

The perfluorinated trityl cation accessible as a triflate derivative

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Supporting Information

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1 General Methods

Melting points were determined using a Gallenkamp standard melting point apparatus and are uncorrected. Proton NMR spectra were recorded on a Bruker Avance III HD UltraShield Ascend 400 MHz (400.23 MHz) spectrometer using the solvent peak as internal reference (CDCl₃: δ H 7.26 and CD₃CN: δ H 1.94). Multiplicities are indicated, s (singlet), d (doublet), t (triplet), app. t (apparent triplet); coupling constants (*J*) are in Hertz (Hz). Due to the highly fluorinated nature of all synthesised compounds, which results in extensive carbon-fluorine coupling, ¹³C NMR analysis was not recorded as it provides no distinctive resonances and hence no meaningful data. ¹⁹F NMR spectra were recorded on the previously mentioned instrument at 376.5 Hz. TLC analysis was performed on precoated 60F₂₅₄ slides, and visualised under a UV lamp. Flash chromatography was carried out using silica gel, particle size 0.2-0.063 mm and using the indicated mobile phase as correlated with TLC analysis.

All commercially available compounds were used as provided without further purification. THF, acetonitrile and toluene were dried using an Innovative Technology PureSolv 7 Solvent System and then stored over 3Å molecular sieves under N₂ for 24 hours if more stringent anhydrous conditions were required. *p*-Xylene was dried over CaH₂ overnight, filtered and stored over 3Å molecular sieves for 24 hours prior to use. Anhydrous *ortho*-dichlorobenzene was purchased from Sigma-Aldrich (1 L, lot number SHBH9726) and used as received.

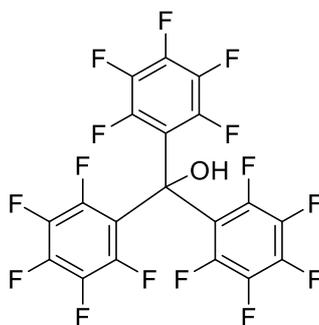
Ag₂[B₁₂Cl₁₂] was prepared according to the procedure employed by Ozerov *et al.*¹

[C₆H₇][CHB₁₁Cl₁₁] was prepared according to the procedure employed by Reed.²

2 Synthesis

Tris(perfluorophenyl)methanol (1OH)

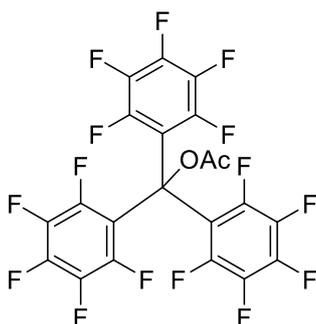
*Note: This compound can be synthesised, as previously described in the literature,³ using bromopentafluorobenzene and *n*-butyllithium to prepare lithium pentafluorobenzene in situ. However, LiC_6F_5 is prone to degrade explosively through elimination of LiF . Despite maintaining a cooling bath temperature of $-75\text{ }^\circ\text{C}$, we have experienced quite a violent explosion when preparing LiC_6F_5 on a 2 g scale. Therefore, we describe a safer, albeit lower yielding, procedure below utilising the more stable Grignard reagent.*



To an oven-dried two-necked 100 mL Schlenk flask equipped with a magnetic stirring bar and reflux condenser was added magnesium (292 mg, 12.0 mmol, 1.2 equiv.). The flask was sealed and evacuated/backflushed with N_2 x 3 before THF (26 mL) was added *via* syringe with stirring. 400 μL bromopentafluorobenzene was then also added *via* syringe and the suspension heated at $35 - 40\text{ }^\circ\text{C}$ (can be done by hand or using a heating bath) until an exotherm was observed. The vessel was then removed from heat and 100 μL aliquots of bromopentafluorobenzene were added periodically up to a total volume of 1.5 mL (12.0 mmol, 1.2 equiv.) over the course of 15 mins. Once addition was complete, the reaction mixture had developed the typical brown colour of a Grignard reagent. It was then heated to reflux for 1 hour before cooling to room temperature and subsequently to $0 - 5\text{ }^\circ\text{C}$ in an ice bath. After stirring on ice for 5 mins, a solution of decafluorobenzophenone (3.62 g, 10.0 mmol, 1.0 equiv.) in THF (7 mL) was added dropwise *via* syringe over 5 mins. No distinctive colour change was observed over the course of the addition. The reaction mixture was allowed to warm back to room temperature before stirring overnight. It was then quenched

through dropwise addition of 6M HCl (10 mL). 25 mL Et₂O was added and, after stirring at room temperature for 2 mins, the layers were separated. The aqueous layer was washed with 2 x 10 mL Et₂O, after which the combined organics were washed with 1 x 10 mL saturated aqueous bicarbonate solution and 2 x 20 mL H₂O. They were then dried over 6 g (~ 2 wts) MgSO₄, filtered and the filter cake washed with 2 x 5 mL Et₂O. The filtrate was concentrated under reduced pressure at 40 °C to obtain an orange oil. ¹⁹F NMR analysis of this oil showed it to be primarily the desired product with small unknown impurities. ¹H NMR analysis also showed residual THF present, which may prevent solidification. Therefore, *n*-hexane (20 mL) was added to the oil, which dissolved, before concentrating again under reduced pressure at 40 °C. Repeating this procedure thrice further yields an orange solid upon final concentration. This solid was covered with ~ 4 mL hexane and cooled to 0 -5 °C for 2 hours. The supernatant was then removed and the solid triturated with a further 2 mL cold hexane. Removing the supernatant once more and drying the solid under reduced pressure at room temperature overnight provided the title compound as a beige solid in 3.42 g (65%) yield. Crystals suitable for X-ray crystallography studies were grown from a concentrated solution of the material in *n*-hexane at -10 °C or *via* slow vapour diffusion from a concentrated CH₂Cl₂ solution into MeCN. M.p. 117 - 118 °C (lit.³ 116.5-117.5 °C). δ_H (400 MHz, CDCl₃): 4.26 (s, 1H). δ_F (376 MHz, CD₃CN): -140.17 (d, *J*_{FF} 18.70), -154.14 (t, *J*_{FF} 21.28), -163.20 (app. t.).

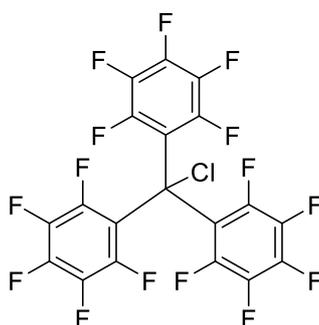
Tris(perfluorophenyl)methyl acetate (10Ac)



To a 5 mL round-bottom flask equipped with a magnetic stirring bar was charged tris(perfluorophenyl)methanol (**10H**, 90 mg, 0.17 mmol, 1.0 equiv.) and acetyl bromide (1 mL, 13.5 mmol, 79.4 equiv.). This mixture was refluxed for 16 hours before removing the excess acetyl bromide under reduced pressure at room temperature to give a light yellow

solid. This was purified further by flash column chromatography using *n*-hexane/CH₂Cl₂ (98:2) eluent. After concentrating the relevant fractions under reduced pressure at 40 °C, the title compound was obtained as a light yellow solid in 40 mg (41%) yield. Crystals suitable for X-ray crystallography studies were grown from a concentrated solution of the material in Et₂O at -10 °C. M.p. 152 – 155 °C. δ_{H} (400 MHz, CDCl₃): 2.17 (s). δ_{F} (376 MHz, CDCl₃): -137.90 (d, J_{FF} 19.5), -151.23 (t, J_{FF} 21.0), -160.84 (app. t.).

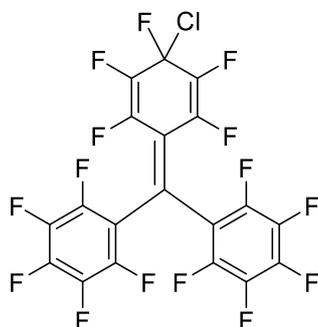
6,6',6''-(chloromethanetriyl)tris(1,2,3,4,5-pentafluorobenzene) (1Cl)



Prior to mixing the reactants, an oil bath was heated to 142.0 °C. Once at temperature, tris(pentafluorophenyl)methanol (**1OH**, 902 mg, 1.7 mmol, 1.0 equiv.) was charged to a 250 mL round-bottom flask equipped with a magnetic stirring bar. *p*-Xylene (60 mL) was added and the solid dissolved readily to form a pale yellow solution. Pyridine (13.7 μ L, 0.17 mmol, 0.1 equiv.) was added *via* micropipette with no change in the appearance of the reaction mixture. Thionyl chloride (9.0 mL, 124.2 mmol, 73.0 equiv.) was then charged in one portion and the flask equipped with a reflux condenser before being placed in the pre-heated oil bath. After approximately 3 mins, reflux was underway and after a further 3 mins the reaction mixture was observed to darken in colour to a pale brown-yellow. After heating for 24 hours, the vessel was allowed to cool to room temperature. The reaction mixture was observed to be orange-yellow at this point. It was concentrated under reduced pressure at 60 °C to obtain a brown-yellow residue that was dried further under hi-vacuum at room temperature. ¹⁹F NMR analysis of this residue showed it to be primarily the desired product with no starting material observed. TLC analysis revealed three primary components of this mixture, each separated by < 0.05 R_F value using a 100% hexane mobile phase. The least polar of these is 6,6'-((4-chloro-2,3,4,5,6-pentafluorocyclohexa-2,5-dien-1-ylidene)methylene)bis(1,2,3,4,5-pentafluorobenzene) (*para*-chloro isomer, **2**), while the most polar is a mix of 1-

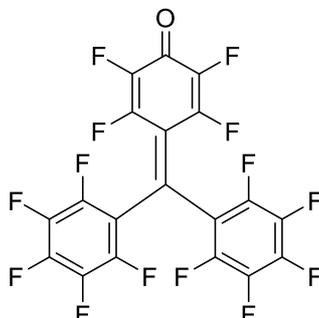
(chloromethyl)-4-methylbenzene and 1-(dichloromethyl)-4-methylbenzene, presumably formed through chlorination of the *p*-xylene solvent under the harsh reaction conditions. The middle spot is the desired product. To the crude material (crude weight: 1.67 g) was therefore charged 4 mL hexane to form a suspension which was filtered to remove the less soluble *para*-chloro isomer **2**. After concentrating the filtrate, the resulting residue was purified *via* flash column chromatography using a column 4 cm (d) x 33 cm (h) and 100% hexane as the eluent. Collecting ~12 mL fractions, the desired product eluted in fractions 29 – 37. Concentration of these fractions under reduced pressure at 40 °C followed by drying further under hi-vacuum at room temperature provided the title compound as a pale yellow solid in 337 mg (36%) yield. Crystal suitable for X-ray crystallography studies were grown from a concentrated solution of the material in CH₂Cl₂ at -10 °C or *via* slow vapour diffusion from a concentrated *n*-hexane solution into toluene. M.p. 104 - 106 °C. δ_F (376 MHz, CDCl₃): -135.50 (d, J_{FF} 18.29), -150.07 (app. t.), -160.38 (app. t.).

6,6'-((4-chloro-2,3,4,5,6-pentafluorocyclohexa-2,5-dien-1-ylidene)methylene)bis(1,2,3,4,5-pentafluorobenzene) (2)



The title compound was isolated as described above as a white solid (yield not determined). Crystals suitable for X-ray crystallography studies were grown from a concentrated solution of the material in Et₂O at -10 °C. M.p. 204 – 205 °C. δ_F (376 MHz, CDCl₃): -104.72 (app. t), -139.42 (app. t), -145.65 (d, J_{FF} 33.24), -146.34 (s), -149.07 (app. t), -160.26 (s).

4-(bis(perfluorophenyl)methylene)-2,3,5,6-tetrafluorocyclohexa-2,5-dien-1-one (6)



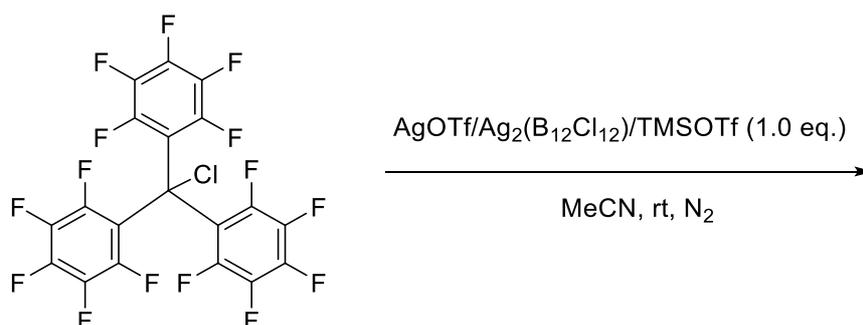
This compound was isolated as part of studies conducted into the reaction between tris(perfluorophenyl)methanol and methanesulfonic acid. To a 25 mL Schlenk flask equipped with a magnetic stirring bar was charged tris(perfluorophenyl)methanol (**1OH**, 59 mg, 0.11 mmol, 1.0 equiv.). The flask was sealed and evacuated/backflushed with N₂ x 3. Neat methanesulfonic acid (1.0 mL, 15.4 mmol, 140.0 equiv.) was added *via* syringe to form a suspension that was sonicated for 5 mins to disperse the solid. The flask was then equipped with a reflux condenser under a positive N₂ flow and the reaction mixture heated at 75.0 °C for 20 hours. Upon cooling, the reaction mixture was dark red with a solid present. This solid was filtered and washed with H₂O before pulling dry to give the title compound as a light tan solid in undetermined yield. Crystals suitable for X-ray crystallography studies were grown from a concentrated solution of the material in CH₂Cl₂ at -10 °C. δ_F (376 MHz, CDCl₃): -130.03 (s), -139.15 (d, J_{FF} 18.97), -147.05 (app. t), -147.45 (s), -159.38 (app. t).

MgSO₄ (2 wts) before filtering and washing the filter cake with 1 x 1 mL CH₂Cl₂. The filtrate was then concentrated under reduced pressure at 40 °C to obtain a beige solid which was dried further under hi-vacuum at room temperature. The vessel was then cooled to 0 – 5 °C in an ice/water bath and triturated with 400 μL cold hexane. The solid was then dried further under reduced pressure at 40 °C before sampling for NMR spectroscopy (CDCl₃, 10 mg/mL). ¹⁹F NMR showed the presence of two separate, symmetrical perfluorinated aromatic compounds, one of which corresponded to tris(perfluorophenyl)methanol. ¹H NMR showed a resonance at 6.22 ppm and tris(perfluorophenyl)methanol at 4.26 ppm. The presence of triethylsilane was also observed. The crude material was allowed to dry at room temperature under reduced pressure overnight before being sampled again for NMR analysis. ¹⁹F revealed no change, but ¹H showed the triethylsilane to have been removed while the resonances at 6.22 ppm and 4.26 ppm remained. The material was then purified further by flash column chromatography using a 97.5:2.5 hexane/EtOAc eluent (column radius: 0.75 cm, column height: 18 cm). 6 mL fractions were collected. The compound of interest eluted in fractions 2 – 4, which were then concentrated under a stream of N₂ before drying further under hi-vacuum at room temperature to provide tris(perfluorophenyl)methane as a white solid in 23 mg (24%) yield. M.p. 159 – 160 °C (lit.⁴ 158 – 159.5 °C). δ_H (400 MHz, CDCl₃): 6.22 (s, 1H). δ_F (376 MHz, CDCl₃): -141.54 (d, *J*_{FF} 19.56), -152.30 (app. t), -160.74 (t, *J*_{FF} 18.10).

3 General Procedures

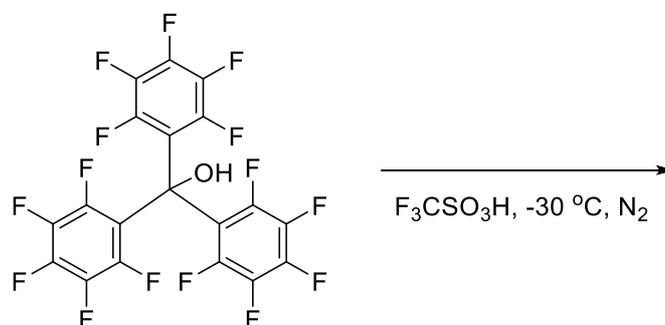
Note: all reactions involving non-acidic reagents were conducted in an N₂-filled glovebox.

Treatment of chloroalkane with halide abstraction agents



To a 20 mL vial equipped with a magnetic stirring bar was charged 6,6',6''-(chloromethanetriyl)tris(1,2,3,4,5-pentafluorobenzene) (**1Cl**, 50 mg, 0.091 mmol, 1.0 equiv.) and the relevant solid halide abstraction agent (AgOTf/Ag₂[B₁₂Cl₁₂], 0.091 mmol, 1.0 equiv.). This mixture was then suspended in acetonitrile (1.0 mL, 20 vol). In reactions utilising TMSOTf, this was then charged *via* micropipette in one portion. The vessel was sealed and stirred at room temperature. ¹⁹F NMR analysis of the crude reaction was performed by removing 250 μL of the reaction mixture and diluting with 250 μL CD₃CN.

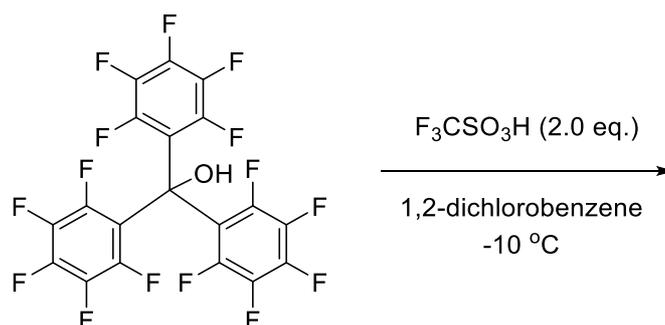
Reaction of tris(perfluorophenyl)methanol in neat triflic acid



To an NMR tube was charged triflic acid (1.0 mL) before sealing and cooling the tube to -30 °C. It was allowed to equilibrate for 10 mins. Tris(perfluorophenyl)methanol (**1OH**, 50 mg,

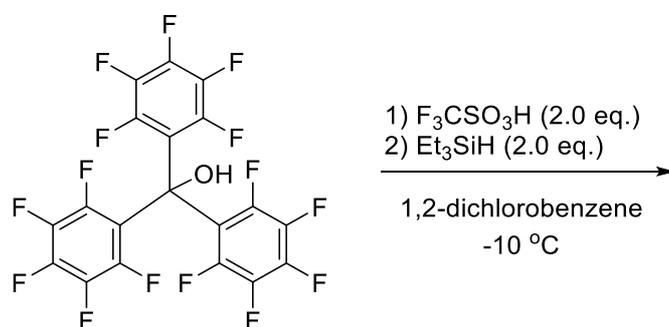
0.095 mmol,) was then charged in one portion. The reaction mixture turned from colourless to deep red immediately. It was agitated lightly by hand to ensure homogeneity before being allowed to stand at -30 °C for 10 mins. It was then analysed by ^{19}F NMR (neat) at -30 °C.

Reaction of tris(perfluorophenyl)methanol with triflic acid in 1,2-dichlorobenzene at -10 °C



To an NMR tube was charged tris(perfluorophenyl)methanol (**1OH**, 25 mg, 0.047 mmol, 1.0 equiv.) and 0.5 mL 1,2-dichlorobenzene (0.5 mL) to form a pale yellow solution. This was then cooled to -10 °C and allowed to equilibrate for 10 mins. Triflic acid (8.3 μL , 0.094 mmol, 2.0 equiv.) was then charged *via* micropipette in one portion. The pale yellow solution immediately turned a very deep red and was homogenous. The sample was subsequently analysed by ^{19}F NMR at -10 °C, which revealed the presence of a new symmetrical species (see NMR spectral data below). Upon allowing the sample to warm to ambient temperature and re-analysing by ^{19}F NMR, the resulting spectrum showed a complex mixture of resonances. Allowing the sample to stand at room temperature for 2 days and subsequently re-analysing by ^{19}F NMR revealed five primary aromatic resonances indicating degradation to the dienone **6**.

Reaction of tris(perfluorophenyl)methanol with 1) triflic acid and 2) triethylsilane in 1,2-dichlorobenzene at -10 °C



Tris(perfluorophenyl)methanol (**1OH**, 100 mg, 0.19 mmol, 1.0 equiv.) was charged to a 10 mL Schlenk flask equipped with a magnetic stirring bar. The flask was sealed and evacuated/backflushed with N₂ x 3. 1,2-dichlorobenzene (2.0 mL) was then charged *via* syringe to form a pale yellow solution which was then cooled to -10 °C and allowed to equilibrate for 10 mins with stirring. Triflic acid (33.6 μL, 0.38 mmol, 2.0 equiv.) was then charged dropwise *via* micropipette under a positive flow of N₂. The pale yellow solution immediately turned deep red and was homogenous. This mixture was stirred at -10 °C for 10 mins before triethylsilane (60.7 μL, 0.38 mmol, 2.0 equiv.) was charged dropwise *via* micropipette under a positive flow of N₂. The red colour of the reaction began to fade and gradually becomes orange/beige. However, a gummy red residue formed down the bottom of the flask which trapped the magnetic stirring bar and caused stirring to halt. The flask was therefore agitated by hand for ~ 5 mins to achieve homogeneity, by which point the red colour had disappeared and the stirring bar had loosened again. The reaction mixture was then stirred at -10 °C for 90 mins before sampling for ¹⁹F NMR analysis (neat). The resulting spectrum revealed the presence of tris(perfluorophenyl)methanol **1OH** and tris(perfluorophenyl)methane **1H** as the primary components of the mixture (see NMR spectral data below).

Protonation of tris(perfluorophenyl)methanol by [C₆H₇][CHB₁₁Cl₁₁]

The described manipulations and characterization via FT-IR were carried out in dry-boxes (H₂O, O₂ < 0.5 ppm) at room temperature. ATR-FT-IR characterization was carried out using an ABB MB3000 spectrometer in the 4000 – 525 cm⁻¹ frequency range using a diamond crystal. In a solvent free method of protonation, a 1 dram vial containing a teflon stir bar was

charged with approx. 30.0 mg freshly prepared $[\text{C}_6\text{H}_7][\text{CHB}_{11}\text{Cl}_{11}]$, and either approx. 26.5 or 13.2 mg **1OH** (0.05 mmol, 1.0 equiv.; or 0.025 mmol, 0.5 equiv.). The solids were allowed to thoroughly mix by stirring with no solvent added. Analysis of the solid suggests protonation of **1OH** was unsuccessful by this method indicated by the presence of the CH_2^+ symmetric stretch at approx. 2780 cm^{-1} . The second method of protonation considered the first method with **1OH** mixed with $[\text{C}_6\text{H}_7][\text{CHB}_{11}\text{Cl}_{11}]$ in 1:1 and 1:2 ratios while mixing in approx. 0.5 mL of benzene. Partial dissolution of the solids was observed with a blue color persisting for minutes. Removal of volatiles under vacuum yielded a dark solid that appears stable at low temperature ($-38.5\text{ }^\circ\text{C}$). ATR-FT-IR analysis shown in Figures S2 and S3 suggests the presence of unreacted $[\text{C}_6\text{H}_7][\text{CHB}_{11}\text{Cl}_{11}]$, **1OH** (minimal), and a new material, potentially the perfluorotrityl cation, based on a comparative analysis to $[(\text{C}_6\text{H}_5)_3\text{C}][\text{CHB}_{11}\text{Cl}_{11}]$ described in Figure S4. Reactions between **1OH** and $[\text{C}_6\text{H}_7][\text{CHB}_{11}\text{Cl}_{11}]$ in a 1:2 ratio mixing in toluene or 1,2-dichlorobenzene resulted in a maroon or green solution, respectively, though as above, the color persisted for only a short time in solution. Small plate-like crystals were obtained via slow cooling, though attempts to obtain diffraction data of the crystal proved unsuccessful during mounting.

4 Infrared data

Figure S1: tris(perfluorophenyl)methanol (**10H**)

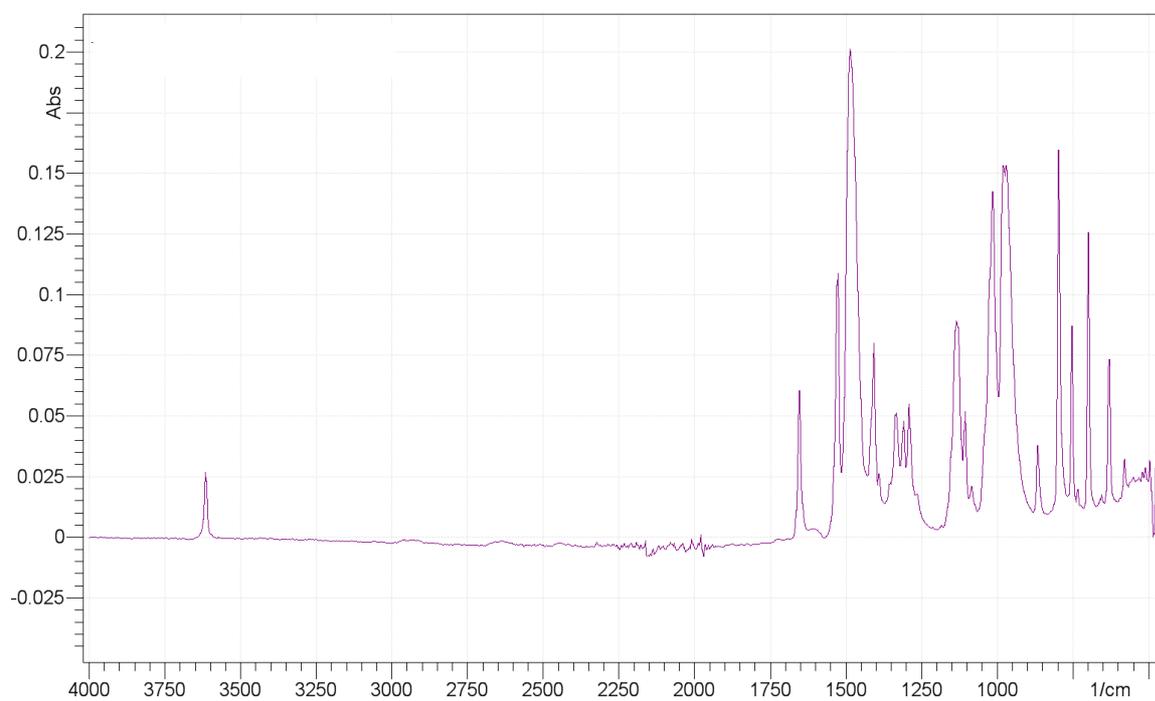


Figure S2: Rxn of tris(perfluorophenyl)methanol (**10H**) + [C₆H₇][CHB₁₁Cl₁₁] in benzene followed by evaporation

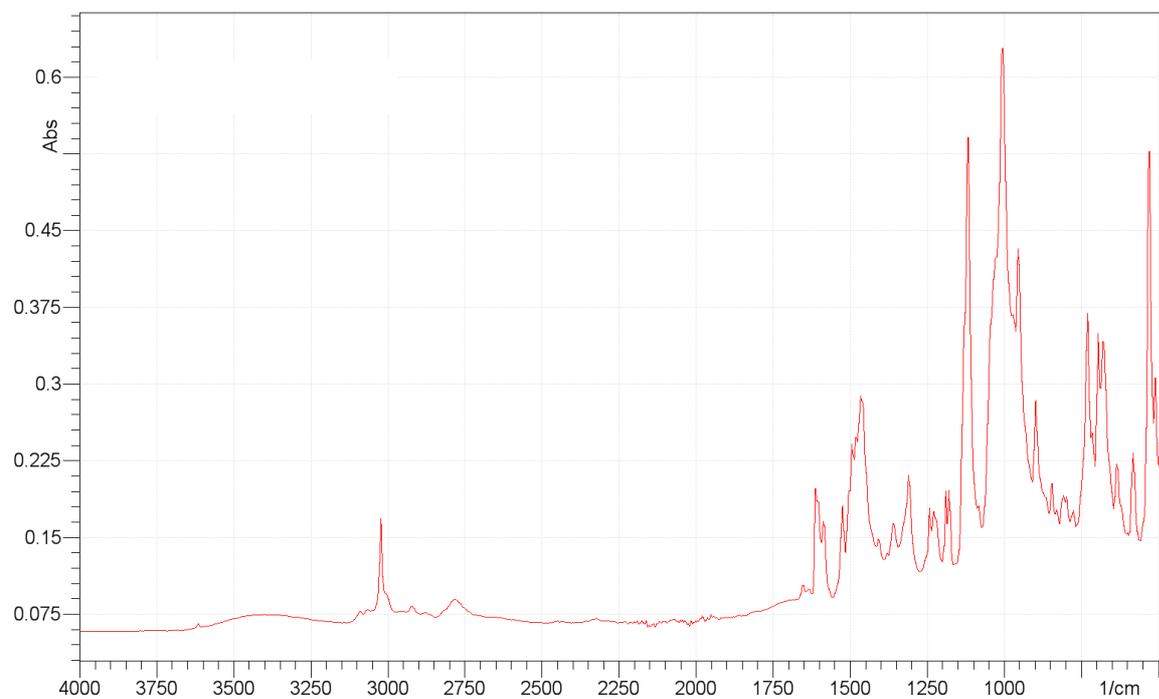


Figure S3: Expanded region of 1250 to 1700 cm^{-1} for overlay of FT-IR spectra for **1OH** (purple), $[\text{C}_6\text{H}_7][\text{CHB}_{11}\text{Cl}_{11}]$ (blue), rxn of 1OH and $[\text{C}_6\text{H}_7][\text{CHB}_{11}\text{Cl}_{11}]$ prior to solvent inclusion (black) and rxn of 1OH and $[\text{C}_6\text{H}_7][\text{CHB}_{11}\text{Cl}_{11}]$ after mixing in benzene and subsequent evaporation (red).

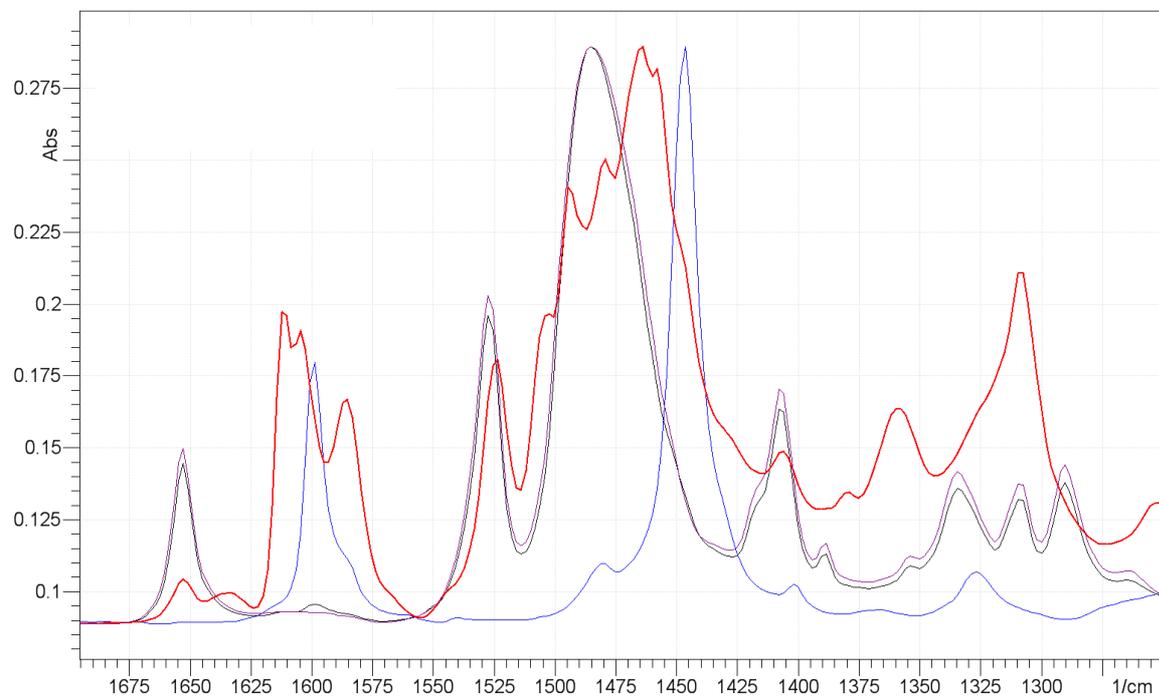
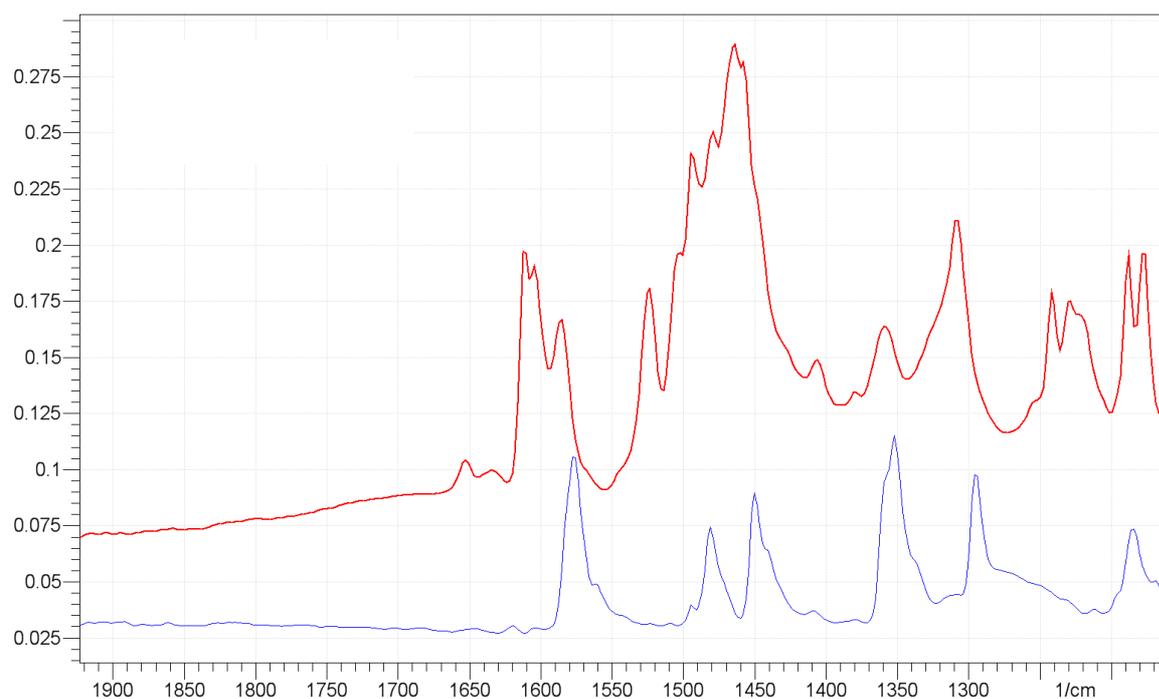


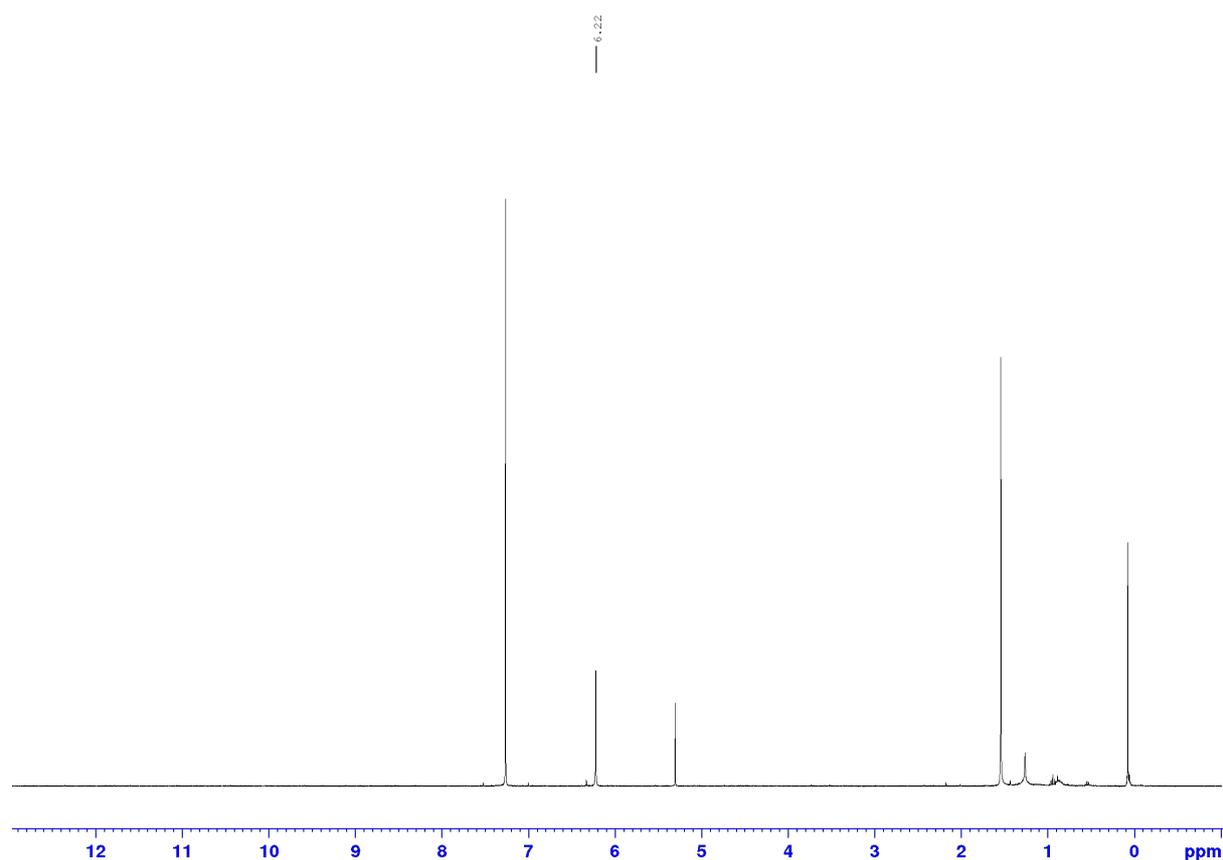
Figure S4: Expanded region of 1250 to 1900 cm^{-1} for overlay spectra of FT-IR for **1OH** mixed with $[\text{C}_6\text{H}_7][\text{CHB}_{11}\text{Cl}_{11}]$ after addition of benzene and subsequent evaporation (red). Known sample of $[(\text{C}_6\text{H}_5)_3\text{C}][\text{CHB}_{11}\text{Cl}_{11}]$ (blue).



5 ^1H NMR data for tris(perfluorophenyl)methane

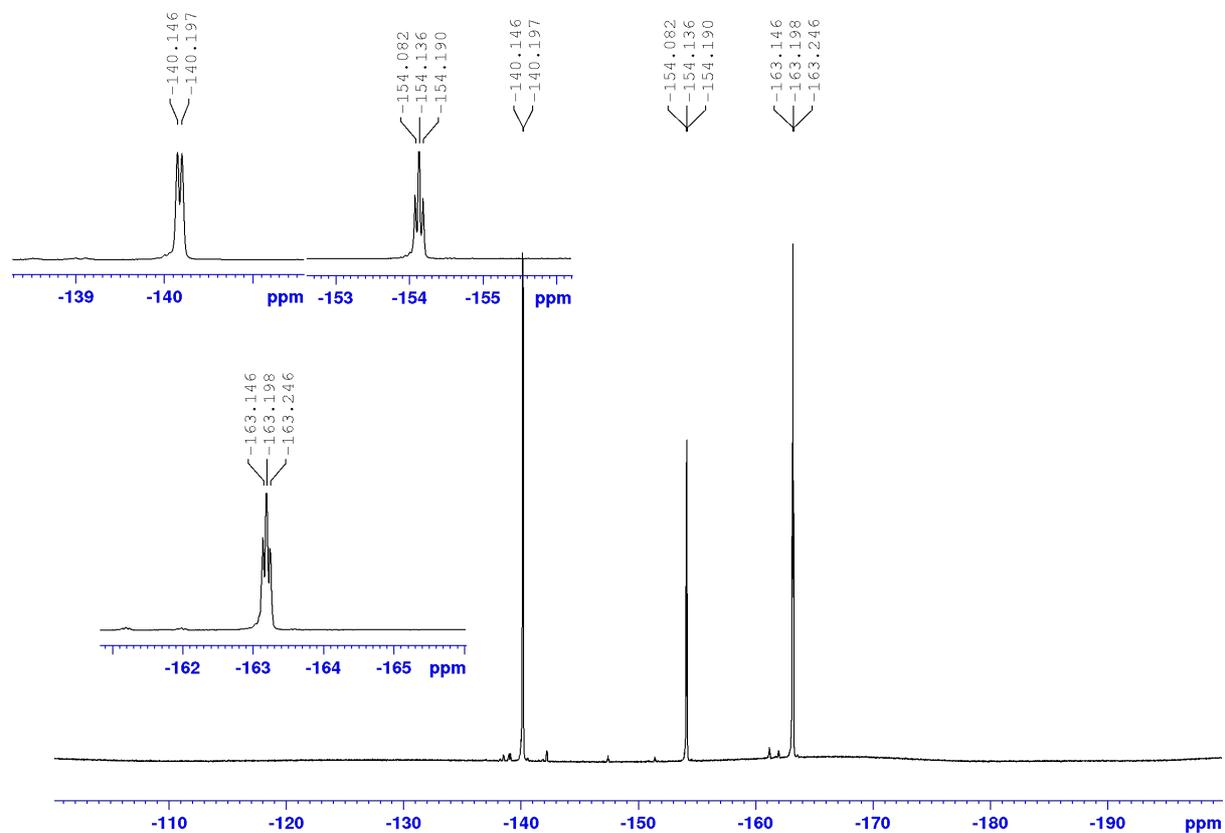
Note: the high molecular mass of tris(perfluorophenyl)methane and the fact that it contains only one proton means the resonance signal is very weak relative to the mass of material used to prepare a sample for NMR analysis. Trace impurities and residual solvents therefore appear much more prominent than is actually the case.

Tris(perfluorophenyl)methane (1H)

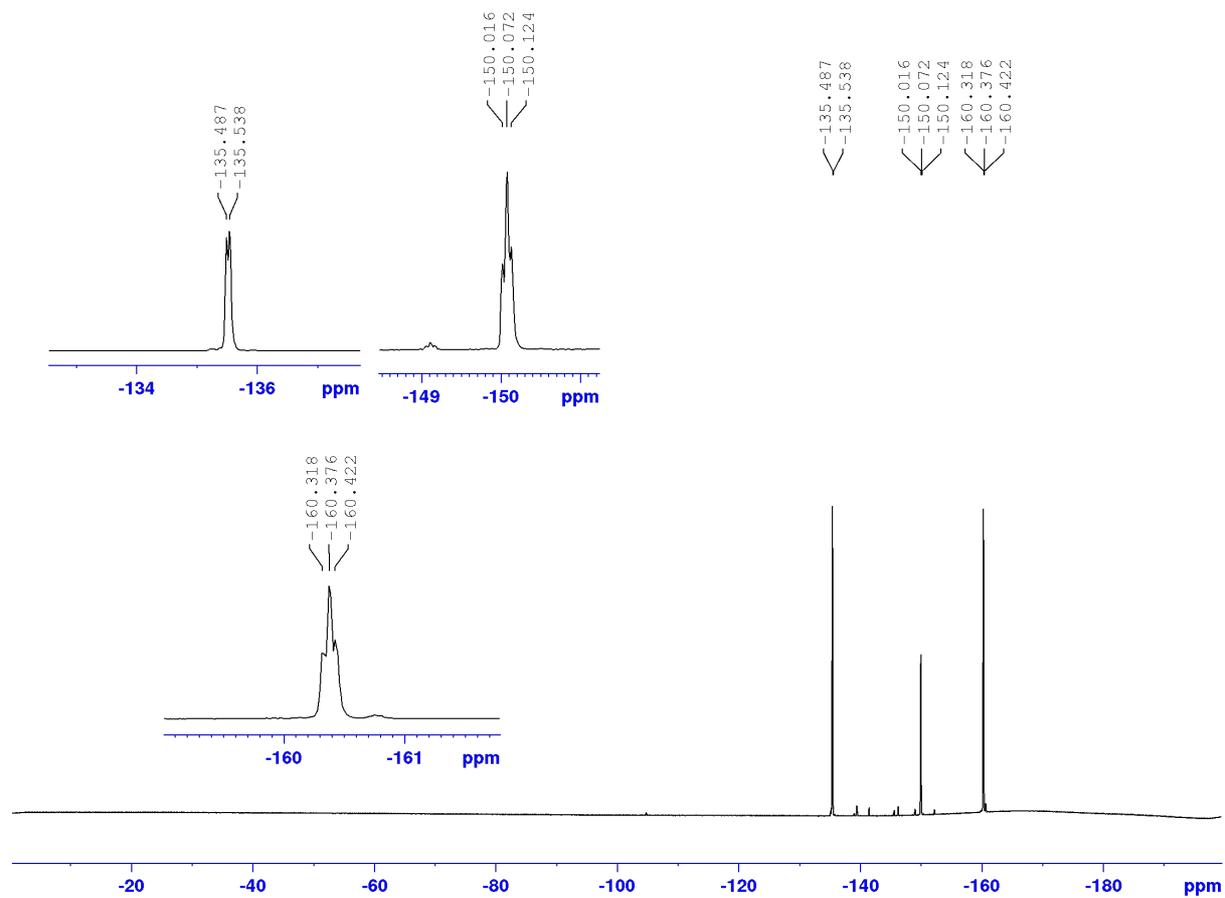


6 ¹⁹F NMR data

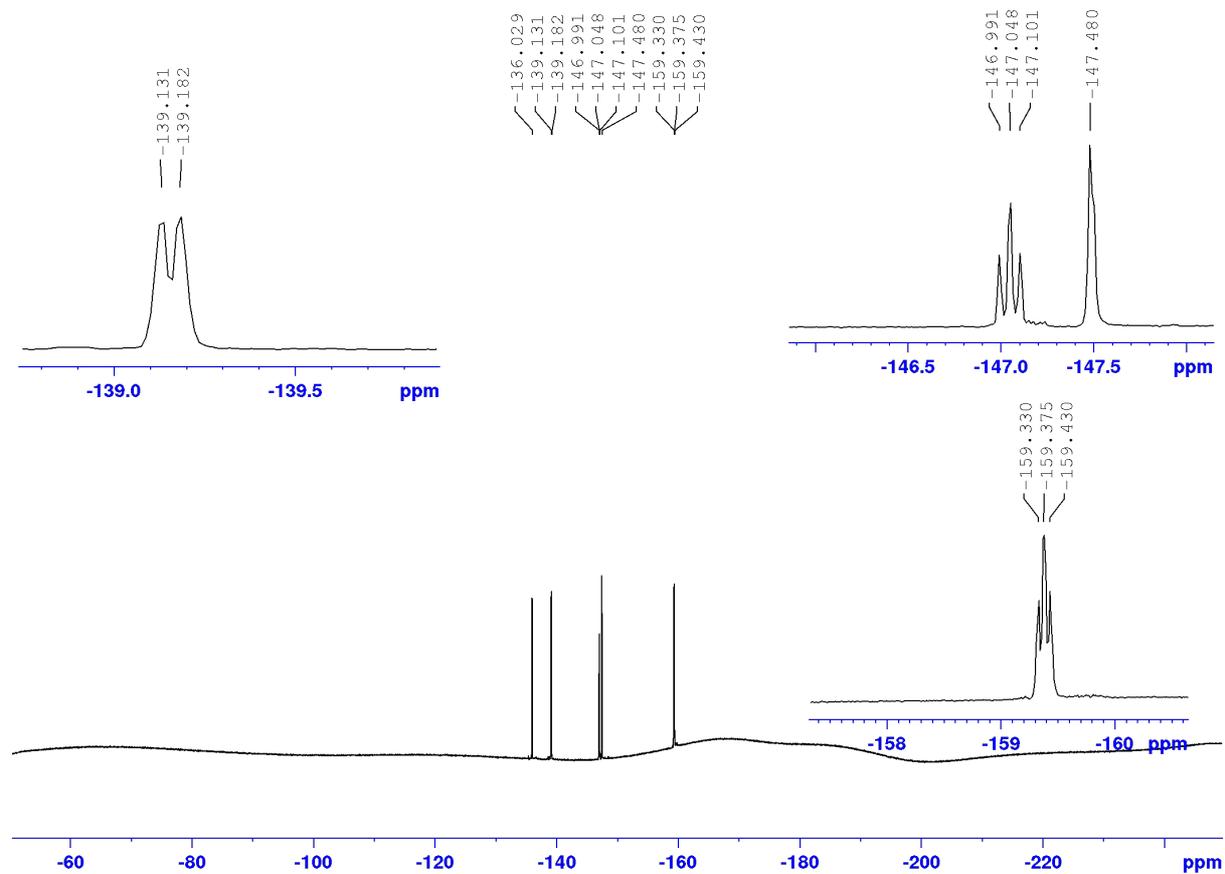
Tris(perfluorophenyl)methanol (10H)



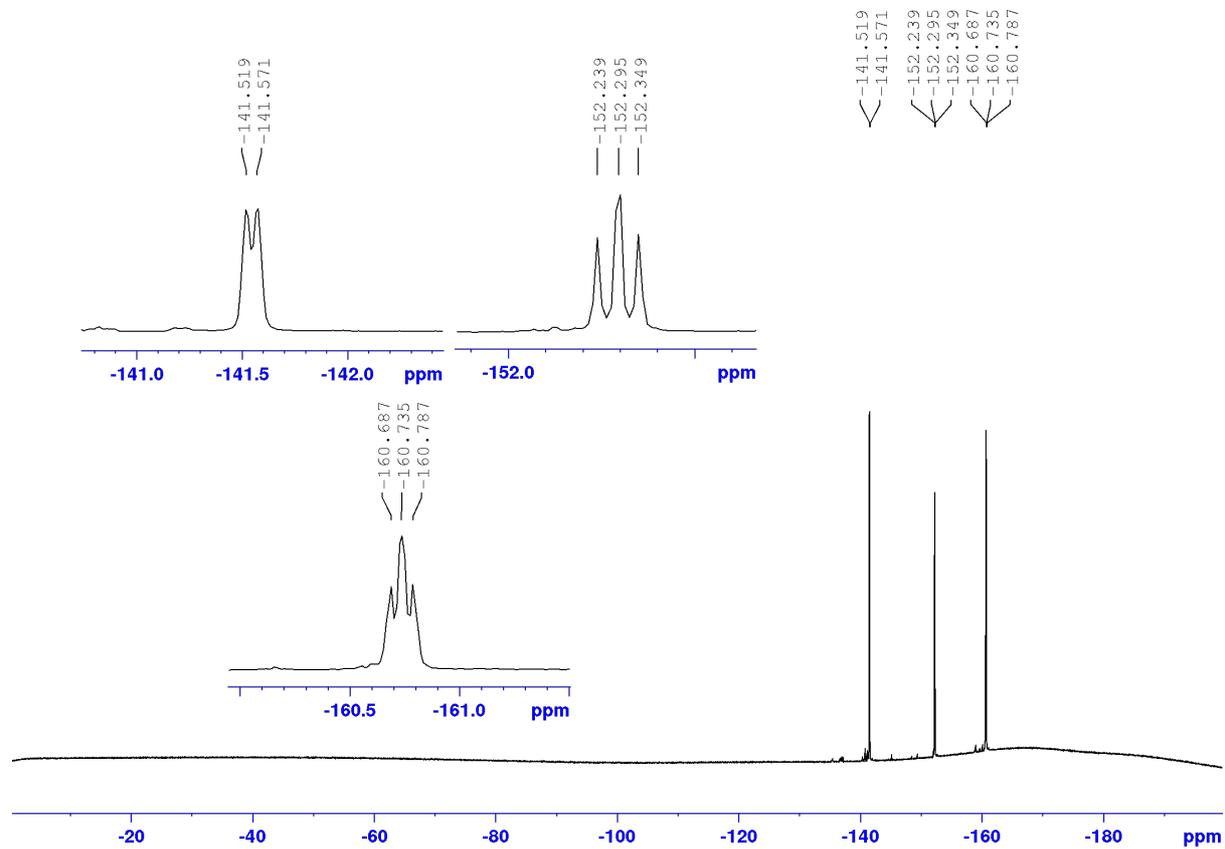
6,6',6''-(chloromethanetriyl)tris(1,2,3,4,5-pentafluorobenzene) (1Cl)



4-(bis(perfluorophenyl)methylene)-2,3,5,6-tetrafluorocyclohexa-2,5-dien-1-one (2)

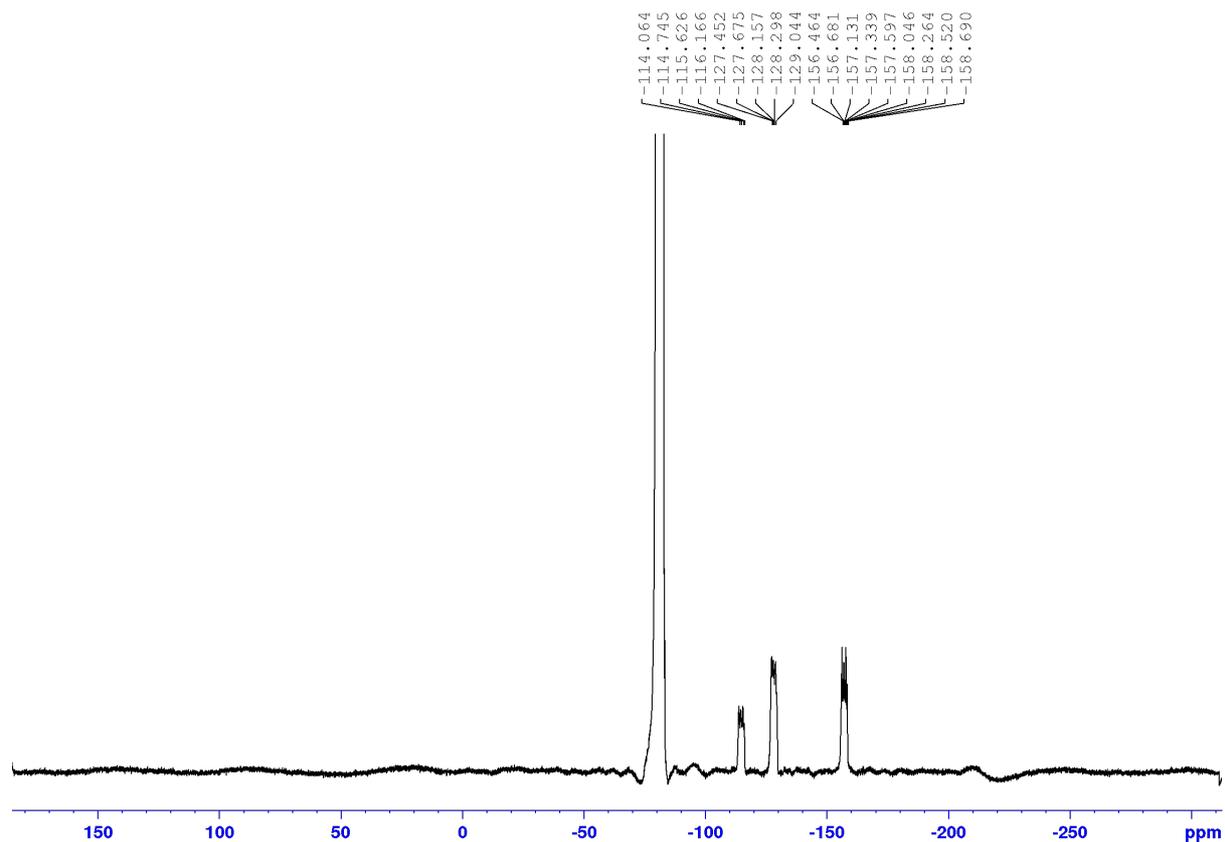


Tris(perfluorophenyl)methane (1H)



Reaction of tris(perfluorophenyl)methanol in neat triflic acid @ - 30 °C

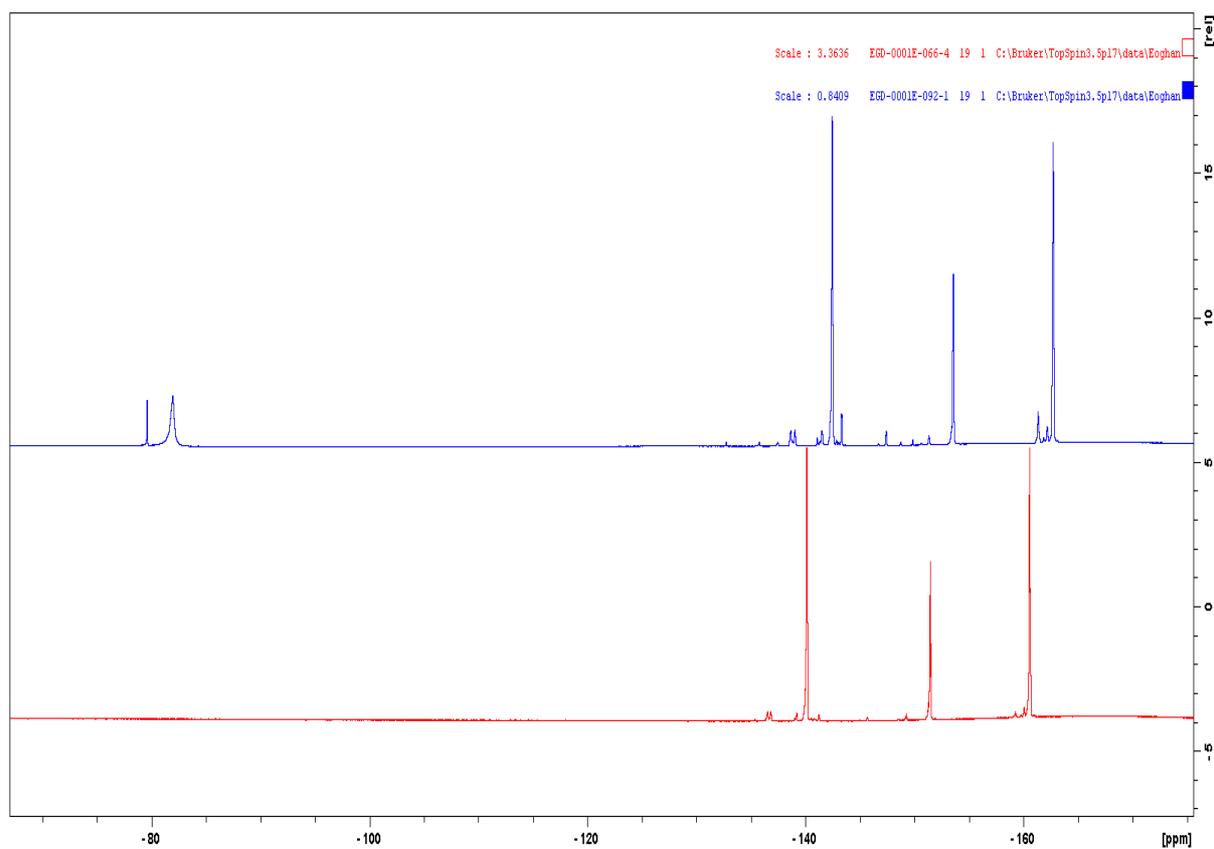
Note: this spectrum has been further baseline corrected post-automatic processing.



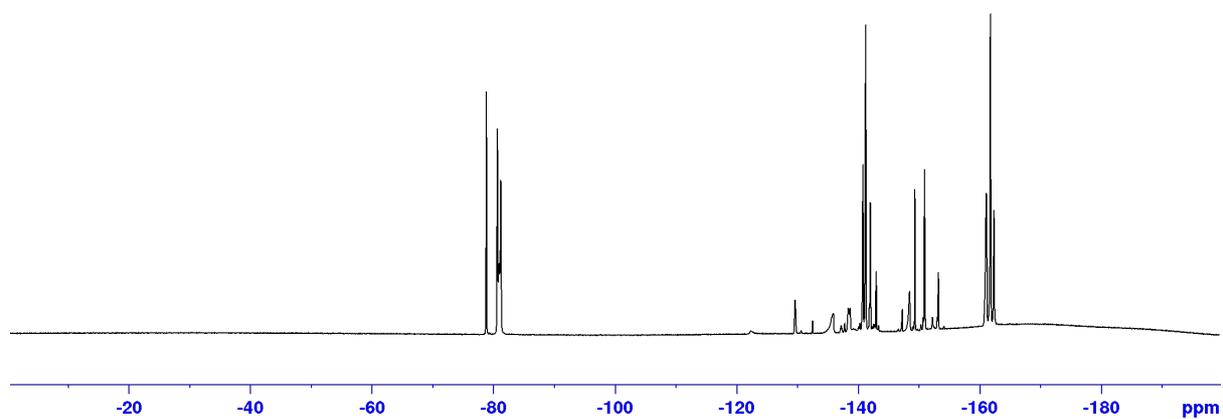
Reaction of tris(perfluorophenyl)methanol with triflic acid in 1,2-dichlorobenzene @ -10 °C

Blue = crude reaction mixture

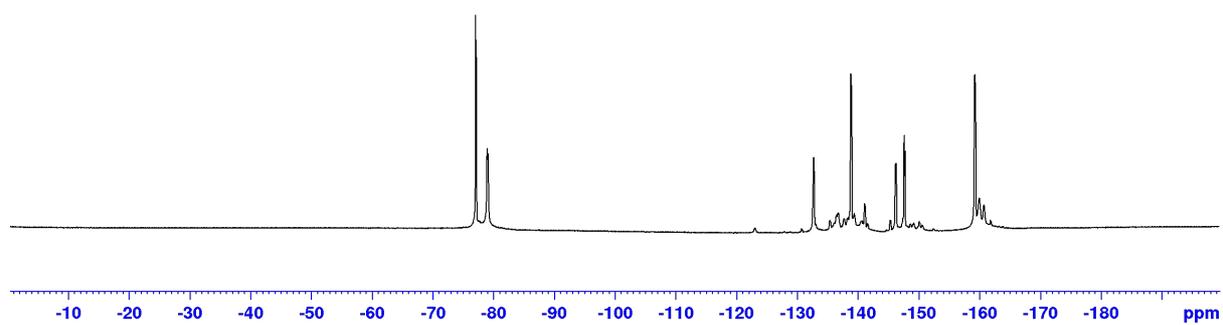
Red = tris(perfluorophenyl)methanol in 1,2-dichlorobenzene



After warming the above sample to ambient temperature and analysing immediately



Above sample after standing at room temperature for 2 days



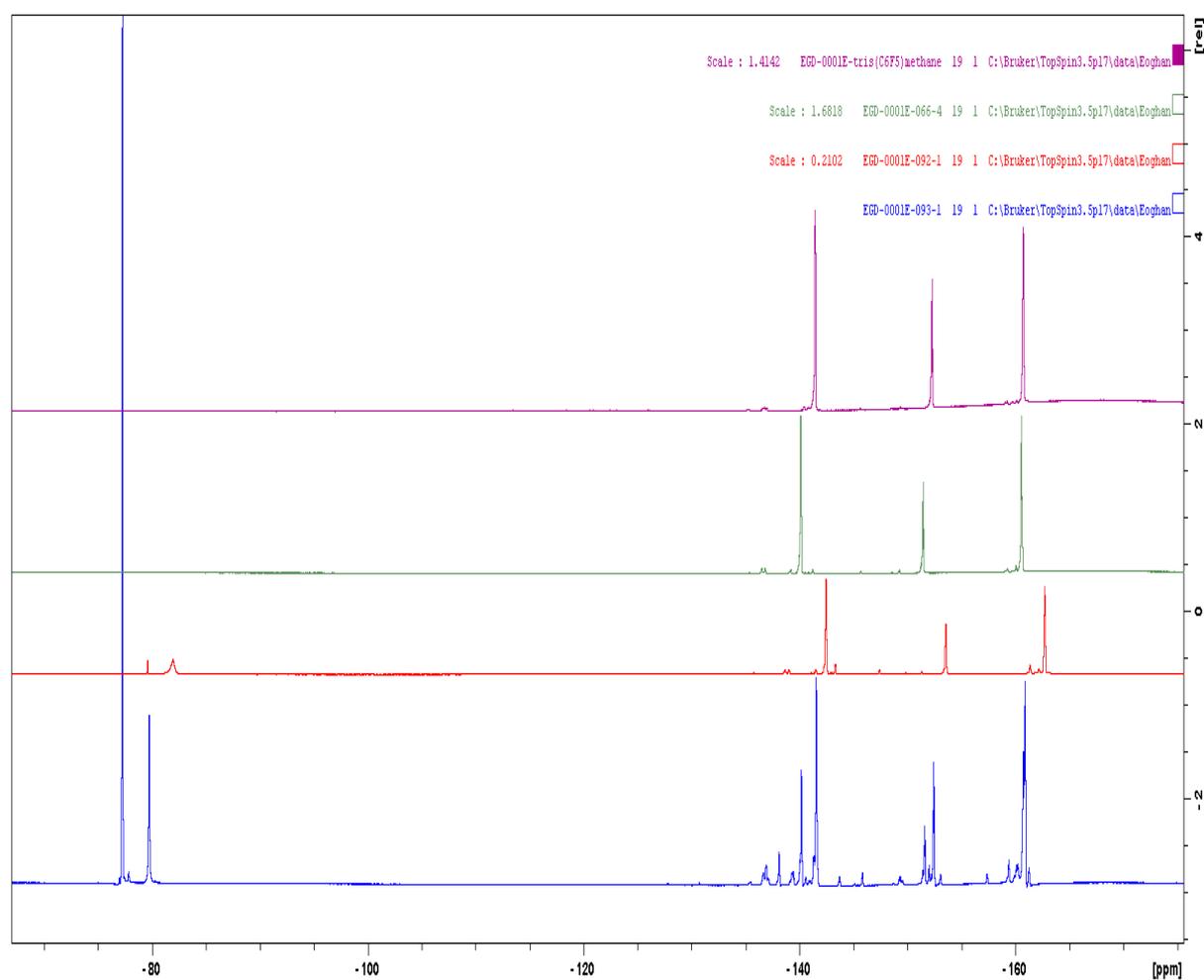
Reaction of tris(perfluorophenyl)methanol with 1) triflic acid and 2) triethylsilane in 1,2-dichlorobenzene @ -10 °C

Blue = crude reaction mixture after Et₃SiH addition

Red = crude reaction mixture before Et₃SiH addition

Green = tris(perfluorophenyl)methanol in 1,2-dichlorobenzene

Purple = tris(perfluorophenyl)methane in 1,2-dichlorobenzene



7. Computational Methods

All calculations were performed with Gaussian 09,⁵ with an ultrafine DFT integration grid. Geometry optimizations were carried out using the B3LYP density functional^{6,7} with the def2-TZVPP basis set.^{8,9} Dispersion was included with Grimme's D3 dispersion, including Becke-Johnson damping,¹⁰ denoted as B3LYP-D3(BJ). Stationary points were all characterized as minima by calculating the Hessian matrix analytically at the same level of theory.

8. Cartesian coordinates of optimized geometries

Trityl cation
C(Ph)₃

```
1 1
6   0.000000  0.000000  0.000000
6   0.000000  1.440415  0.000000
6  -1.011978  2.160237  0.672627
6   1.011978  2.160237 -0.672627
6  -0.998538  3.540843  0.683157
1  -1.767676  1.622616  1.225256
6   0.998538  3.540843 -0.683157
1   1.767676  1.622616 -1.225256
6   0.000000  4.232828  0.000000
1  -1.758784  4.083424  1.226453
1   1.758784  4.083424 -1.226453
1   0.000000  5.314109  0.000000
6   1.247436 -0.720207  0.000000
6   1.364831 -1.956518 -0.672627
6   2.376810 -0.203720  0.672627
6   2.567191 -2.635180 -0.683157
1   0.521389 -2.342160 -1.225256
6   3.565729 -0.905662  0.683157
1   2.289065  0.719544  1.225256
6   3.665737 -2.116414  0.000000
1   2.656957 -3.564863 -1.226453
1   4.415741 -0.518560  1.226453
1   4.602154 -2.657055  0.000000
6  -1.247436 -0.720207  0.000000
6  -1.364831 -1.956518  0.672627
6  -2.376810 -0.203720 -0.672627
6  -2.567191 -2.635180  0.683157
1  -0.521389 -2.342160  1.225256
6  -3.565729 -0.905662 -0.683157
1  -2.289065  0.719544 -1.225256
6  -3.665737 -2.116414  0.000000
```

1	-2.656957	-3.564863	1.226453
1	-4.415741	-0.518560	-1.226453
1	-4.602154	-2.657055	0.000000

C(C₆F₅)₃ cation

1	1		
6	0.000000	0.000000	0.000000
6	0.000000	1.438234	0.000000
6	-0.956903	2.184113	0.730216
6	0.956903	2.184113	-0.730216
6	-0.951001	3.561620	0.751340
9	-1.857921	1.562075	1.479733
6	0.951001	3.561620	-0.751340
9	1.857921	1.562075	-1.479733
6	0.000000	4.254843	0.000000
9	-1.830074	4.230083	1.473886
9	1.830074	4.230083	-1.473886
9	0.000000	5.562951	0.000000
6	1.245547	-0.719117	0.000000
6	1.413045	-1.920759	-0.730216
6	2.369949	-0.263354	0.730216
6	2.608953	-2.604401	-0.751340
9	0.423836	-2.390044	-1.479733
6	3.559954	-0.957219	0.751340
9	2.281757	0.827969	1.479733
6	3.684802	-2.127421	0.000000
9	2.748322	-3.699932	-1.473886
9	4.578396	-0.530151	1.473886
9	4.817657	-2.781476	0.000000
6	-1.245547	-0.719117	0.000000
6	-1.413045	-1.920759	0.730216
6	-2.369949	-0.263354	-0.730216
6	-2.608953	-2.604401	0.751340
9	-0.423836	-2.390044	1.479733
6	-3.559954	-0.957219	-0.751340
9	-2.281757	0.827969	-1.479733
6	-3.684802	-2.127421	0.000000
9	-2.748322	-3.699932	1.473886
9	-4.578396	-0.530151	-1.473886
9	-4.817657	-2.781476	0.000000

C(C₆F₅)₃OH

0	1		
6	0.028478	0.000058	-0.759341
6	1.421238	0.486264	-0.313035
6	1.669070	1.505162	0.603476
6	2.551973	-0.112568	-0.880725
6	2.953656	1.938469	0.907278
6	3.840281	0.303269	-0.592340

6	4.045727	1.341482	0.304210
6	-0.278333	-1.442464	-0.329407
6	-1.360568	-2.100138	-0.919843
6	0.436884	-2.167687	0.618089
6	-1.678903	-3.416125	-0.626376
6	0.134941	-3.486440	0.927638
6	-0.922686	-4.119145	0.298378
6	-1.097068	0.960385	-0.311023
6	-1.949707	0.728326	0.764628
6	-1.305096	2.155603	-0.995658
6	-2.977588	1.598367	1.101953
6	-2.319030	3.043124	-0.683546
6	-3.171327	2.758836	0.372424
9	-1.796444	-0.335954	1.562281
9	-3.770863	1.324113	2.135188
9	-4.150946	3.597607	0.688538
9	-2.468958	4.168171	-1.379145
9	-0.471251	2.525623	-1.991135
9	-2.174449	-1.462459	-1.763914
9	-2.719956	-4.002474	-1.215396
9	-1.220601	-5.380830	0.589313
9	0.857019	-4.140412	1.836781
9	1.443732	-1.620635	1.313146
9	2.430374	-1.162918	-1.694024
9	4.884034	-0.302495	-1.155233
9	5.277486	1.748593	0.588416
9	3.133522	2.926932	1.782244
9	0.679965	2.118696	1.268308
8	0.033610	-0.081784	-2.182724
1	0.205494	0.791575	-2.547193

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