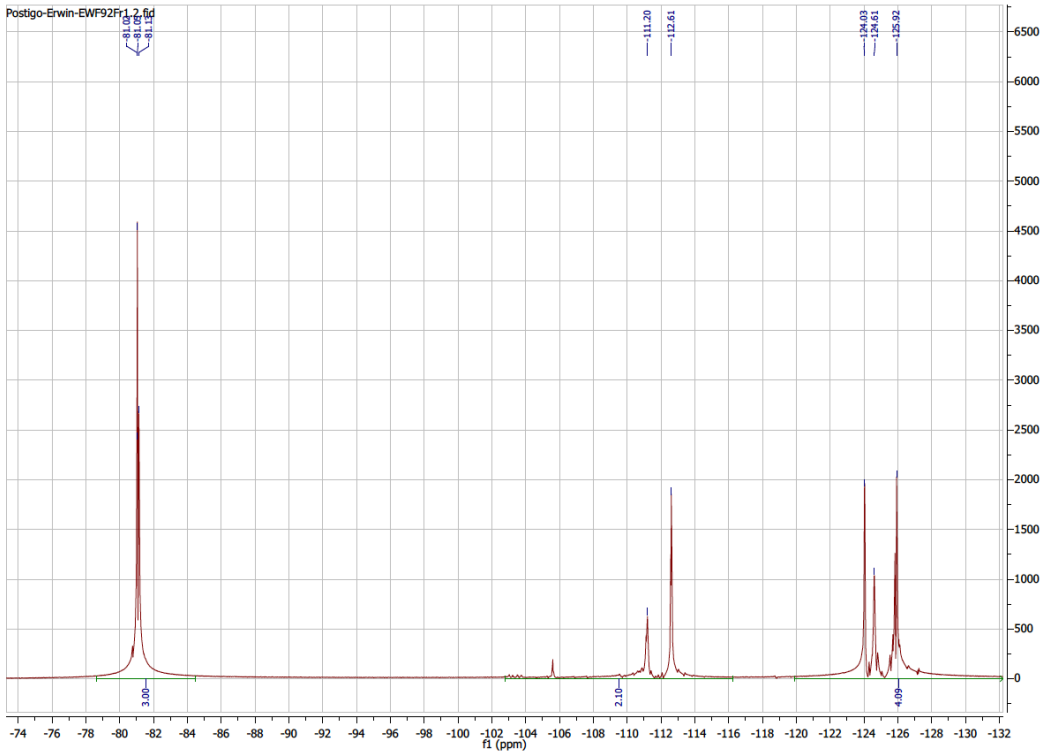


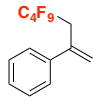
^{19}F NMR (564.686 MHz) spectrum of **4A** in $CDCl_3$..





^{19}F NMR (564.686 MHz) spectrum of **4A** in $CDCl_3$.





HSQC spectrum of **4A** in $CDCl_3$